HEC MONTRÉAL

Statistical Modelling

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Welcome

This course is about statistical modelling.

A famous quote attributed to George Box claims that

> All models are wrong, but some are useful.

This standpoint is reductive: Peter McCullagh and John Nelder wrote in the preamble of their book (emphasis mine)

> Modelling in science remains, partly at least, an art. Some principles do exist, however, to guide the modeller. The first is that all models are wrong; **some, though, are better** than others and we can **search for the better ones**. At the same time we must recognize that eternal truth is not within our grasp.

And this quote by David R. Cox adds to the point:

> ...it does not seem helpful just to say that all models are wrong. The very word model implies simplification and idealization. The idea that complex physical, biological or sociological systems can be exactly described by a few formulae is patently absurd. The construction of idealized representations that **capture important stable aspects of such systems** is, however, a vital part of general scientific analysis and statistical models, especially substantive ones, do not seem essentially different from other kinds of model.

Why use models? Paul Krugman wrote in 2010 in his blog

> The answer I'd give is that models are an enormously important tool for clarifying your thought. You don't have to literally believe your model — in fact, you're a fool if you do — to believe that putting together a simplified but complete account of how things work, with all the eyes crossed and teas dotted or something, helps you gain a much more sophisticated understanding of the real situation. People who don't use models end up relying on slogans that are much more simplistic than the models

Course content

There are two main data type: **experimental** data are typically collected in a control environment following a research protocol with a particular experimental design: they serve to answer questions specified ahead of time. This approach is highly desirable to avoid the garden of forking paths (researchers unfortunately tend to refine or change their hypothesis in light of data, which invalidates their findings — preregistration alleviates this somewhat). While experimental data are highly desirable, it is not always possible to collect experimental data: for example, an economist cannot modify interest rates to see how it impacts consumer savings. When data have been collected beforehand without intervention (for other purposes), these are called **observational**. These will be the ones most frequently encountered.

A stochastic model will comprise two ingredients: a distribution for the random data and a formula linking the parameters or the conditional expectation of a response variable Y to a set of explanatories $\mathbf{X}$. A model can serve to either predict new outcomes (predictive modelling) or else to test research hypothesis about the effect of the explanatory variables on the response (explanatory model). These two objectives are of course not mutually exclusive even if we distinguish in practice inference and prediction.

A predictive model gives predictions of Y for different combinations of explanatory variables or future data. For example, one could try to forecast the enery consumption of a house as a function of weather, the number of inhabitants and its size. Black boxes used in machine learning are often used solely for prediction: these models are not easily interpreted and they often ignore the data structure.

By constrast, explicative models are often simple and interpretable: regression models are often used for inference purpose and we will focus on these. The following examples will be covered in class or as part of the exercices:

- Are sequential decisions in online shop (buying or not, then selecting the quantity) preferable to integrated decisions (Duke and Amir 2023)?
- Determining what is the most distracting for road users: talking on a cellphone, texting or checking your smartwatch (Brodeur et al. 2021)?
- What is the impact of inconsistencies between product description and the displayed image (Lee and Choi 2019)?
- Is the price of gasoline more expensive in the Gaspé peninsula than in the rest of Quebec? A report of the *Régie de l'énergie* examines the question
- Are driving tests in the UK easier if you live in a rural area? An analysis of *The Guardian* hints that it is the case.
- What is the environmental perception of a package that includes cardboard over a plastic container (Sokolova, Krishna, and Döring 2023)?

- What is the psychological impact of suggested amounts on donations (Moon and VanEpps 2023)?
- What are the benefits of face-to-face meetings, rather than via videoconference tools? Brucks and Levav (2022) suggests a decrease in the number of creative ideas and interactions when meeting online.

1 Introduction

This chapter reviews some basic notions of probability and statistics that are normally covered in undergraduate or college.

1.1 Population and samples

Statistics is the science of uncertainty quantification: of paramount importance is the notion of randomness. Generally, we will seek to estimate characteristics of a population using only a sample (a sub-group of the population of smaller size).

The **population of interest** is a collection of individuals which the study targets. For example, the Labour Force Survey (LFS) is a monthly study conducted by Statistics Canada, who define the target population as "all members of the selected household who are 15 years old and older, whether they work or not." Asking every Canadian meeting this definition would be costly and the process would be long: the characteristic of interest (employment) is also a snapshot in time and can vary when the person leaves a job, enters the job market or become unemployed.

In general, we therefore consider only **samples** to gather the information we seek to obtain. The purpose of **statistical inference** is to draw conclusions about the population, but using only a share of the latter and accounting for sources of variability. George Gallup made this great analogy between sample and population:

> One spoonful can reflect the taste of the whole pot, if the soup is well-stirred

A **sample** is a random sub-group of individuals drawn from the population. Creation of sampling plans is a complex subject and semester-long sampling courses would be required to evens scratch the surface of the topic. Even if we won't be collecting data, keep in mind the following information: for a sample to be good, it must be representative of the population under study. Selection bias must be avoided, notably samples of friends or of people sharing opinions.

Because the individuals are selected at **random** to be part of the sample, the measurement of the characteristic of interest will also be random and change from one sample to the next. However, larger samples of the same quality carry more information and our estimator will be more precise. Sample size is not guarantee of quality, as the following example demonstrates.

Example 1.1 (Polling for the 1936 USA Presidential Election)**.** *The Literary Digest* surveyed 10 millions people by mail to know voting preferences for the 1936 USA Presidential Election. A sizeable share, 2.4 millions answered, giving Alf Landon (57%) over incumbent President Franklin D. Roosevelt (43%). The latter nevertheless won in a landslide election with 62% of votes cast, a 19% forecast error. Biased sampling and differential non-response are mostly responsible for the error: the sampling frame was built using "phone number directories, drivers' registrations, club memberships, etc.", all of which skewed the sample towards rich upper class white people more susceptible to vote for the GOP.

In contrast, Gallup correctly predicted the outcome by polling (only) 50K inhabitants. Read the full story here.

1.1.1 Variable type

- a **variable** represents a characteristic of the population, for example the sex of an individual, the price of an item, etc.
- an **observation** is a set of measures (variables) collected under identical conditions for an individual or at a given time.

Table 1.1: First lines of the `renfe` database, which contains the price of 10K train tickets between Madrid and Barcelona. The columns `price` and `duration` represent continuous variables, all others are categorical.

price	type	class	fare	dest	duration	wday
143.4	AVE	Preferente	Promo	Barcelona-Madrid	190	6
181.5	AVE	Preferente	Flexible	Barcelona-Madrid	190	2
86.8	AVE	Preferente	Promo	Barcelona-Madrid	165	7
86.8	AVE	Preferente	Promo	Barcelona-Madrid	190	7
69.0	AVE-TGV	Preferente	Promo	Barcelona-Madrid	175	4

The choice of statistical model and test depends on the underlying type of the data collected. There are many choices: quantitative (discrete or continuous) if the variables are numeric, or qualitative (binary, nominal, ordinal) if they can be described using an adjective; I prefer the term categorical, which is more evocative.

Most of the models we will deal with are so-called regression models, in which the mean of a quantitative variable is a function of other variables, termed explanatories. There are two types of numerical variables

- a discrete variable takes a finite or countable number of values, prime examples being binary variables or count variables.
- a continuous variable can take (in theory) an infinite possible number of values, even when measurements are rounded or measured with a limited precision (time, width, mass). In many case, we could also consider discrete variables as continuous if they take enough values (e.g., money).

Categorical variables take only a finite of values. They are regrouped in two groups,

- nominal if there is no ordering between levels (sex, color, country of origin) or
- ordinal if they are ordered (Likert scale, salary scale) and this ordering should be reflected in graphs or tables.

We will bundle every categorical variable using arbitrary encoding for the levels: for modelling, these variables taking K possible values (or levels) must be transformed into a set of $K-1$ binary 0/1 variables, the omitted level corresponding to a baseline. Failing to declare categorical variables in your favorite software is a common mistake, especially when these are saved in the database using integers rather than strings.

1.2 Random variable

Suppose we wish to describe the behaviour of a stochastic phenomenon. To this effect, one should enumerate the set of possible values taken by the variable of interest and their probability: this is what is encoded in the distribution.

Random variables are denoted using capital letters: for example $Y \sim \mathsf{normal}(\mu, \sigma^2)$ indicates that Y follows a normal distribution with parameters μ and $\sigma > 0$. If the values of the latter are left unspecified, we talk about the family of distributions. When the values are given, for example $\mu = 0$ and $\sigma = 1$, we deal with a single distribution for which a function encode the probability of the underlying variable.

Definition 1.1 (Distribution function, mass function and density)**.** The (cumulative) distribution function $F(y)$ gives the cumulative probability that an event doesn't exceed a given numerical value y, $F(y) = \mathsf{Pr}(Y \leq y)$.

If Y is discrete, then it has atoms of non-zero probability and we call f the mass function, and $f(y) = \mathsf{Pr}(Y = y)$ gives the probability of each outcome y. In the continuous case, no numerical value has non-zero probability and so we consider intervals instead. The density function $f(x)$ is non-negative and satisfies $\int_{\mathbb{R}} f(x)\mathrm{d}x = 1$: the integral over a set B (the area under the curve) gives the probability of Y falling inside $B \in \mathbb{R}$. It follows that the distribution function of a continuous random variable is simply $F(y) = \int_{-\infty}^{y} f(x)\mathrm{d}x$.

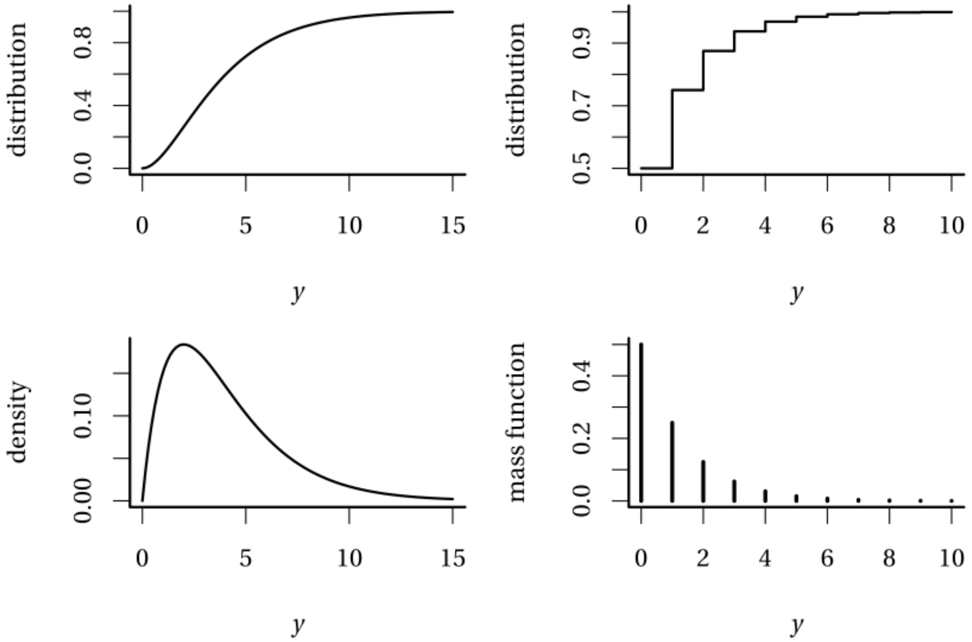


Figure 1.1: (Cumulative) distribution functions (top) and density/mass functions (bottom) of continuous (left) and discrete (right) random variables.

One of the first topics covered in introductory statistics is descriptive statistics such as the mean and standard deviation. These are estimators of (centered) moments, which characterise a random variable. In the case of the standard normal distribution, the expectation and variance fully characterize the distribution.

Definition 1.2 (Moments)**.** Let Y be a random variable with density (or mass) function $f(x)$. The **expectation** (or theoretical mean) of a continuous random variable Y is

$$\mathsf{E}(Y) = \int_{\mathbb{R}} x f(x)\mathrm{d}x.$$

In the discrete case, we set rather $\mu = \mathsf{E}(Y) = \sum_{x\in\mathcal{X}} x\mathsf{Pr}(X = x)$, where $\mathcal{X}$ denotes the support of Y, the set of numerical values at which the probability of Y is non-zero. More generally, we can look at the expectation of a function $g(x)$ for Y, which is nothing but the integral (or sum in the discrete case) of $g(x)$ weighted by the density or mass function of $f(x)$. In the same fashion, provided the integral is finite, the variance is

$$\mathsf{Va}(Y) = \mathsf{E}\{Y - \mathsf{E}(Y)\}^2 \equiv \int_{\mathbb{R}} (x-\mu)^2 f(x)\mathrm{d}x.$$

The **standard deviation** is the square root of the variance, $\mathsf{sd}(Y) = \sqrt{\mathsf{Va}(Y)}$: it units are the same as those of Y and are thus more easily interpreted.

The notion of moments can be extended to higher dimensions. Consider an n-vector $\boldsymbol{Y}$. In the regression setting, the response $\boldsymbol{Y}$ would usually comprise repeated measures on an individual, or even observations from a group of individuals.

The expected value (theoretical mean) of the vector $\boldsymbol{Y}$ is calculated componentwise, i.e.,

$$\mathsf{E}(\boldsymbol{Y}) = \boldsymbol{\mu} = \begin{pmatrix} \mathsf{E}(Y_1) & \cdots & \mathsf{E}(Y_n) \end{pmatrix}^\top$$

whereas the second moment of $\boldsymbol{Y}$ is encoded in the $n \times n$ **covariance** matrix

$$\mathsf{Va}(\boldsymbol{Y}) = \boldsymbol{\Sigma} = \begin{pmatrix} \mathsf{Va}(Y_1) & \mathsf{Co}(Y_1, Y_2) & \cdots & \mathsf{Co}(Y_1, Y_n) \\ \mathsf{Co}(Y_2, Y_1) & \mathsf{Va}(Y_2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ \mathsf{Co}(Y_n, Y_1) & \mathsf{Co}(Y_n, Y_2) & \cdots & \mathsf{Va}(Y_n) \end{pmatrix}$$

The ith diagonal element of $\boldsymbol{\Sigma}$, $\sigma_{ii} = \sigma_i^2$, is the variance of Y_i, whereas the off-diagonal entries $\sigma_{ij} = \sigma_{ji}$ $(i \neq j)$ are the covariance of pairwise entries, with

$$\mathsf{Co}(Y_i, Y_j) = \int_{\mathbb{R}^2} (y_i - \mu_i)(y_j - \mu_j) f_{Y_i, Y_j}(y_i, y_j)\mathrm{d}y_i \mathrm{d}y_j.$$

The covariance matrix $\boldsymbol{\Sigma}$ is thus symmetric. It is customary to normalize the pairwise dependence so they do not depend on the component variance. The linear **correlation** between Y_i and Y_j is

$$\rho_{ij} = \mathsf{Cor}(Y_i, Y_j) = \frac{\mathsf{Co}(Y_i, Y_j)}{\sqrt{\mathsf{Va}(Y_i)}\sqrt{\mathsf{Va}(Y_j)}} = \frac{\sigma_{ij}}{\sigma_i \sigma_j}.$$

The correlation matrix of $\boldsymbol{Y}$ is an $n \times n$ symmetric matrix with ones on the diagonal and the pairwise correlations off the diagonal,

$$\mathsf{Cor}(\boldsymbol{Y}) = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \cdots & \rho_{1n} \\ \rho_{21} & 1 & \rho_{23} & \cdots & \rho_{2n} \\ \rho_{31} & \rho_{32} & 1 & \ddots & \rho_{3n} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \rho_{n1} & \rho_{n2} & \rho_{n3} & \cdots & 1 \end{pmatrix}.$$

One of the most important parts of modelling correlated (or longitudinal) data is the need to account for within-group correlations. This basically comes down to modelling a covariance matrix for observations within the same group (or within the same individual in the case of repeated measures), which is the object of Chapter 5.

Definition 1.3 (Bias)**.** The bias of an estimator $\hat{\theta}$ for a parameter θ is

$$\mathsf{bias}(\hat{\theta}) = \mathsf{E}(\hat{\theta}) - \theta$$

The estimator is unbiased if its bias is zero.

Example 1.2 (Unbiased estimators)**.** The unbiased estimator of the mean and the variance of Y are

$$\begin{aligned} \overline{Y}_n &= n^{-1}\sum_{i=1}^n Y_i \\ S_n &= (n-1)^{-1}\sum_{i=1}^n (Y_i - \overline{Y})^2. \end{aligned}$$

While unbiasedness is a desirable property, there may be cases where no unbiased estimator exists for a parameter! Often, rather, we seek to balance bias and variance: recall that an estimator is a function of random variables and thus it is itself random: even if it is unbiased, the numerical value obtained will vary from one sample to the next.

Definition 1.4. We often seek an estimator that minimises the **mean squared error**,

$$\mathsf{MSE}(\hat{\theta}) = \mathsf{E}\{(\hat{\theta} - \theta)^2\} = \mathsf{Va}(\hat{\theta}) + \{\mathsf{E}(\hat{\theta})\}^2.$$

The mean squared error is an objective function consisting of the sum of the squared bias and the variance.

Most estimators we will considered are so-called maximum likelihood estimator. These estimator are asymptotically efficient, in the sense that they have the lowest mean squared error of all estimators for large samples. Other properties of maximum likelihood estimators also make them attractive default choice for estimation.

1.3 Discrete distributions

Many distributions for discrete random variables have a simple empirical justification, stemming from simple combinatorial arguments (counting). We revisit the most common ones.

Definition 1.5 (Bernoulli distribution)**.** We consider a binary event such as coin toss (heads/tails). In general, the two events are associated with success/failure. By convention, failures are denoted by zeros and successes by ones, the probability of success being p so $\mathsf{Pr}(Y=1)=p$ and $\mathsf{Pr}(Y=0)=1-p$ (complementary event). The mass function of the Bernoulli distribution is thus

$$\mathsf{Pr}(Y=y)=p^y(1-p)^{1-y}, \quad y=0,1.$$

A rapid calculation shows that $\mathsf{E}(Y)=p$ and $\mathsf{Va}(Y)=p(1-p)$. Indeed,

$$\mathsf{E}(Y)=\mathsf{E}(Y^2)=p\cdot 1+(1-p)\cdot 0=p.$$

Many research questions have binary responses, for example:

- did a potential client respond favourably to a promotional offer?
- is the client satisfied with service provided post-purchase?
- will a company go bankrupt in the next three years?
- did a study participant successfully complete a task?

Oftentimes, we will have access to aggregated data.

Definition 1.6 (Binomial distribution)**.** If we consider the sum of independent and identically distributed Bernoulli events, the number of sucesses Y out of m trials is binomial, denoted $\mathsf{Bin}(m,p)$; the mass function of the binomial distribution is

$$\mathsf{Pr}(Y=y)=\binom{m}{y}p^y(1-p)^{1-y}, \quad y=0,1.$$

The likelihood of a sample from a binomial distribution is (up to a normalizing constant that doesn't depend on p) the same as that of m independent Bernoulli trials. The expectation of the binomial random variable is $\mathsf{E}(Y)=mp$ and its variance $\mathsf{Va}(Y)=mp(1-p)$.

As examples, we could consider the number of successful candidates out of m who passed their driving license test or the number of customers out of m total which spent more than 10$ in a store.

More generally, we can also consider count variables whose realizations are integer-valued, for examples the number of

- insurance claims made by a policyholder over a year,
- purchases made by a client over a month on a website,
- tasks completed by a study participant in a given time frame.

Definition 1.7 (Poisson distribution)**.** If the probability of success p of a Bernoulli event is small in the sense that $mp \to \lambda$ when the number of trials m increases, then the number of success follows approximately a Poisson distribution with mass function

$$\mathsf{Pr}(Y=y) = \frac{\exp(-\lambda)\lambda^y}{\Gamma(y+1)}, \quad y=0,1,2,\ldots$$

where $\Gamma(\cdot)$ denotes the gamma function. The parameter λ of the Poisson distribution is both the expectation and the variance of the distribution, meaning $\mathsf{E}(Y) = \mathsf{Va}(Y) = \lambda$.

Definition 1.8 (Negative binomial distribution)**.** The negative binomial distribution arises if we consider the number of Bernoulli trials with probability of success p until we obtain m success. Let Y denote the number of failures: the order of success and failure doesn't matter, except for the latest trial which must be a success. The mass function of the negative binomial is

$$\mathsf{Pr}(Y=y) = \binom{m-1+y}{y} p^m (1-p)^y.$$

The negative binomial distribution also appears as the unconditional distribution of a two-stage hierarchical gamma-Poisson model, in which the mean of the Poisson distribution is random and follows a gamma distribution. In notation, this is $Y \mid \Lambda = \lambda \sim \mathsf{Po}(\lambda)$ and Λ follows a gamma distribution with shape r and scale θ, whose density is

$$f(x) = \theta^{-r} x^{r-1} \exp(-x/\theta)/\Gamma(r).$$

The unconditional number of success is then negative binomial.

In the context of generalized linear models, we will employ yet another parametrisation of the distribution, with the mass function

$$\mathsf{Pr}(Y=y) = \frac{\Gamma(y+r)}{\Gamma(y+1)\Gamma(r)} \left(\frac{r}{r+\mu}\right)^r \left(\frac{\mu}{r+\mu}\right)^y, y=0,1,\ldots,\mu,r>0,$$

where Γ is the gamma function and the parameter $r>0$ is not anymore integer valued. The expectation and variance of Y are $\mathsf{E}(Y)=\mu$ et $\mathsf{Va}(Y)=\mu+k\mu^2$, where $k=1/r$. The variance of the negative binomial distribution is thus higher than its expectation, which justifies the use of the negative binomial distribution for modelling overdispersion.

1.4 Continuous distributions

We will encounter many continuous distributions that arise as (asymptotic) null distribution of test statistics because of the central limit theorem, or that follow from transformation of Gaussian random variables.

Definition 1.9 (Beta distribution)**.** The beta distribution $\mathsf{Beta}(\alpha,\beta)$ is a distribution supported on the unit interval $[0,1]$ with shape parameters $\alpha>0$ and $\beta>0$. It's density is

$$f(x)=\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}x^{\alpha-1}(1-x)^{1-\beta},\qquad x\in[0,1].$$

The case $\alpha=\beta=1$, also denoted $\mathsf{unif}(0,1)$, corresponds to a standard uniform distribution.

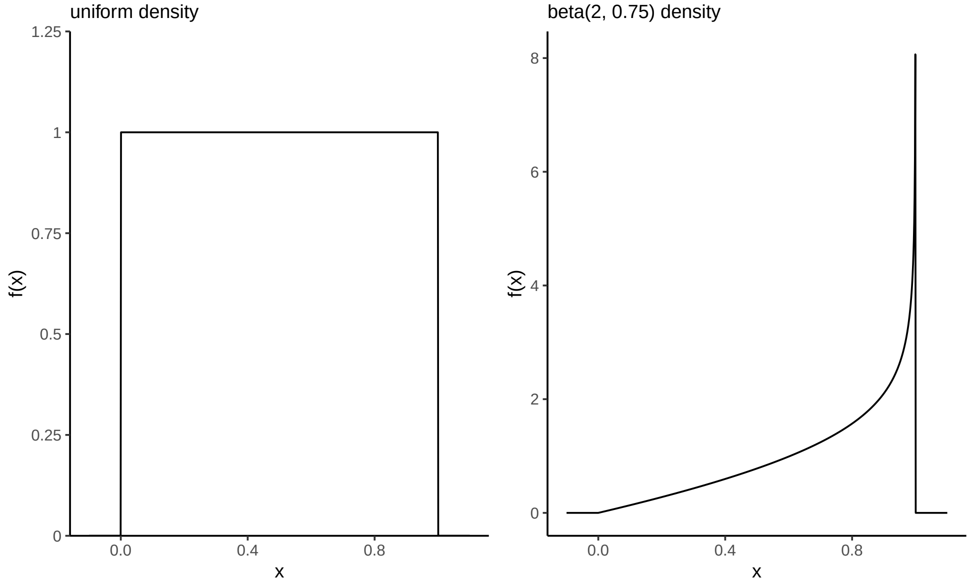


Figure 1.2: Density fonction of uniform (left) and beta(2, 3/4) random variables on the unit interval.

Definition 1.10 (Exponential distribution)**.** The exponential distribution plays a prominent role in the study of waiting time of Poisson processes, and in survival analysis. One caracteristic of the distribution is it's absence of memory: $\Pr(Y\geq y+u\mid Y>u)=\Pr(Y>u)$ for $y,u>0$.

The distribution function of the exponential distribution with scale $\lambda > 0$, denoted $Y \sim \mathsf{Exp}(\lambda)$, is $F(x) = 1 - \exp(-x/\lambda)$ and the corresponding density function is $f(x) = \lambda^{-1}\exp(-x/\lambda)$ for $x > 0$. The expected value of Y is simply λ.

Definition 1.11 (Normal distribution)**.** Ths most well known distribution, the normal distribution is ubiquitous in statistics because of the central limit theorem (CLT), which describes the behaviour of the sample mean in large sample.The parameters μ and $\sigma > 0$ that fully characterize the distribution of the normal distribution and they correspond to the expectation and standard deviation. The density of a normal distribution is symmetric around μ, while σ describes the dispersion around this mode. The bell-shaped density function is

$$f(x) = (2\pi\sigma^2)^{-1/2}\exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}, \qquad x \in \mathbb{R}.$$

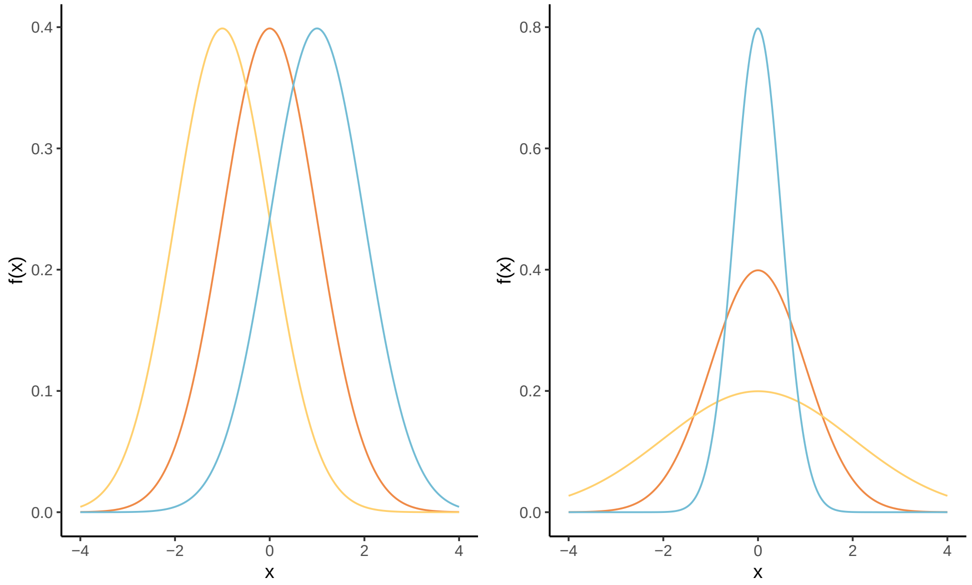


Figure 1.3: Densities of normal distributions with different mean parameters (left) and different scale parameters (right).

The distribution function of the normal distribution is not available in closed-form. The normal distribution is a location-scale distribution: if $Y \sim \mathsf{normal}(\mu, \sigma^2)$, then $Z = (Y - \mu)/\sigma \sim \mathsf{normale}(0,1)$. Conversely, if $Z \sim \mathsf{normal}(0,1)$, then $Y = \mu + \sigma Z \sim \mathsf{normal}(\mu, \sigma^2)$.

We will also encounter the multivariate normal distribution; for a d dimensional vector

$\boldsymbol{Y} \sim \mathsf{normal}_d(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, the density is

$$f(\boldsymbol{x}) = (2\pi)^{-d/2}|\boldsymbol{\Sigma}|^{-1/2} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right\}$$

The mean vector $\boldsymbol{\mu}$ is the vector of expectation of individual observations, whereas $\boldsymbol{\Sigma}$ is the $d \times d$ covariance matrix of $\boldsymbol{Y}$. A unique property of the multivariate normal distribution is the link between independence and the covariance matrix: if Y_i and Y_j are independent, the (i,j) off-diagonal entry of $\boldsymbol{\Sigma}$ is zero.

Definition 1.12 (Chi-square distribution)**.** The chi-square distribution with $\nu > 0$ degrees of freedom, denoted χ^2_ν or $\mathsf{chi} - \mathsf{square}(\nu)$. It's density is

$$f(x;\nu) = \frac{1}{2^{\nu/2}\Gamma(\nu/2)} x^{\nu/2-1}\exp(-x/2), \qquad x > 0.$$

It can be obtained for ν integer by considering the following: if we consider k independent and identically distributed standard normal variables, $Y_i \sim \mathsf{normal}(0,1)$, then $\sum_{i=1}^k Y_i^2$ follows a chi-square distribution with k degrees of freedom, denote χ^2_k. The square of a standard normal variate likewise follows a χ^2_1 distribution. The expectation of χ^2_k random variable is k.

If we consider a sample of n normally distributed observations, the scaled sample variance $(n-1)S^2/\sigma^2 \sim \chi^2_{n-1}$.

Definition 1.13 (Student-t distribution)**.** The Student-t distribution with $\nu > 0$ degrees of freedom is a location-scale family. The standard version is denoted by $\mathsf{Student}(\nu)$.

The name "Student" comes from the pseudonym used by William Gosset in Gosset (1908), who introduced the asymptotic distribution of the t-statistic. The density of the standard T with ν degrees of freedom is

$$f(y;\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)\sqrt{\nu\pi}}\left(1+\frac{y^2}{\nu}\right)^{-\frac{\nu+1}{2}}$$

the distribution has polynomial tails, is symmetric around 0 and unimodal. As $\nu \to \infty$, the Student distribution converges to a normal distribution. It has heavier tails than the normal distribution and only the first $\nu - 1$ moments of the distribution exist, so a Student distribution with $\nu = 2$ degrees of freedom has infinite variance.

For normally distributed data, the centered sample mean divided by the sample variance, $(\overline{Y} - \mu)/S^2$ follows a Student-t distribution with $n-1$ degrees of freedom, which explains the terminology t-tests.

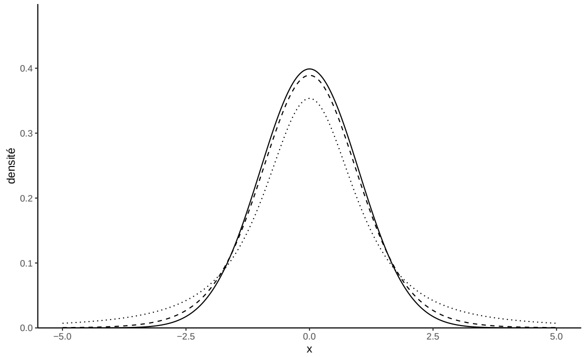


Figure 1.4: Comparison between the Student-t density for varying degrees of freedom, with $\nu = 2$ (dotted), $\nu = 10$ (dashed) and the normal density ($\nu = \infty$).

Definition 1.14 (Fisher distribution)**.** The Fisher or F distribution is used to determine the large sample behaviour of test statistics for comparing different group averages (in analysis of variance) assuming data are normally distributed.

The F distribution, denoted $\mathsf{Fisher}(\nu_1, \nu_2)$, is obtained by dividing two independent chi-square random variables with respective degrees of freedom ν_1 and ν_2. Specifically, if $Y_1 \sim \chi^2_{\nu_1}$ and $Y_2 \sim \chi^2_{\nu_2}$, then

$$F = \frac{Y_1/\nu_1}{Y_2/\nu_2} \sim \mathsf{Fisher}(\nu_1, \nu_2)$$

The Fisher distribution tends to a $\chi^2_{\nu_1}$ when $\nu_2 \to \infty$.

1.5 Graphs

This section reviews the main graphical representation of random variables, depending on their type.

The main type of graph for representing categorical variables is bar plot (and modifications thereof). In a bar plot, the frequency of each category is represented in the y-axis as a function of the (ordered) levels on the x-axis. This representation is superior to the ignominious pie chart, a nuisance that ought to be banned (humans are very bad at comparing areas and a simple rotation changes the perception of the graph)!

Continuous variables can take as many distinct values as there are observations, so we cannot simply count the number of occurences by unique values. Instead, we bin them

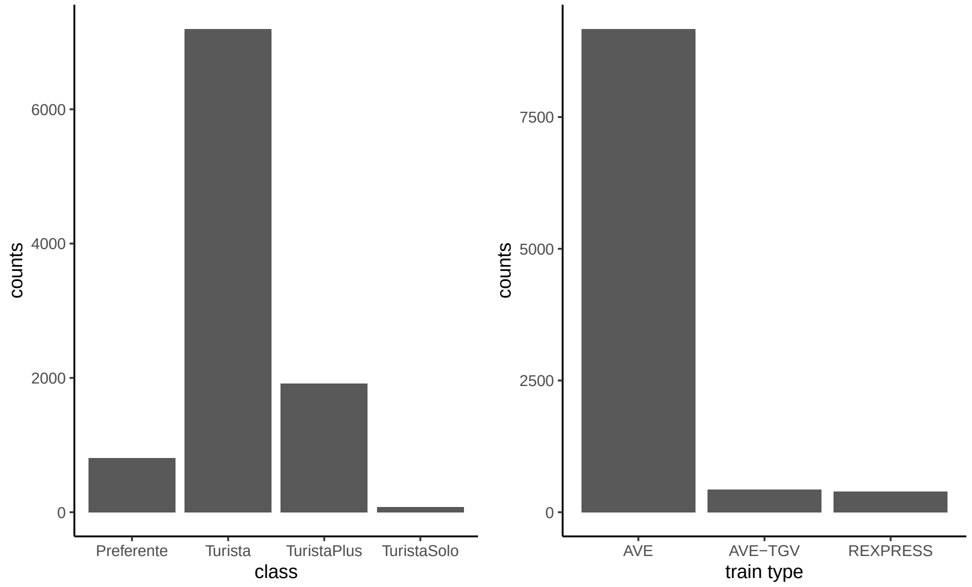


Figure 1.5: Bar plot of ticket class for Renfe tickets data

into distinct intervals so as to obtain an histogram. The number of class depends on the number of observations: as a rule of thumb, the number of bins should not exceed $\sqrt{n}$, where n is the sample size. We can then obtain the frequency in each class, or else normalize the histogram so that the area under the bands equals one: this yields a discrete approximation of the underlying density function. Varying the number of bins can help us detect patterns (rounding, asymmetry, multimodality).

Since we bin observations together, it is sometimes difficult to see where they fall. Adding rugs below or above the histogram will add observation about the range and values taken, where the heights of the bars in the histogram carry information about the (relative) frequency of the intervals.

If we have a lot of data, it sometimes help to focus only on selected summary statistics.

Definition 1.15 (Box-and-whiskers plot)**.** A box-and-whiskers plot (or boxplot) represents five numbers

- The box gives the quartiles q_1, q_2, q_3 of the distribution. The middle bar q_2 is thus the median, so 50% of the observations are smaller or larger than this number.
- The length of the whiskers is up to 1.5 times the interquartiles range $q_3 - q_1$ (the whiskers extend until the latest point in the interval, so the largest observation that is smaller than $q_3 + 1.5(q_3 - q_1)$, etc.)

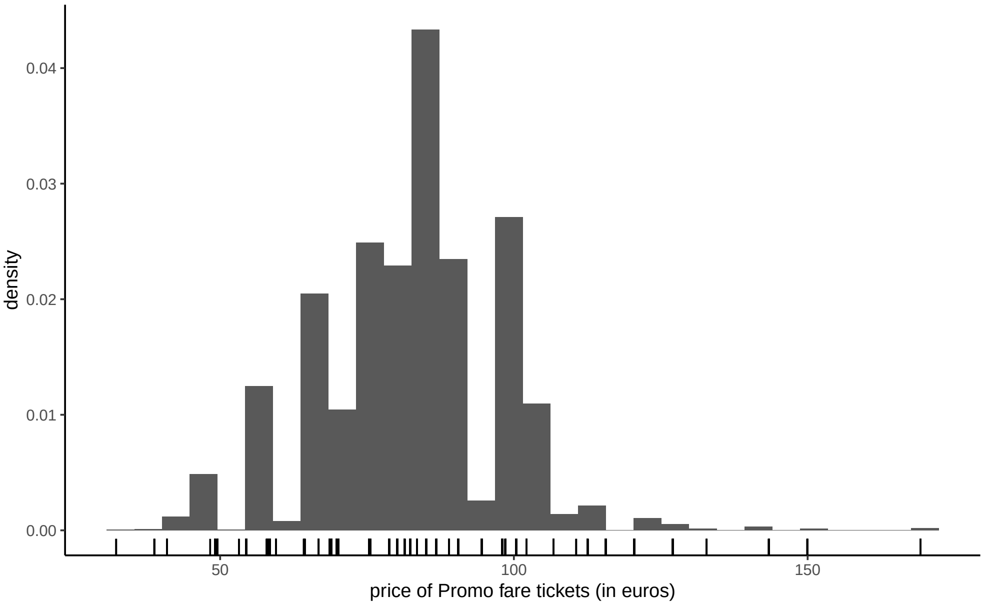


Figure 1.6: Histogram of Promo tickets for Renfe ticket data

- Observations beyond the whiskers are represented by dots or circles, sometimes termed outliers. However, beware of this terminology: the larger the sample size, the more values will fall outside the whiskers. This is a drawback of boxplots, which was conceived at a time where the size of data sets was much smaller than what is current standards.

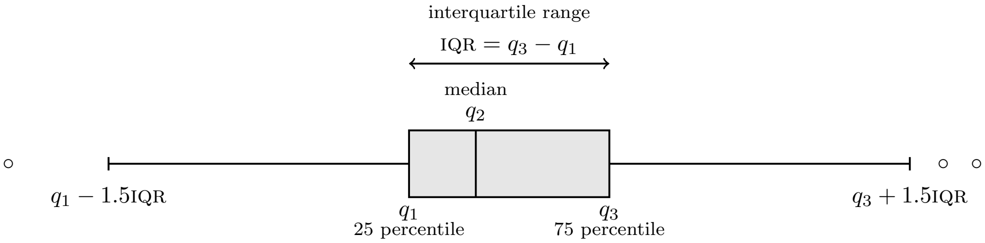


Figure 1.7: Box-and-whiskers plot

We can represent the distribution of a response variable as a function of a categorical variable by drawing a boxplot for each category and laying them side by side. A third variable, categorical, can be added via a color palette, as shown in Figure 1.8.

Scatterplots are used to represent graphically the co-variation between two continuous

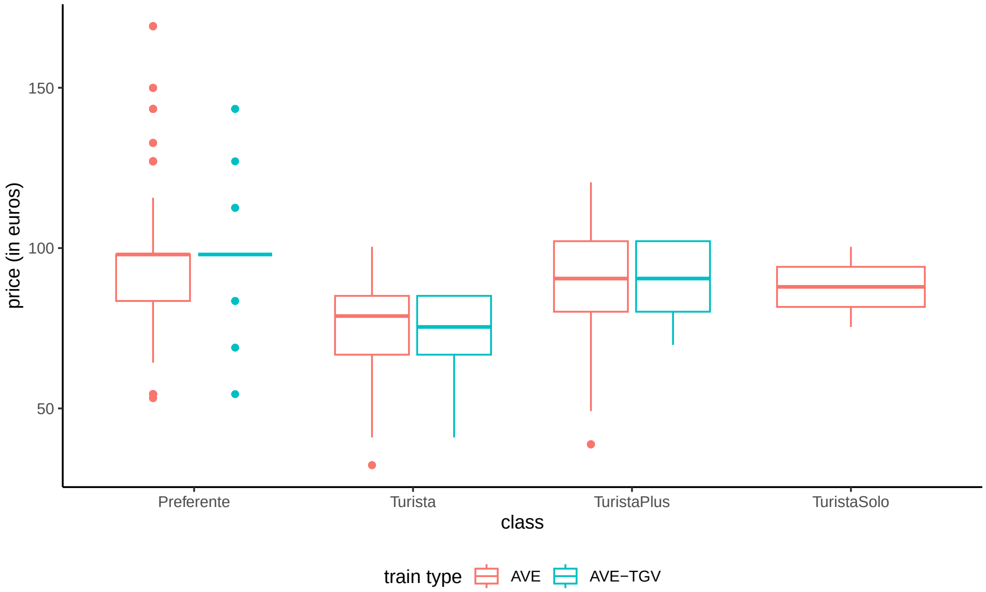


Figure 1.8: Box-and-whiskers plots for Promo fare tickets as a function of class and type for the Renfe tickets data.

variables: each tuple gives the coordinate of the point. If only a handful of large values are visible on the graph, a transformation may be useful: oftentimes, you will encounter graphs where the x- or y-axis is on the log-scale when the underlying variable is positive. If the number of data points is too large, it is hard to distinguish points because they are overlaid: adding transparency, or binning using a two-dimensional histogram with the frequency represented using color are potential solutions. The left panel of Figure 1.9 shows the 100 simulated observations, whereas the right-panel shows a larger sample of 10 000 points using hexagonal binning, an analog of the bivariate density.

Models are (at best) an approximation of the true data generating mechanism and we will want to ensure that our assumptions are reasonable and the quality of the fit decent.

Definition 1.16 (Quantiles-quantiles plots)**.** Quantile-quantile plots are graphical goodness-of-fit diagnostics that are based on the following principle: if Y is a continuous random variable with distribution function F, then the mapping $F(Y) \sim \mathsf{unif}(0,1)$ yields standard uniform variables. Similarly, the quantile transform applied to a uniform variable provides a mean to simulating samples from F, viz. $F^{-1}(U)$. Consider then a random sample of size n from the uniform distribution ordered from smallest to largest, with $U_{(1)} \leq \cdots \leq U_{(n)}$. One can show these ranks have marginally a Beta distribution, $U_{(k)} \sim \mathsf{beta}(k, n+1-k)$ with expectation $k/(n+1)$.

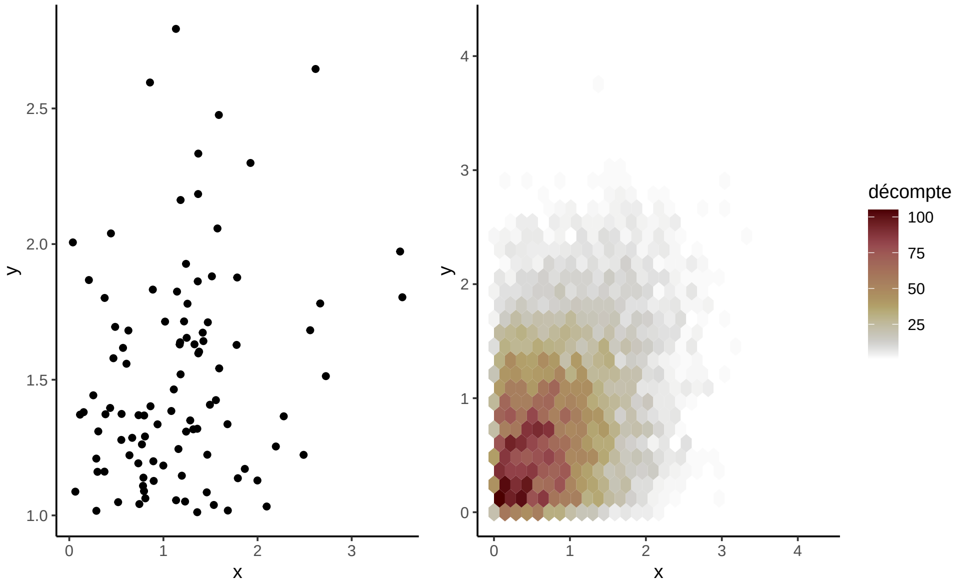


Figure 1.9: Scatterplot (left) and hexagonal heatmap of bidimensional bin counts (right) of simulated data.

In practice, we don't know F and, even if we did, one would need to estimate the parameters. We consider some estimator $\widehat{F}$ for the model and apply the inverse transform to an approximate uniform sample $\{i/(n+1)\}_{i=1}^{n}$. The quantile-quantile plot shows the data as a function of the (first moment) of the transformed order statistics:

- on the x-axis, the theoretical quantiles $\widehat{F}^{-1}\{\mathrm{rank}(y_i)/(n+1)\}$
- on the y-axis, the empirical quantiles y_i

If the model is adequate, the ordered values should follow a straight line with unit slope passing through the origin.

Even if we knew the true distribution of the data, the sample variability makes it very difficult to spot if deviations from the model are abnormal or compatible with the model. A simple point estimate with no uncertainty measure can lead to wrong conclusions. As such, we add approximate pointwise or simultaneous confidence intervals. The simplest way to do this is by simulation, by repeating the following steps B times:

1. simulate a sample $\{Y_i^{(b)}\}(i=1,\ldots,n)$ from $\widehat{F}$
2. re-estimate the parameters of F to obtain $\widehat{F}_{(b)}$
3. calculate and save the plotting positions $\widehat{F}_{(b)}^{-1}\{i/(n+1)\}$.

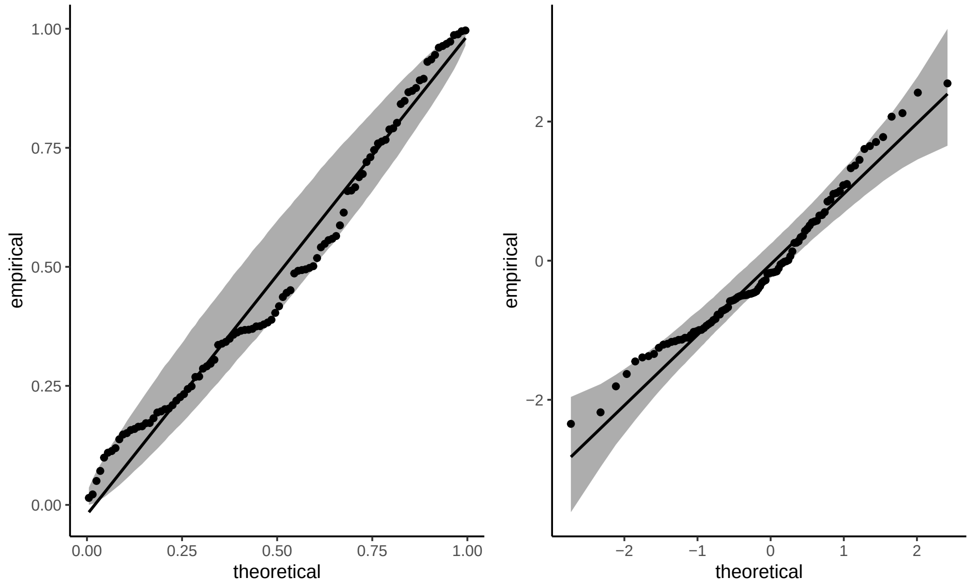


Figure 1.10: Probability-probability plot (left) on uniform margins, and ormal quantile-quantile plot (right) for the same dataset.

The result of this operation is an $n \times B$ matrix of simulated data. We obtain a symmetric $(1-\alpha)$ confidence interval by keeping the empirical quantile of order $\alpha/2$ and $1-\alpha/2$ from each row. The number B should be larger than 999, say, and be chosen so that B/α is an integer.

For the pointwise interval, each order statistic from the sample is a statistic and so the probability of any single one falling outside the confidence interval is approximately α. However, order statistics are not independent (they are ordered), so its common to see neighbouring points falling outside of their respective intervals. The intervals shown in Figure 1.10 are pointwise and derived (magically) using a simple function. The uniform order statistics have larger variability as we move away from 0.5, but the uncertainty in the quantile-quantile plot largely depends on F.

Interpretation of quantile-quantile plots requires practice and experience: this post by *Glen_b* on StackOverflow nicely summarizes what can be detected (or not) from them.

1.6 Laws of large numbers

An estimator for a parameter θ is **consistent** if the value obtained as the sample size increases (to infinity) converges to the true value of θ. Mathematically speaking, this translates into convergence in probability, meaning $\hat{\theta} \overset{\mathsf{Pr}}{\to} \theta$. In common language, we say that the probability that $\hat{\theta}$ and θ differ becomes negligible as n gets large.

Consistency is the *a minima* requirement for an estimator: when we collect more information, we should approach the truth. The law of large number states that the sample mean of n (independent) observations with common mean μ, say $\overline{Y}_n$, converges to μ, denoted $\overline{Y}_n \to \mu$. Roughly speaking, our approximation becomes less variable and asymptotically unbiased as the sample size (and thus the quantity of information available for the parameter) increases. The law of large number is featured in Monte Carlo experiments: we can approximate the expectation of some (complicated) function $g(x)$ by simulating repeatedly independent draws from Y and calculating the sample mean $n^{-1}\sum_{i=1}^n g(Y_i)$.

If the law of large number tells us what happens in the limit (we get a single numerical value), the result doesn't contain information about the rate of convergence and the uncertainty at finite levels.

1.7 Central Limit Theorem

The central limit theorem gives the approximate large sample distribution of the sample mean. Consider a random sample of size n $\{Y_i\}_{i=1}^n$ of independent random variables with common expectation μ and variance σ^2. The sample mean $\overline{Y} = n^{-1}\sum_{i=1}^n Y_i$ converges to μ by the law of large number, but we also have that

- the estimator $\overline{Y}$ is centered around μ,
- the standard error is $\sigma/\sqrt{n}$; the rate of convergence is thus $\sqrt{n}$. For a sample of size 100, the standard error of the sample mean will be 10 times smaller than that of the underlying random variable.
- the sample mean, once properly scaled, follows approximately a normal distribution

Mathematically, the central limit theorem states $\sqrt{n}(\overline{Y} - \mu) \overset{\mathrm{d}}{\rightarrow} \mathsf{normal}(0, \sigma^2)$. If n is large (a rule of thumb is $n > 30$, but this depends on the underlying distribution of Y), then $\overline{Y} \stackrel{\cdot}{\sim} \mathsf{normal}(\mu, \sigma^2/n)$.

How do we make sense of this result? Let us consider the mean travel time of high speed Spanish trains (AVE) between Madrid and Barcelona that are operated by Renfe.

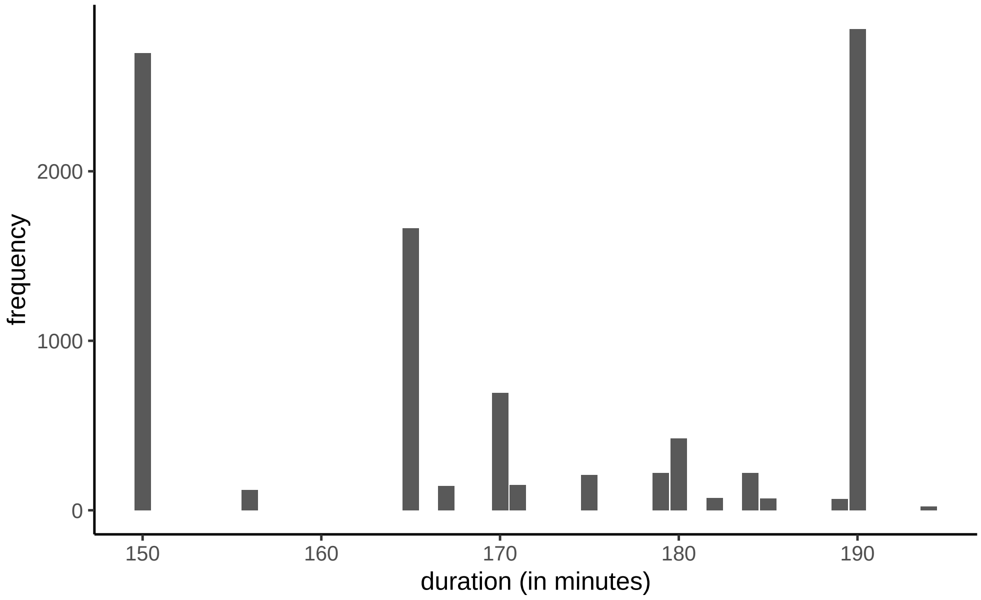


Figure 1.11: Empirical distribution of travel times of high speed trains.

Our exploratory data analysis showed previously that the duration is the one advertised on the ticket: there are only 15 unique travel time. Based on 9603 observations, we estimate the mean travel time to be 170 minutes and 41 seconds. Figure 1.11 shows the empirical distribution of the data.

Consider now samples of size $n = 10$, drawn repeatedly from the population: in the first sample, the sample mean is 169.3 minutes, whereas we get an estimate of 167 minutes in our second , 157.9 minutes in the third, etc.

We draw $B = 1000$ different samples, each of size $n = 5$, from two millions records, and calculate the sample mean in each of them. The top right panel of Figure 1.12 is a histogram of the sample means when $n = 5$, whereas the bottom left panel shows the same thingfor $n = 20$. The last graph of Figure 1.12 shows the impact of the increase in sample size: whereas the normal approximation is okay-ish for $n = 5$, it is indistinguishable from the normal approximation for $n = 20$. As n increases and the sample size gets bigger, the quality of the approximation improves and the curve becomes more concentrated around the true mean. Even if the distribution of the travel time is discrete, the mean is approximately normal.

We considered a single distribution in the example, but you could play with other distributions and vary the sample size to see when the central limit theorem kicks in usng this applet.

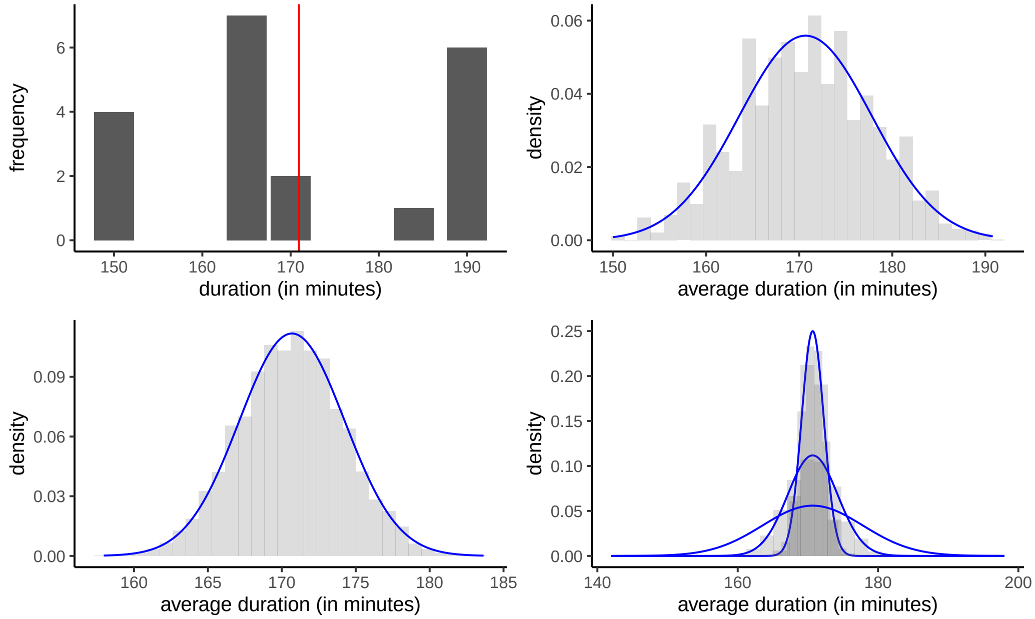


Figure 1.12: Graphical representation of the central limit theorem. The upper left panel shows a sample of 20 observations with its sample mean (vertical red). The three other panels show the histograms of the sample mean from repeated samples of size 5 (top right), 20 (bottom left) and 20, 50 and 100 overlaid, with the density approximation provided by the central limit theorem.

The central limit theorem underlies why scaled test statistics which have sample mean zero and sample variance 1 have a standard null distribution in large sample: this is what guarantees the validity of our inference!

2 Statistical inference

In most applied domains, empirical evidences drive the advancement of the field and data from well designed experiments contribute to the built up of science. In order to draw conclusions in favour or against a theory, researchers turn (often unwillingly) to statistics to back up their claims. This has led to the prevalence of the use of the null hypothesis statistical testing (NHST) framework. One important aspect of the reproducibility crisis is the misuse of p-values in journal articles: falsification of a null hypothesis is not enough to provide substantive findings for a theory.

Because introductory statistics course typically present hypothesis tests without giving much thoughts to the underlying construction principles of such procedures, users often have a reductive view of statistics as a catalogue of pre-determined procedures. To make a culinary analogy, users focus on learning recipes rather than trying to understand the basics of cookery. This chapter focuses on understanding of key ideas related to testing.

! Important

Learning objectives:

- Understanding the role of uncertainty in decision making.
- Understanding the importance of signal-to-noise ratio as a measure of evidence.
- Knowing the basic ingredients of hypothesis testing and being capable of correctly formulating and identifying these components in a paper.
- Correctly interpreting p-values and confidence intervals for a parameter.

The first step of a design is formulating a research question. Generally, this hypothesis will specify potential differences between population characteristics due to some intervention (a treatment) that the researcher wants to quantify. This is the step during which researchers decide on sample size, choice of response variable and metric for the measurement, write down the study plan, etc.

It is important to note that most research questions cannot be answered by simple tools. Researchers wishing to perform innovative methodological research should contact experts and consult with statisticians **before** they collect their data to get information on how best to proceed for what they have in mind so as to avoid the risk of making misleading and false claims based on incorrect analysis or data collection.

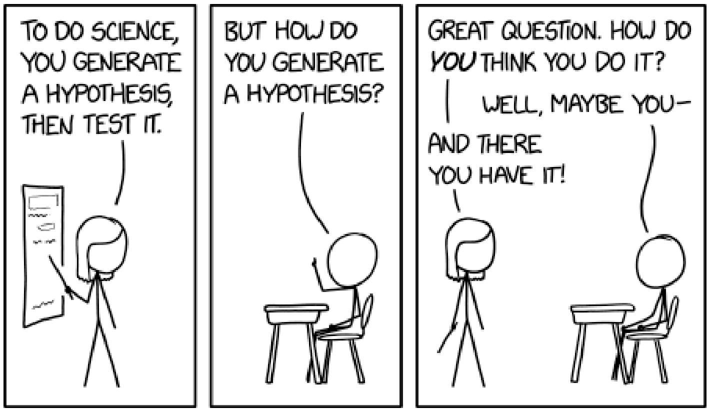

TO DO SCIENCE, YOU GENERATE A HYPOTHESIS, THEN TEST IT.
BUT HOW DO YOU GENERATE A HYPOTHESIS?
GREAT QUESTION. HOW DO YOU THINK YOU DO IT?
WELL, MAYBE YOU—
AND THERE YOU HAVE IT!

Figure 2.1: xkcd comic 2569 (Hypothesis generation) by Randall Munroe. Alt text: Frazzled scientists are requesting that everyone please stop generating hypotheses for a little bit while they work through the backlog. Cartoon reprinted under the CC BY-NC 2.5 license.

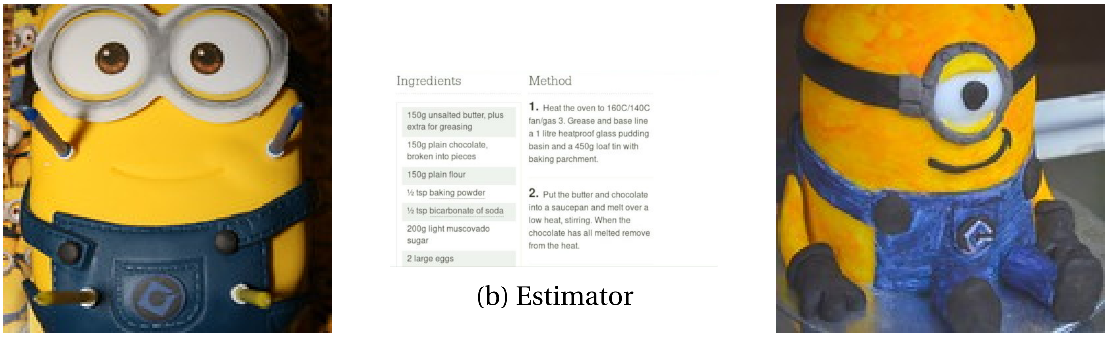
2.1 Sampling variability

Given data, a researcher will be interested in estimating particular characteristics of the population. We can characterize the set of all potential values their measurements can take, together with their frequency, via a distribution.

The purpose of this section is to illustrate how we cannot simply use raw differences between groups to make meaningful comparisons: due to sampling variability, samples will be alike even if they are generated in the same way, but there will be always be differences between their summary statistics. Such differences tend to attenuate (or increase) as we collect more sample. Inherent to this is the fact that as we gather more data (and thus more information) about our target, the portrait becomes more precise. This is ultimately what allows us to draw meaningful conclusions but, in order to do so, we need first to determine what is likely or plausible and could be a stroke of luck, and what is not likely to occur solely due to randomness.

We call numerical summaries of the data **statistics**. Its important to distinguish between procedures/formulas and their numerical values. An **estimator** is a rule or formula used to calculate an estimate of some parameter or quantity of interest based on observed data (like a recipe for cake). Once we have observed data we can actually compute the sample mean, that is, we have an estimate — an actual value (the cake), which is a single realization and not random. In other words,

- an estimand is our conceptual target, like the population characteristic of interest (population mean).
- an estimator is the procedure or formula telling us how to transform the sample data into a numerical summary that is a proxy of our target.
- an estimate is a number, the numerical value obtained once we apply the formula to observed data.



Ingredients

- 150g unsalted butter, plus extra for greasing
- 150g plain chocolate, broken into pieces
- 150g plain flour
- ½ tsp baking powder
- ½ tsp bicarbonate of soda
- 200g light muscovado sugar
- 2 large eggs

Method

1. Heat the oven to 160C/140C fan/gas 3. Grease and base line a 1 litre heatproof glass pudding basin and a 450g loaf tin with baking parchment.
2. Put the butter and chocolate into a saucepan and melt over a low heat, stirring. When the chocolate has all melted remove from the heat.

(a) Estimand

(b) Estimator

(c) Estimate

Figure 2.2: Estimand (left), estimator (middle) and estimate (right) illustrated with cakes and based on an original idea of Simon Grund. Cake photos shared under CC BY-NC 2.0 license.

For example, we may use as estimand the population average of $Y_1, \ldots,$ say μ. The estimator will be sample mean, i.e., the sum of the elements in the sample divided by the sample size, $\overline{Y} = (Y_1 + \cdots + Y_n)/n$. The estimate will be a numerical value, say 4.3.

Because the inputs of the estimator are random, the output is also random and change from one sample to the next: even if you repeat a recipe, you won't get the exact same result every time, as in Figure 2.3.

To illustrate this point, Figure 2.4 shows five simple random samples of size $n = 10$ drawn from an hypothetical population with mean μ and standard deviation σ, along with their sample mean $\overline{y}$. Because of the sampling variability, the sample means of the subgroups will differ even if they originate from the same distribution. You can view sampling variability as noise: our goal is to extract the signal (typically differences in means) but accounting for spurious results due to the background noise.

The astute eye might even notice that the sample means (thick horizontal segments) are less dispersed around the full black horizontal line representing the population average μ

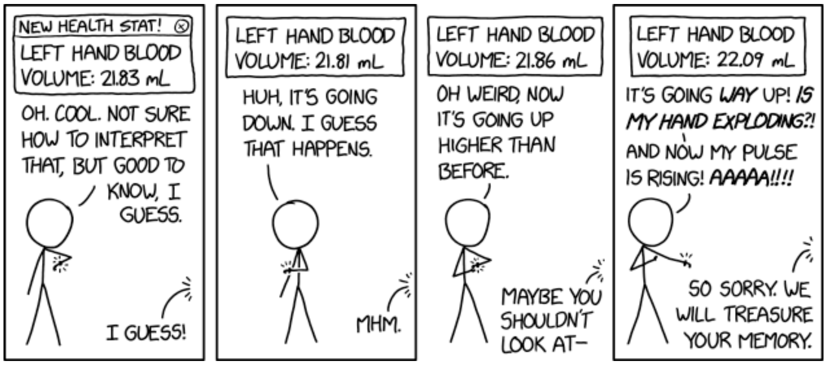

NEW HEALTH STAT!
LEFT HAND BLOOD VOLUME: 21.83 mL
OH. COOL. NOT SURE HOW TO INTERPRET THAT, BUT GOOD TO KNOW, I GUESS.
I GUESS!
LEFT HAND BLOOD VOLUME: 21.81 mL
HUH, IT'S GOING DOWN. I GUESS THAT HAPPENS.
MHM.
LEFT HAND BLOOD VOLUME: 21.86 mL
OH WEIRD, NOW IT'S GOING UP HIGHER THAN BEFORE.
MAYBE YOU SHOULDN'T LOOK AT—
LEFT HAND BLOOD VOLUME: 22.09 mL
IT'S GOING WAY UP! IS MY HAND EXPLODING?! AND NOW MY PULSE IS RISING! AAAAA!!!!
SO SORRY. WE WILL TREASURE YOUR MEMORY.

Figure 2.3: xkcd comic 2581 (Health Stats) by Randall Munroe. Alt text: You will live on forever in our hearts, pushing a little extra blood toward our left hands now and then to give them a squeeze. Cartoon reprinted under the CC BY-NC 2.5 license.

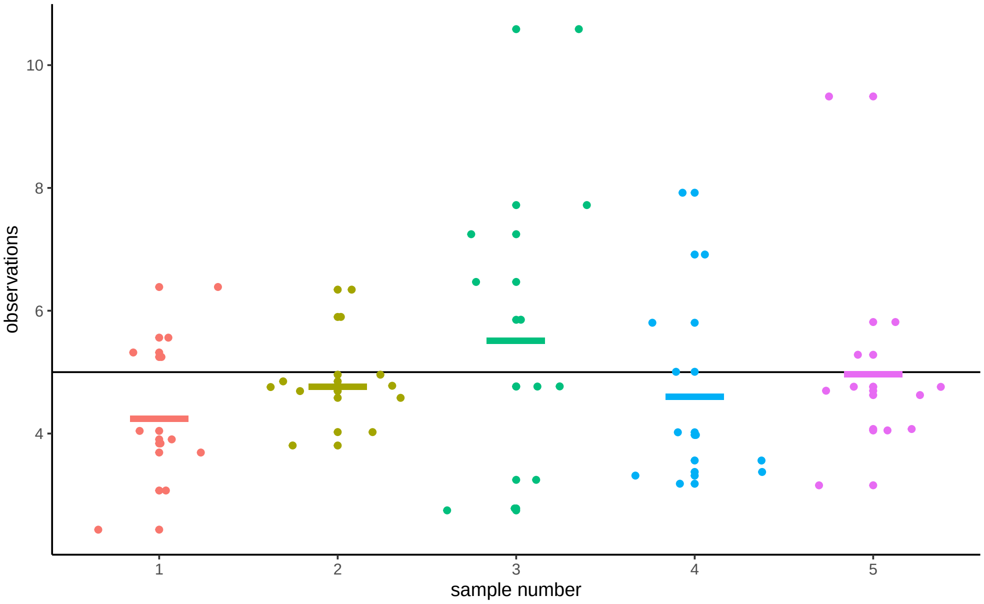


Figure 2.4: Five samples of size $n = 10$ drawn from a common population with mean μ (horizontal line). The colored segments show the sample means of each sample.

than are the individual measurements. This is a fundamental principle of statistics: information accumulates as you get more data.

Values of the sample mean don't tell the whole picture and studying differences in mean (between groups, or relative to a postulated reference value) is not enough to draw conclusions. In most settings, there is no guarantee that the sample mean will be equal to it's true value because it changes from one sample to the next: the only guarantee we have is that it will be on average equal to the population average in repeated samples. Depending on the choice of measurement and variability in the population, there may be considerable differences from one observation to the next and this means the observed difference could be a fluke.

To get an idea of how certain something is, we have to consider the variability of an observation Y_i. This variance of an observation drawn from the population is typically denoted σ^2 and it's square root, the standard deviation, by σ.

The standard deviation *of a statistic* is termed **standard error**; it should not be confused with the standard deviation σ of the population from which the sample observations $Y_1, \ldots, Y_n$ are drawn. Both standard deviation and standard error are expressed in the same units as the measurements, so are easier to interpret than variance. Since the standard error is a function of the sample size, it is however good practice to report the estimated standard deviation in reports.

Example 2.1 (Sample proportion and uniform draws)**.** To illustrate the concept of sampling variability, we follow the lead of Matthew Crump and consider samples from a uniform distribution on $\{1, 2, \ldots, 10\}$ each number in this interval is equally likely to be sampled.

Even if they are drawn from the same population, the 10 samples in Figure 2.5 look quite different. The only thing at play here is the sample variability: since there are $n = 20$ observations in total, there should be on average 10% of the observations in each of the 10 bins, but some bins are empty and others have more counts than expected. This fluctuation is due to randomness, or chance.

How can we thus detect whether what we see is compatible with the model we think generated the data? The key is to collect more observations: the bar height is the sample proportion, an average of 0/1 values with ones indicating that the observation is in the bin and zero otherwise.

Consider now what happens as we increase the sample size: the top panel of Figure 2.6 shows uniform samples for increasing samples size. The scaled bar plot looks more and more like the true underlying distribution (flat, each bin with equal frequency) as the sample size increases. The sample distribution of points is nearly indistinguishable from the theoretical one (straight line) when $n = 10000$.[1] The bottom panel, on the other hand,

[1] The formula shows that the standard error decreases by a tenfold every time the sample size increases by a factor 100.

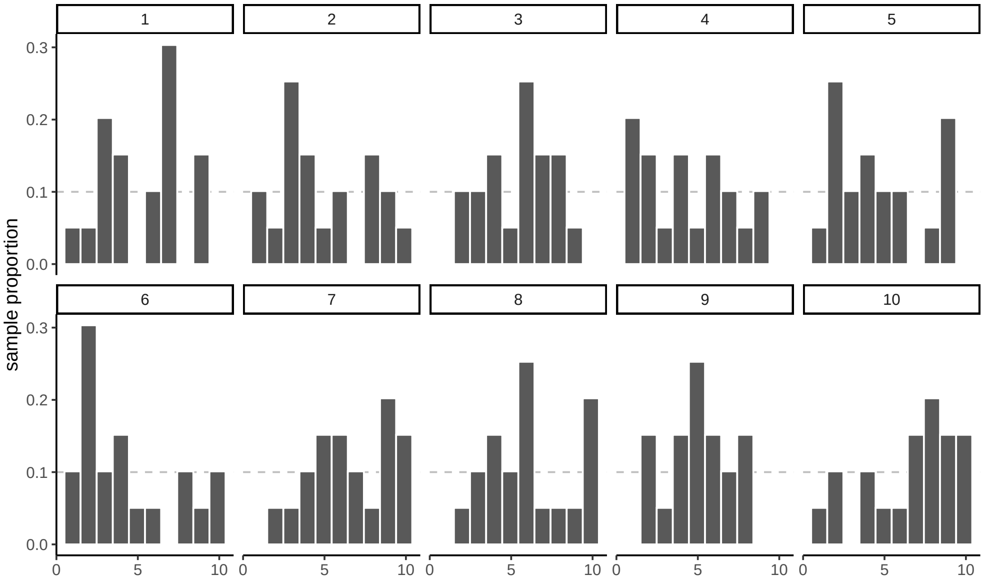


Figure 2.5: Histograms for 10 random samples of size $n = 20$ from a discrete uniform distribution.

isn't from a uniform distribution and larger samples come closer to the population distribution. We couldn't have spotted this difference in the first two plots, since the sampling variability is too important; there, the lack of data in some bins could have been attributed to chance, as they are comparable with the graph for data that are truly uniform. This is in line with most practical applications, in which the limited sample size restricts our capacity to disentangle real differences from sampling variability. We must embrace this uncertainty: in the next section, we outline how hypothesis testing helps us disentangle the signal from the noise.

2.2 Hypothesis testing

An **hypothesis test** is a binary decision rule used to evaluate the statistical evidence provided by a sample to make a decision regarding the underlying population. The main steps involved are:

- define the model parameters
- formulate the alternative and null hypothesis
- choose and calculate the test statistic

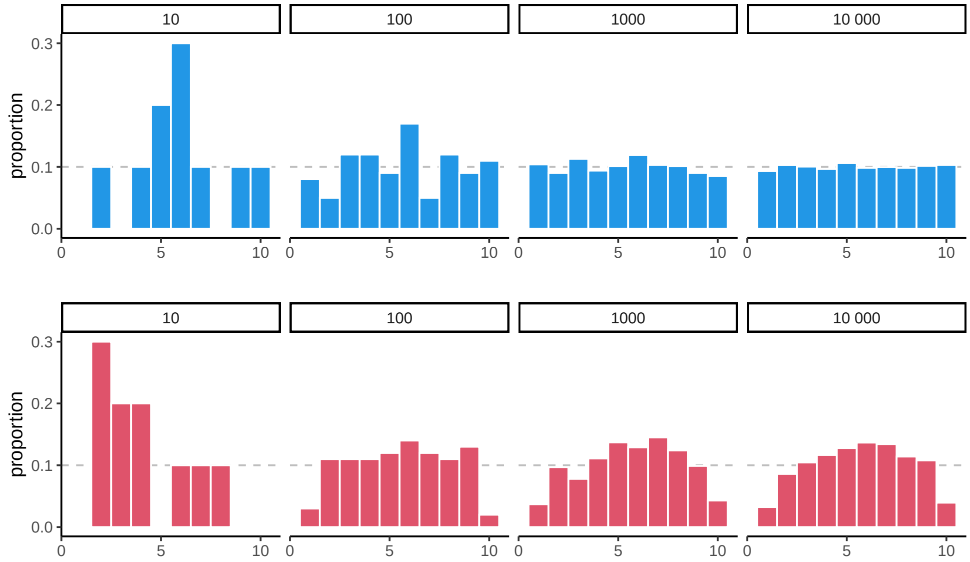


Figure 2.6: Bar plots of data from a uniform distribution (top) and non-uniform (bottom) with increasing sample sizes of 10, 100, 1000 and 10 000 (from left to right).

- obtain the null distribution describing the behaviour of the test statistic under $\mathscr{H}_0$
- calculate the p-value
- conclude (reject or fail to reject $\mathscr{H}_0$) in the context of the problem.

A good analogy for hypothesis tests is a trial for murder on which you are appointed juror.

- The judge lets you choose between two mutually exclusive outcome, guilty or not guilty, based on the evidence presented in court.
- The presumption of innocence applies and evidences are judged under this optic: are evidence remotely plausible if the person was innocent? The burden of the proof lies with the prosecution to avoid as much as possible judicial errors. The null hypothesis $\mathscr{H}_0$ is *not guilty*, whereas the alternative $\mathscr{H}_a$ is *guilty*. If there is a reasonable doubt, the verdict of the trial will be not guilty.
- The test statistic (and the choice of test) represents the summary of the proof. The more overwhelming the evidence, the higher the chance the accused will be declared guilty. The prosecutor chooses the proof so as to best outline this: the choice of evidence (statistic) ultimately will maximise the evidence, which parallels the power of the test.
- The final step is the verdict. This is a binary decision, guilty or not guilty. For an

> hypothesis test performed at level α, one would reject (guilty) if the *p*-value is less than α.

The above description provides some heuristic, but lacks crucial details.

2.3 Hypothesis

In statistical tests we have two hypotheses: the null hypothesis ($\mathscr{H}_0$) and the alternative hypothesis ($\mathscr{H}_1$). Usually, the null hypothesis is the 'status quo' and the alternative is what we're really interested in testing. A statistical hypothesis test allows us to decide whether or not our data provides enough evidence to reject $\mathscr{H}_0$ in favour of $\mathscr{H}_1$, subject to some pre-specified risk of error. Usually, hypothesis tests involve a parameter, say θ, which characterizes the underlying distribution at the population level ans whose value is unknown. A two-sided hypothesis test regarding a parameter θ has the form

$$\mathscr{H}_0 : \theta = \theta_0 \qquad \text{versus} \qquad \mathscr{H}_a : \theta \neq \theta_0.$$

We are testing whether or not θ is precisely equal to the value θ_0. The hypotheses are a statistical representation of our research question.

A common example of two-sided test is one for the regression coefficient β_j associated to an explanatory variable X_j, for which the null and alternative hypothesis are

$$\mathscr{H}_0 : \beta_j = \beta_j^0 \qquad \text{versus} \qquad \mathscr{H}_a : \beta_j \neq \beta_j^0,$$

where β_j^0 is some value that reflects the research question of interest. For example, if $\beta_j^0 = 0$, the underlying question is: is covariate X_j impacting the response Y linearly once other variables have been taken into account?

Note that we can impose direction in the hypotheses and consider alternatives of the form $\mathscr{H}_a : \theta > \theta_0$ or $\mathscr{H}_a : \theta < \theta_0$.

2.4 Test statistic

A test statistic T is a function of the data that summarise the information contained in the sample for θ. The form of the test statistic is chosen such that we know its underlying distribution under $\mathscr{H}_0$, that is, the potential values taken by T and their relative probability if $\mathscr{H}_0$ is true. Indeed, Y is a random variable and its value change from one sample to the next. This allows us to determine what values of T are likely if $\mathscr{H}_0$ is true. Many statistics we will consider are **Wald statistic**, of the form

$$T = \frac{\widehat{\theta} - \theta_0}{\mathrm{se}(\widehat{\theta})}$$

where $\widehat{\theta}$ is an estimator of θ, θ_0 is the postulated value of the parameter and $\mathrm{se}(\widehat{\theta})$ is an estimator of the standard deviation of the test statistic $\widehat{\theta}$.

For example, to test whether the mean of a population is zero, we set

$$\mathscr{H}_0 : \mu = 0, \qquad \mathscr{H}_a : \mu \neq 0,$$

and the Wald statistic is

$$T = \frac{\overline{X} - 0}{S_n/\sqrt{n}}$$

where $\overline{X}$ is the sample mean of $X_1, \ldots, X_n$,

$$\overline{X} = \frac{1}{n}\sum_{i=1}^{n} X_i = \frac{X_1 + \cdots + X_n}{n}$$

and the standard error (of the mean) $\overline{X}$ is $S_n/\sqrt{n}$; the sample variance S_n is an estimator of the standard deviation σ,

$$S_n^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \overline{X})^2.$$

2.5 Null distribution and *p*-value

The *p*-value allows us to decide whether the observed value of the test statistic T is plausible under $\mathscr{H}_0$. Specifically, the *p*-value is the probability that the test statistic is equal or more extreme to the estimate computed from the data, assuming $\mathscr{H}_0$ is true. Suppose that based on a random sample $Y_1, \ldots, Y_n$ we obtain a statistic whose value $T = t$. For a two-sided test $\mathscr{H}_0 : \theta = \theta_0$ vs. $\mathscr{H}_a : \theta \neq \theta_0$, the *p*-value is $\mathrm{Pr}_0(|T| \geq |t|)$.[2]

How do we determine the null distribution given that the true data generating mechanism is unknown to us? We ask a statistician! In simple cases, it might be possible to enumerate all possible outcomes and thus quantity the degree of outlyingness of our observed statistic. In more general settings, we can resort to simulations or to probability theory: the

[2] If the distribution of T is symmetric around zero, the *p*-value reduces to $p = 2 \times \mathrm{Pr}_0(T \geq |t|)$.

central limit theorem says that the sample mean behaves like a normal random variable with mean μ and standard deviation $\sigma/\sqrt{n}$ for n large enough. The central limit theorem has broader applications since most statistics can be viewed as some form of average or transformation thereof, a fact used to derive benchmarks for most commonly used tests. Most software use these approximations as proxy by default: the normal, Student's t, χ^2 and F distributions are the reference distributions that arise the most often.

Figure 2.7 shows the distribution of p-values for two scenarios: one in which there are no differences and the null is true, the other under an alternative. The probability of rejection is obtained by calculating the area under the density curve between zero and $\alpha = 0.1$, here 0.1 on the left. Under the null, the model is calibrated and the distribution of *p*-values is uniform (i.e., a flat rectangle of height 1), meaning all values in the unit interval are equally likely. Under the alternative (right), small *p*-values are more likely to be observed.

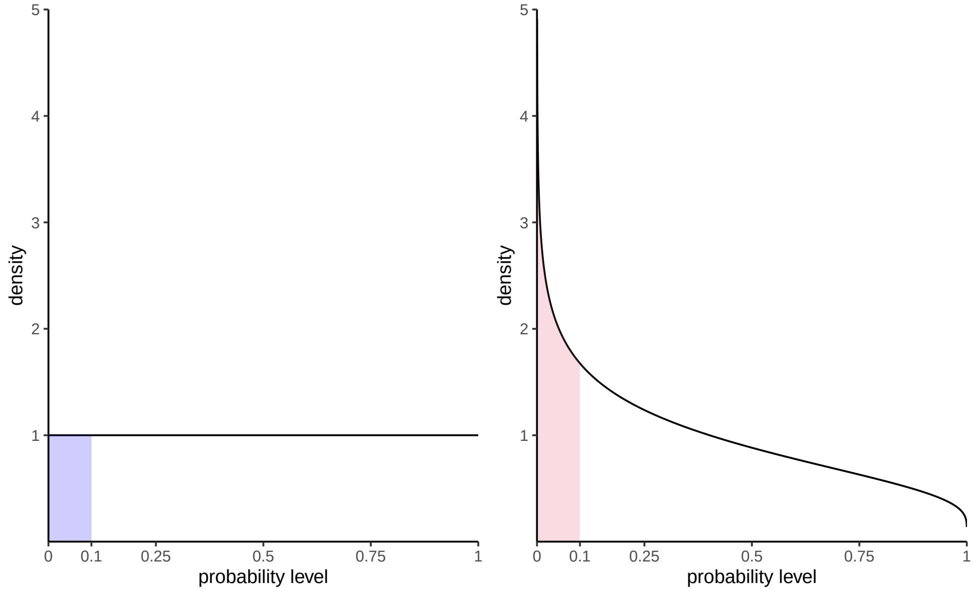


Figure 2.7: Density of *p*-values under the null hypothesis (left) and under an alternative with a signal-to-noise ratio of 0.5 (right).

There are generally three ways of obtaining null distributions for assessing the degree of evidence against the null hypothesis

- exact calculations
- large sample theory (aka 'asymptotics' in statistical lingo)
- simulation

While desirable, the first method is only applicable in simple cases (such as counting the probability of getting two six if you throw two fair die). The second method is most commonly used due to its generality and ease of use (particularly in older times where computing power was scarce), but fares poorly with small sample sizes (where 'too small' is context and test-dependent). The last approach can be used to approximate the null distribution in many scenarios, but adds a layer of randomness and the extra computations costs sometimes are not worth it.

Consider the example of a two-sided test involving the population mean $\mathscr{H}_0 : \mu = 0$ against the alternative $\mathscr{H}_1 : \mu \neq 0$. Assuming the random sample comes from a normal (population) $\mathsf{normal}(\mu, \sigma^2)$, it can be shown that if $\mathscr{H}_0$ is true (that is, if $\mu = 0$), the test statistic

$$T = \frac{\overline{X}}{S/\sqrt{n}}$$

follows a Student-*t* distribution with $n-1$ degrees of freedom. This allows us to calculate the *p*-value (either from a table, or using some statistical software). By virtue of the symmetry, the *p*-value is $P = 2 \times \Pr(T > |t|)$, where $T \sim \mathsf{Student}(n-1)$.

2.6 Confidence intervals

A **confidence interval** is an alternative way to present the conclusions of an hypothesis test performed at significance level α. It is often combined with a point estimator $\widehat{\theta}$ plus or minus a margin of error designed to give an indication of the variability of the estimation procedure. Wald-based $(1-\alpha)$ confidence intervals for a scalar parameter θ are of the form

$$[\widehat{\theta} + \mathfrak{q}_{\alpha/2}\mathrm{se}(\widehat{\theta}), \widehat{\theta} + \mathfrak{q}_{1-\alpha/2} \times \mathrm{se}(\widehat{\theta})]$$

where $\mathfrak{q}_{\alpha/2}$ is the $\alpha/2$ quantile of the null distribution of the Wald statistic W,

$$W = \frac{\widehat{\theta} - \theta}{\mathrm{se}(\widehat{\theta})},$$

and where θ represents the postulated value for the fixed, but unknown value of the parameter. The critical values for a symmetric interval, chosen so that the probability of being more extreme is α, are the $\alpha/2$ and $1-\alpha/2$ quantiles of the null distribution.

For example, for a random sample $X_1, \ldots, X_n$ from a normal distribution $\mathsf{normal}(\mu, \sigma)$, the $(1-\alpha)$ confidence interval for the population mean μ is

$$\overline{X} \pm t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}$$

where $t_{n-1,\alpha/2}$ is the $1-\alpha/2$ quantile of a Student-t distribution with $n-1$ degrees of freedom.

The bounds of the confidence intervals are random variables, since both estimators of the parameter and its standard error, $\widehat{\theta}$ and $\mathrm{se}(\widehat{\theta})$, are random: their values will vary from one sample to the next. Before the interval is calculated, there is a $1-\alpha$ probability that θ is contained in the **random** interval $(\widehat{\theta}-\mathfrak{q}_{\alpha/2}\,\mathrm{se}(\widehat{\theta}), \widehat{\theta}+\mathfrak{q}_{\alpha/2}\,\mathrm{se}(\widehat{\theta}))$, where $\widehat{\theta}$ denotes the estimator. Once we obtain a sample and calculate the confidence interval, there is no more notion of probability: the true value of the parameter θ is either in the confidence interval or not. We can interpret confidence intervals as follows: if we were to repeat the experiment multiple times, and calculate a $1-\alpha$ confidence interval each time, then roughly $1-\alpha$ of the calculated confidence intervals would contain the true value of θ in repeated samples (in the same way, if you flip a coin, there is roughly a 50-50 chance of getting heads or tails, but any outcome will be either). Our confidence is in the *procedure* we use to calculate confidence intervals and not in the actual values we obtain from a sample.

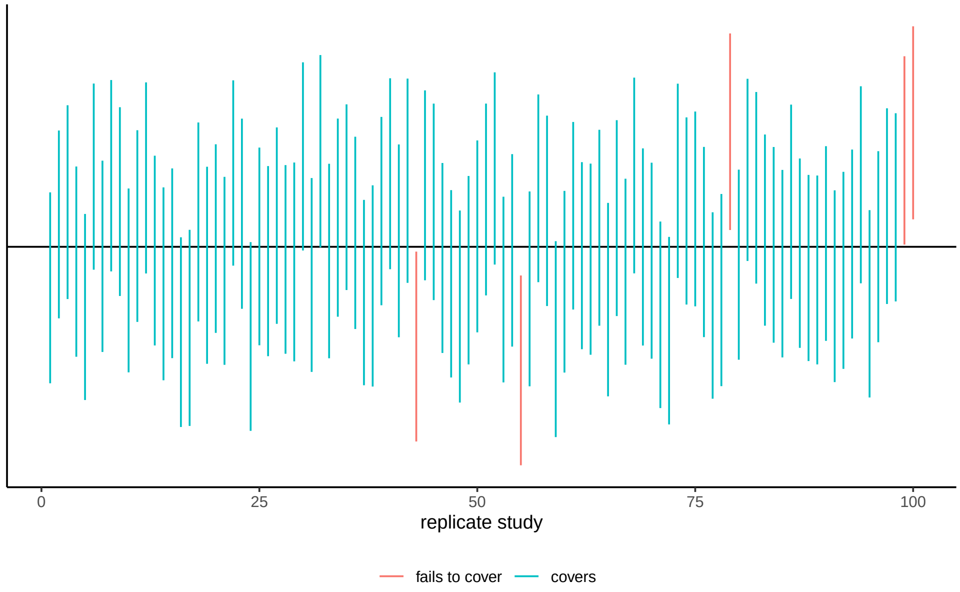


Figure 2.8: 95% confidence intervals for the mean of a standard normal population for 100 random samples. On average, 5% of these intervals fail to include the true mean value of zero (in red).

If we are only interested in the binary decision rule reject/fail to reject $\mathscr{H}_0$, the confidence interval is equivalent to a *p*-value since it leads to the same conclusion. Whereas the $1-\alpha$ confidence interval gives the set of all values for which the test statistic doesn't provide enough evidence to reject $\mathscr{H}_0$ at level α, the *p*-value gives the probability under the null of obtaning a result more extreme than the postulated value and so is more precise for this particular value. If the *p*-value is smaller than α, our null value θ will be outside of the confidence interval and vice-versa.

2.7 Conclusion

The *p*-value allows us to make a decision about the null hypothesis. If $\mathscr{H}_0$ is true, the *p*-value follows a uniform distribution. Thus, if the *p*-value is small, this means observing an outcome more extreme than $T = t$ is unlikely, and so we're inclined to think that $\mathscr{H}_0$ is not true. There's always some underlying risk that we're making a mistake when we make a decision. In statistic, there are two type of errors:

- type I error: we reject $\mathscr{H}_0$ when $\mathscr{H}_0$ is true,
- type II error: we fail to reject $\mathscr{H}_0$ when $\mathscr{H}_0$ is false.

These hypothesis are not judged equally: we seek to avoid error of type I (judicial errors, corresponding to condemning an innocent). To prevent this, we fix the level of the test, α, which captures our tolerance to the risk of committing a type I error: the higher the level of the test α, the more often we will reject the null hypothesis when the latter is true. The value of $\alpha \in (0,1)$ is the probability of rejecting $\mathscr{H}_0$ when $\mathscr{H}_0$ is in fact true,

$$\alpha = \Pr{}_0\left(\text{ reject } \mathscr{H}_0\right).$$

where the subscript $\Pr{}_0$ indicates the probability under the null model. The level α is fixed beforehand, typically 1%, 5% or 10%. Keep in mind that the probability of type I error is α only if the null model for $\mathscr{H}_0$ is correct (sic) and correspond to the data generating mechanism.

The focus on type I error is best understood by thinking about medical trial: you need to prove a new cure is better than existing alternatives drugs or placebo, to avoid extra costs or harming patients (think of Didier Raoult and his unsubstantiated claims that hydrochloroquine, an antipaludean drug, should be recommended treatment against Covid19).

Decision \ true model	$\mathscr{H}_0$	$\mathscr{H}_a$
fail to reject $\mathscr{H}_0$	✓	type II error
reject $\mathscr{H}_0$	type I error	✓

To make a decision, we compare our *p*-value P with the level of the test α:

- if $P < \alpha$, we reject $\mathscr{H}_0$;
- if $P \geq \alpha$, we fail to reject $\mathscr{H}_0$.

Do not mix up level of the test (probability fixed beforehand by the researcher) and the *p*-value. If you do a test at level 5%, the probability of type I error is by definition α and does not depend on the *p*-value. The latter is conditional probability of observing a more extreme likelihood given the null distribution $\mathscr{H}_0$ is true.

Caution

The American Statistical Association (ASA) published a list of principles guiding (mis)interpretation of *p*-values, some of which are reproduced below:

> (2) *P*-values do not measure the probability that the studied hypothesis is true.
>
> (3) Scientific conclusions and business or policy decisions should not be based only on whether a *p*-value passes a specific threshold.
>
> (4) *P*-values and related analyses should not be reported selectively.
>
> (5) *p*-value, or statistical significance, does not measure the size of an effect or the importance of a result.

2.8 Power

There are two sides to an hypothesis test: either we want to show it is not unreasonable to assume the null hypothesis, or else we want to show beyond reasonable doubt that a difference or effect is significative: for example, one could wish to demonstrate that a new website design (alternative hypothesis) leads to a significant increase in sales relative to the status quo. Our ability to detect these improvements and make discoveries depends on the power of the test: the larger the power, the greater our ability to reject $\mathscr{H}_0$ when the latter is false.

Failing to reject $\mathscr{H}_0$ when $\mathscr{H}_a$ is true corresponds to the definition of type II error, the probability of which is $1-$power, say. The **power of a test** is the probability of rejecting $\mathscr{H}_0$ when $\mathscr{H}_0$ is false, i.e.,

$$\mathrm{Pr}_a(\text{reject } \mathscr{H}_0),$$

i.e., the probability under the alternative model of falling in the rejection region. Depending on the alternative models, it is more or less easy to detect that the null hypothesis is false and reject in favor of an alternative.

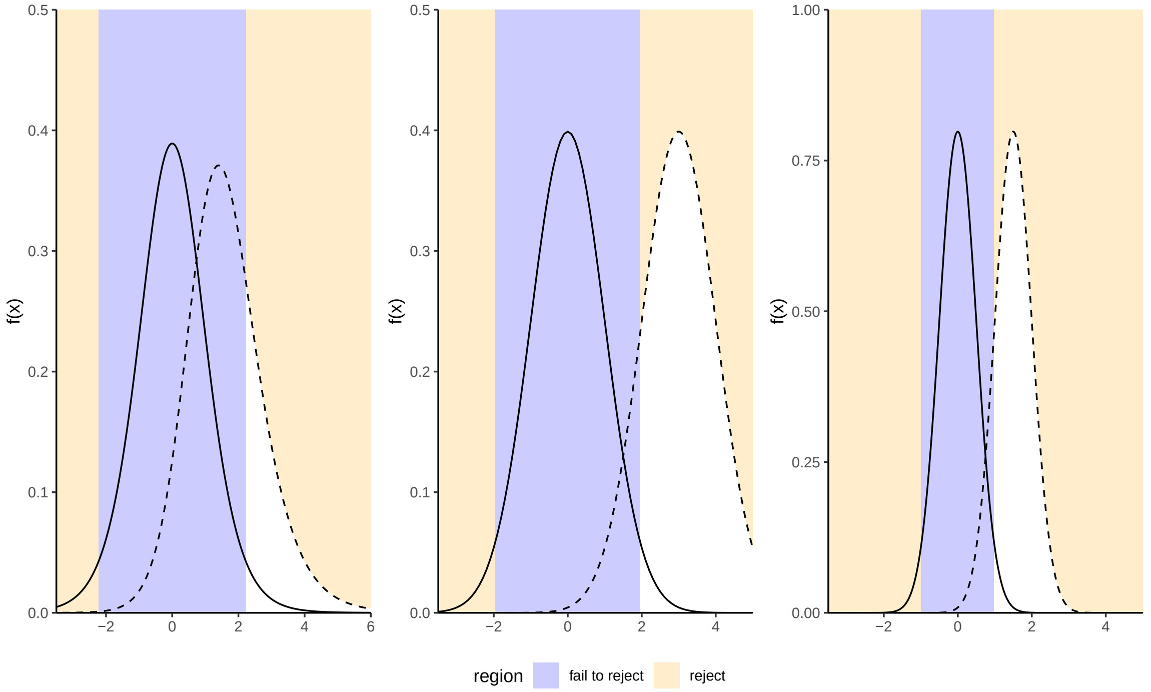


Figure 2.9: Comparison between null distribution (full curve) and a specific alternative for a t-test (dashed line). The power corresponds to the area under the curve of the density of the alternative distribution which is in the rejection area (in white). The middle panel shows an increase in power due to an increase in the mean difference, whereas the right panel shows the change due to a decrease in variability of increase in the sample size.

We want a test to have high power, i.e., that the power should be as close to 1 as possible. Minimally, the power of the test should be α because we reject the null hypothesis α fraction of the time even when $\mathscr{H}_0$ is true. Power depends on many criteria, notably

- the effect size: the bigger the difference between the postulated value for θ_0 under $\mathscr{H}_0$ and the observed behavior, the easier it is to detect it, as in the middle panel of Figure 2.9;
- variability: the less noisy your data, the easier it is to detect differences between the curves (big differences are easier to spot, as the right panel of Figure 2.9 shows);

- the sample size: the more observation, the higher our ability to detect significative differences because the standard error decreases with sample size n at a rate (typically) of $n^{-1/2}$. The null distribution also becomes more concentrated as the sample size increase.
- the choice of test statistic: for example, rank-based statistics discard information about the actual values and care only about relative ranking. Resulting tests are less powerful, but are typically more robust to model misspecification and outliers. The statistics we will choose are standard and amongst the most powerful: as such, we won't dwell on this factor.

To calculate the power of a test, we need to single out a specific alternative hypothesis. In very special case, analytic derivations are possible but typically we compute the power of a test through Monte Carlo methods. For a given alternative, we simulate repeatedly samples from the model, compute the test statistic on these new samples and the associated *p*-values based on the postulated null hypothesis. We can then calculate the proportion of tests that lead to a rejection of the null hypothesis at level α, namely the percentage of *p*-values smaller than α.

2.9 Examples

Example 2.2 (Gender inequality and permutation tests)**.** We consider data from Rosen and Jerdee (1974), who look at sex role stereotypes and their impacts on promotion and opportunities for women candidates. The experiment took place in 1972 and the experimental units, which consisted of 95 male bank supervisors, were submitted to various memorandums and asked to provide ratings or decisions based on the information provided.

We are interested in Experiment 1 related to promotion of employees: managers were requested to decide on whether or not to promote an employee to become branch manager based on recommendations and ratings on potential for customer and employee relations.

The authors intervention focused on the description of the nature (complexity) of the manager's job (either simple or complex) and the sex of the candidate (male or female): all files were otherwise similar.

We consider for simplicity only sex as a factor and aggregate over job for the $n = 93$ replies. Table 2.2 shows the counts for each possibility.

Table 2.2: Promotion recommandation to branch manager based on sex of the applicant.

	male	female
promote	32	19

hold file	12	30

The null hypothesis of interest here that sex has no impact, so the probability of promotion is the same for men and women. Let p_{m} and p_{w} denote these respective probabilities; we can thus write mathematically the null hypothesis as $\mathscr{H}_0 : p_{\mathrm{m}} = p_{\mathrm{w}}$ against the alternative $\mathscr{H}_a : p_{\mathrm{m}} \neq p_{\mathrm{w}}$.

The test statistic typically employed for contingency tables is a chi-square test[3], which compares the overall proportions of promoted to that in for each subgroup. The sample proportion for male is 32/42 = ~76%, compared to 19/49 or ~49% for female. While it seems that this difference of 16% is large, it could be spurious: the standard error for the sample proportions is roughly 3.2% for male and 3.4% for female.

If there was no discrimination based on sex, we would expect the proportion of people promoted to be the same overall; this is 51/93 =0.55 for the pooled sample. We could simply do a test for the mean difference, but rely instead on the Pearson contingency X^2_p (aka chi-square) test, which compares the expected counts (based on equal promotion rates) to the observed counts, suitably standardized. If the discrepancy is large between expected and observed, than this casts doubt on the validity of the null hypothesis.

If the counts of each cell are large, the null distribution of the chi-square test is well approximated by a χ^2 distribution. The output of the test includes the value of the statistic, 10.79, the degrees of freedom of the χ^2 approximation and the *p*-value, which gives the probability that a random draw from a χ^2_1 distribution is larger than the observed test statistic **assuming the null hypothesis is true**. The *p*-value is very small, 0.001, which means such a result is quite unlikely to happen by chance if there was no sex-discrimination.

Another alternative to obtain a benchmark to assess the outlyingness of the observed odds ratio is to use simulations: permutation tests are well illustrated by Jared Wilber. Consider a database containing the raw data with 93 rows, one for each manager, with for each an indicator of `action` and the `sex` of the hypothetical employee presented in the task.

Table 2.3: First five rows of the database in long format for experiment 1 of Rosen and Jerdee.

action	sex
promote	male
hold file	female
promote	male

[3] If you have taken advanced modelling courses, this is a score test obtained by fitting a Poisson regression with `sex` and `action` as covariates; the null hypothesis corresponding to lack of interaction term between the two.

hold file	female
hold file	male

Under the null hypothesis, sex has no incidence on the action of the manager. This means we could get an idea of the "what-if" world by shuffling the sex labels repeatedly. Thus, we could obtain a benchmark by repeating the following steps multiple times:

1. permute the labels for `sex`,
2. recreate a contingency table by aggregating counts,
3. calculate a test statistic for the simulated table.

As test statistic, we use odds ratio: the odds of an event is the ratio of the number of success over failure: in our example, this would be the number of promoted over held files. The odds of promotion for male is $32/12$, whereas that of female is $19/30$. The odds ratio for male versus female is thus $\mathsf{OR} = (32/12)/(19/30) = 4.21$. Under the null hypothesis, $\mathscr{H}_0 : \mathsf{OR} = 1$ (same probability of being promoted) (why?)

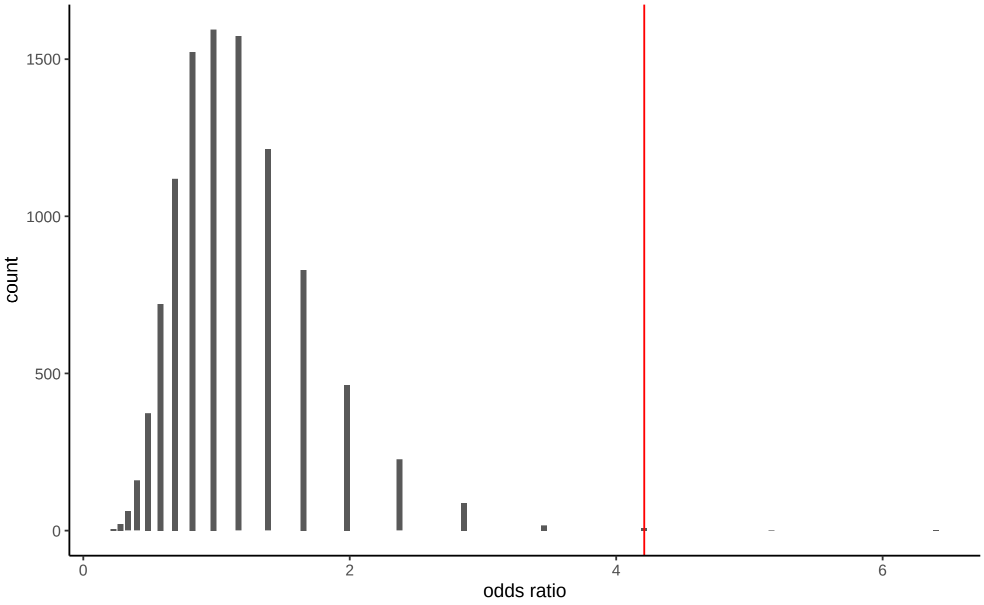


Figure 2.10: Histogram of the simulated null distribution of the odds ratio statistic obtained using a permutation test; the vertical red line indicates the sample odds ratio.

The histogram in Figure 2.10 shows the distribution of the odds ratio based on 10 000 permutations. Reassuringly, we again get roughly the same approximate *p*-value, here 0.002.[4]

The article concluded (in light of the above and further experiments)

> Results confirmed the hypothesis that male administrators tend to discriminate against female employees in personnel decisions involving promotion, development, and supervision.

Recap

- Model parameters: probability of promotion for men and women, respectively p_{m} and p_{w}.
- Hypotheses: no discrimination based on gender, meaning equal probability of promotion (null hypothesis $\mathscr{H}_0 : p_{\mathrm{m}} = p_{\mathrm{w}}$, versus alternative hypothesis $\mathscr{H}_a : p_{\mathrm{m}} \neq p_{\mathrm{w}}$).
- Test statistic: (1) chi-square test for contingency tables and (2) odds ratio.
- p-value: (1) $.0010$ and (2) $.0024$ based on permutation test.
- Conclusion: reject null hypothesis, as there is evidence of a gender-discrimination with different probability of promotion for men and women.

Following the APA guidelines, the χ^2 statistic would be reported as $\chi^2(1, n = 93) = 10.79$, $p = .001$ along with counts and sample proportions.

Example 2.3 ("The Surprise of Reaching Out")**.** Liu et al. (2023) studies social interactions and the impact of surprise on people reaching out if this contact is unexpected. Experiment 1 focuses on questionnaires where the experimental condition is the perceived appreciation of reaching out to someone (vs being reached to). The study used a questionnaire administered to 200 American adults recruited on the Prolific Academic platform. The response index consists of the average of four questions measured on a Likert scale ranging from 1 to 7, with higher values indicating higher appreciation.

We can begin by inspecting summary statistics for the sociodemographic variables (gender and age) to assess whether the sample is representative of the general population as a whole. The proportion of `other` (including non-binary people) is much higher than that of the general census, and the population skews quite young according to Table 2.4.

Table 2.4: Summary statistics of the age of participants, and counts per gender

gender	min	max	mean	n
male	18	78	32.0	105

[4] The *p*-value obtained for the permutation test would change from one run to the next since it's input is random. However, the precision of the proportion statistic is sufficient for decision making purposes.

female	19	68	36.5	92
other	24	30	27.7	3

Table 2.5: Mean ratings, standard deviation and number of participants per experimental condition.

role	mean	sd	n
initiator	5.50	1.28	103
responder	5.87	1.27	97

Since there are only two groups, initiator and responder, we are dealing with a pairwise comparison. The logical test one could use is a two sample t-test, or a variant thereof. Using Welch two sample t-test statistic, both group average and standard deviation are estimated using the data provided.

The software returns $t(197.52) = -2.05$, $p = .041$, which leads to the rejection of the null hypothesis of no difference in appreciation depending on the role of the individual (initiator or responder). The estimated mean difference is $\Delta M = -0.37$, 95% CI $[-0.73, -0.01]$; since 0 is not included in the confidence interval, we also reject the null hypothesis at level 5%. The estimate suggests that initiators underestimate the appreciation of reaching out.[5]

Recap

- Model parameters: average expected appreciation score μ_{i} and μ_{r} of initiators and responder, respectively
- Hypothesis: expected appreciation score is the same for initiator and responders, $\mathscr{H}_0 : \mu_{\mathrm{i}} = \mu_{\mathrm{r}}$ against alternative $\mathscr{H}_a : \mu_{\mathrm{i}} \neq \mu_{\mathrm{r}}$ that they are different.
- Test statistic: Welch two sample t-test
- p-value: 0.041
- Conclusion: reject the null hypothesis, average appreciation score differs depending on the role

Example 2.4 (Virtual communication curbs creative idea generation)**.** A Nature study performed an experiment to see how virtual communications teamwork by comparing the output both in terms of ideas generated during a brainstorming session by pairs and of the quality of ideas, as measured by external referees. The sample consisted of 301 pairs of participants who interacted via either videoconference or face-to-face.

[5] Assuming that the variance of each subgroup were equal, we could have used a two-sample t-test instead. The difference in the conclusion is immaterial, with a nearly equal p-value.

The authors compared the number of creative ideas, a subset of the ideas generated with creativity score above average. The mean number of the number of creative ideas for face-to-face 7.92 ideas (sd 3.40) relative to videoconferencing 6.73 ideas (sd 3.27).

Brucks and Levav (2022) used a negative binomial regression model: in their model, the expected number creative ideas generated is

$$\mathsf{E}(\texttt{ncreative}) = \exp(\beta_0 + \beta_1 \texttt{video})$$

where $\texttt{video} = 0$ if the pair are in the same room and $\texttt{video} = 1$ if they interact instead via videoconferencing.

The mean number of ideas for videoconferencing is thus $\exp(\beta_1)$ times that of the face-to-face: the estimate of the multiplicative factor is $\exp(\beta_1)$ is 0.85 95% CI $[0.77, 0.94]$.

No difference between experimental conditions translates into the null hypothesis as $\mathscr{H}_0 : \beta_1 = 0$ vs $\mathscr{H}_0 : \beta_1 \neq 0$ or equivalently $\mathscr{H}_0 : \exp(\beta_1) = 1$. The likelihood ratio test comparing the regression model with and without `video` the statistic is $R = 9.89$ (p-value based on χ^2_1 of $.002$). We conclude the average number of ideas is different, with summary statistics suggesting that virtual pairs generate fewer ideas.

If we had resorted to a two sample t-test, we would have found a mean difference in the number of creative idea of $\Delta M = 1.19$, 95% CI $[0.43, 1.95]$, $t(299) = 3.09$, $p = .002$.

Both tests come with slightly different sets of assumptions, but yield similar conclusions: there is evidence of a smaller number of creative ideas when people interact via videoconferencing.

Example 2.5 (Price of Spanish high speed train tickets)**.** The Spanish national railway company, Renfe, manages regional and high speed train tickets all over Spain and The Gurus harvested the price of tickets sold by Renfe. We are interested in trips between Madrid and Barcelona and, for now, ask the question: are tickets more expensive one way or another? To answer this, we consider a sample of 8059 AVE tickets sold at Promo rate. Our test statistic will again be the mean difference between the price (in euros) for a train ticket for Madrid–Barcelona (μ_1) and the price for Barcelona–Madrid (μ_2), i.e., $\mu_1 - \mu_2$. The null hypothesis is that there are no difference in price, so $\mathscr{H}_0 : \mu_1 - \mu_2 = 0$.

We use Welch's t test statistic for two samples: the sample mean of the price of Barcelona-Madrid tickets is 82.15 euros, that of Madrid-Barcelona tickets is 82.54 euros and the Welch statistic is worth -1.15. If we use a normal approximation, the *p*-value is 0.25.

Rather than use the asymptotic distribution, whose validity stems from the central limit theorem, we could consider another approximation under the less restrictive assumption that the data are exchangeable: under the null hypothesis, there is no difference between the two destinations and so the label for destination (a binary indicator) is arbitrary. The reasoning underlying permutation tests is as follows: to create a benchmark, we will consider observations with the same number in each group, but permuting the labels. We then compute the test statistic on each of these datasets. If there are only a handful in each group (fewer than 10), we could list all possible permutations of the data, but otherwise we can repeat this procedure many times, say 9999, to get a good approximation. This gives an approximate distribution from which we can extract the *p*-value by computing the rank of our statistic relative to the others.

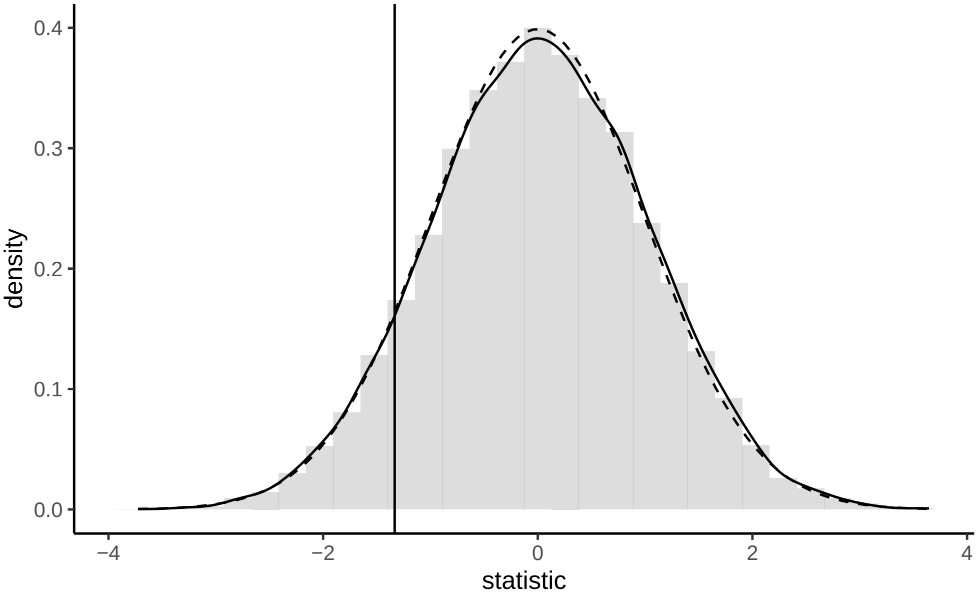


Figure 2.11: Permutation-based approximation to the null distribution of Welch two-sample t-test statistic (histogram and black curve) with standard normal approximation (dashed curve) for the price of AVE tickets at promotional rate between Madrid and Barcelona. The value of the test statistic calculated using the original sample is represented by a vertical line.

The so-called bootstrap approximation to the *p*-value of the permutation test, 0.186, is the proportion of statistics that are more extreme than the one based on the original sample. It is nearly identical to that obtained from the Satterthwaite approximation, 0.249 (the Student-t distribution is numerically equivalent to a standard normal with that many degrees of freedom), as shown in Figure 2.11. Even if our sample is very large ($n = 8059$ observations), the difference is not statistically significative. With a bigger sample (the database has more than 2 million tickets), we could estimate more precisely the average difference, up to 1/100 of an euro: the price difference would eventually become statistically significative, but this says nothing about practical difference: 0.28 euros relative to an

Promo ticket priced on average 82.56 euros is a negligible amount.

3 Likelihood-based inference

This chapter is dedicated to the basics of statistical modelling using likelihood-based inference, arguably the most popular estimation paradigm in statistics.

> ❗ Important
>
> **Learning objectives**:
>
> - Learn the terminology associated with likelihood-based inference
> - Derive closed-form expressions for the maximum likelihood estimator in simple models
> - Using numerical optimization, obtain parameter estimates and their standards errors using maximum likelihood
> - Use large-sample properties of the likelihood to derive confidence intervals and tests
> - Use information criteria for model selection

A statistical model starts with the specification of a data generating mechanism. We postulate that the data has been generated from a probability distribution with p-dimensional parameter vector $\boldsymbol{\theta}$. The sample space is the set in which the n vector observations lie, while the parameter space $\boldsymbol{\Theta} \subseteq \mathbb{R}^p$ is the set in which the parameter takes values.

As motivating example, consider the time a passenger must wait at the *Université de Montréal* station if that person arrives at 17:59 sharp every weekday, just in time for the metro train. The measurements in `waiting` represent the time in seconds before the next train leaves the station. The data were collected over three months and can be treated as an independent sample. The left panel of Figure 3.1 shows an histogram of the $n = 62$ observations, which range from 4 to 57 seconds. The data are positive, so our model must account for this feature.

Example 3.1 (Exponential model for waiting times)**.** To model the waiting time, we may consider for example an exponential distribution with scale λ (Definition 1.10), which rep-

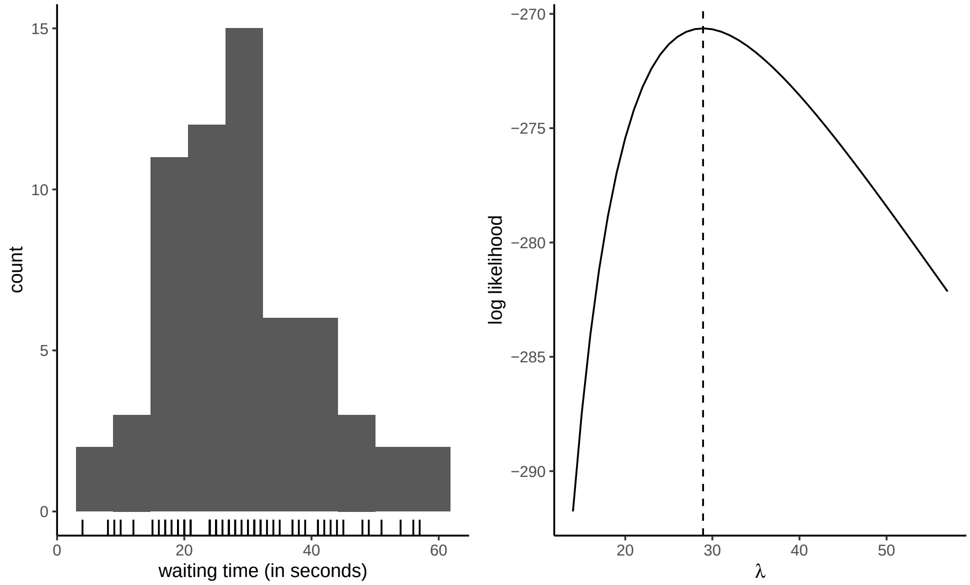


Figure 3.1: Histogram of waiting time with rugs for the observations (left) and exponential log likelihood function for the waiting time, with the maximum likelihood estimate at dashed vertical line (right).

resents the theoretical mean. Under independence[1], the joint density for the observations $y_1, \ldots, y_n$ is

$$f(\boldsymbol{y}) = \prod_{i=1}^{n} f(y_i) = \prod_{i=1}^{n} \lambda^{-1} \exp(-y_i/\lambda) = \lambda^{-n} \exp\left(-\sum_{i=1}^{n} y_i/\lambda\right)$$

The sample space is $\mathbb{R}_+^n = [0, \infty)^n$, while the parameter space is $(0, \infty)$.

To estimate the scale parameter λ and obtain suitable uncertainty measures, we need a modelling framework. We turn to likelihood-based inference.

3.1 Maximum likelihood estimation

For any given value of $\boldsymbol{\theta}$, we can obtain the probability mass or density of the sample observations, and we use this to derive an objective function for the estimation.

[1] Recall that, if A and B are independent random variables, the joint probability is the product of the probability of the events, $\Pr(A \cup B) = \Pr(A)\Pr(B)$. The same holds for density or mass function, since the latter are defined as the derivative of the distribution function.

Definition 3.1 (Likelihood)**.** The **likelihood** $L(\boldsymbol{\theta})$ is a function of the parameter vector $\boldsymbol{\theta}$ that gives the probability (or density) of observing a sample under a postulated distribution, treating the observations as fixed,

$$L(\boldsymbol{\theta};\boldsymbol{y}) = f(\boldsymbol{y};\boldsymbol{\theta}),$$

where $f(\boldsymbol{y};\boldsymbol{\theta})$ denotes the joint density or mass function of the n-vector containing the observations.

If the latter are independent, the joint density factorizes as the product of the density of individual observations, and the likelihood becomes

$$L(\boldsymbol{\theta};\boldsymbol{y}) = \prod_{i=1}^{n} f_i(y_i;\boldsymbol{\theta}) = f_1(y_1;\boldsymbol{\theta}) \times \cdots \times f_n(y_n;\boldsymbol{\theta}).$$

The corresponding log likelihood function for independent and identically distributions observations is

$$\ell(\boldsymbol{\theta};\boldsymbol{y}) = \sum_{i=1}^{n} \ln f(y_i;\boldsymbol{\theta})$$

Example 3.2 (Dependent data)**.** The joint density function only factorizes for independent data, but an alternative sequential decomposition can be helpful. For example, we can write the joint density $f(y_1, \ldots, y_n)$ using the factorization

$$f(\boldsymbol{y}) = f(y_1) \times f(y_2 \mid y_1) \times \ldots f(y_n \mid y_1, \ldots, y_n)$$

in terms of conditional. Such a decomposition is particularly useful in the context of time series, where data are ordered from time 1 until time n and models typically relate observation y_n to it's past. For example, the $\mathsf{AR}(1)$ process, states that $Y_t \mid Y_{t-1} = y_{t-1} \sim \mathsf{normal}(\alpha + \beta y_{t-1}, \sigma^2)$ and we can simplify the log likelihood using the Markov property, which states that the current realization depends on the past, $Y_t \mid Y_1, \ldots, Y_{t-1}$, only through the most recent value Y_{t-1}. The log likelihood thus becomes

$$\ell(\boldsymbol{\theta}) = \ln f(y_1) + \sum_{i=2}^{n} f(y_i \mid y_{i-1}).$$

Definition 3.2 (Maximum likelihood estimator)**.** The **maximum likelihood estimator** $\widehat{\boldsymbol{\theta}}$ is the vector value that maximizes the likelihood,

$$\widehat{\boldsymbol{\theta}} = \mathrm{argmax}_{\boldsymbol{\theta}\in\boldsymbol{\Theta}} L(\boldsymbol{\theta};\boldsymbol{y}).$$

The natural logarithm $\ln$ is a monotonic transformation, so the maximum likelihood estimator $\boldsymbol{\theta}$ for likelihood $L(\boldsymbol{\theta}; \boldsymbol{y})$ is the same as that of the log likelihood $\ell(\boldsymbol{\theta}; \boldsymbol{y}) = \ln L(\boldsymbol{\theta}; \boldsymbol{y})$.[2]

If we suppose that our model is correct, than we expect to observe whatever was realized, so we find the parameter vector that makes the sample the most likely to have been generated by our model. Several properties of maximum likelihood estimator makes it appealing for inference. The maximum likelihood estimator is efficient, meaning it has the smallest asymptotic mean squared error. The maximum likelihood estimator is also **consistent**, i.e., it converges to the correct value as the sample size increase (asymptotically unbiased).

We can resort to numerical optimization routines to find the value of the maximum likelihood estimate, or sometimes derive closed-form expressions for the estimator, starting from the log likelihood. The right panel of Figure 3.1 shows the exponential log likelihood, which attains a maximum at $\widehat{\lambda} = 28.935$ second, the sample mean of the observations. The function decreases to either side of these values as the data become less compatible with the model. Given the values achieved here with a small sample, it is easy to see that direct optimization of the likelihood function (rather than it's natural logarithm) could lead to numerical underflow, since already $\exp(-270) \approx 5.5 \times 10^{-118}$, and log values smaller than -746 would be rounded to zero.

Example 3.3 (Calculation of the maximum likelihood of an exponential distribution)**.** As Figure 3.1 reveals that the exponential log likelihood function is unimodal and thus achieves a single maximum, we can use calculus to derive an explicit expression for $\widehat{\lambda}$ based on the log likelihood

$$\ell(\lambda) = -n \ln \lambda - \frac{1}{\lambda} \sum_{i=1}^{n} y_i.$$

Taking first derivative and setting the result to zero, we find

$$\frac{\mathrm{d}\ell(\lambda)}{\mathrm{d}\lambda} = -\frac{n}{\lambda} + \frac{1}{\lambda^2} \sum_{i=1}^{n} y_i = 0.$$

Rearranging this expression by taking $-n/\lambda$ to the right hand side of the equality and multiplying both sides by $\lambda^2 > 0$, we find that $\widehat{\lambda} = \sum_{i=1}^{n} y_i/n$. The second derivative of the log likelihood is $\mathrm{d}^2\ell(\lambda)/\mathrm{d}\lambda^2 = n(\lambda^{-2} - 2\lambda^{-3}\overline{y})$, and plugging $\lambda = \overline{y}$ gives $-n/\overline{y}^2$, which is negative. Therefore, $\widehat{\lambda}$ is indeed a maximizer.

[2] Since in most instances we deal with a product of densities, taking the log leads to a sum of log density contributions, which facilitates optimization.

Example 3.4 (Normal samples)**.** Suppose we have an independent normal sample of size n with mean μ and variance σ^2, where $Y_i \sim \mathsf{normal}(\mu, \sigma^2)$ are independent. Recall that the density of the normal distribution is

$$f(y; \mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}.$$

For an simple random sample of size n, whose realization is $y_1, \ldots, y_n$, the likelihood is

$$\begin{aligned} L(\mu, \sigma^2; \boldsymbol{y}) =& \prod_{i=1}^n \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(y_i-\mu)^2\right\} \\ =& (2\pi\sigma^2)^{-n/2} \exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^n (y_i-\mu)^2\right\}. \end{aligned}$$

and the log likelihood is

$$\ell(\mu, \sigma^2; \boldsymbol{y}) = -\frac{n}{2}\ln(2\pi) - \frac{n}{2}\ln(\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^n (y_i-\mu)^2.$$

One can show that the maximum likelihood estimators for the two parameters are

$$\widehat{\mu} = \overline{Y} = \frac{1}{n}\sum_{i=1}^n Y_i, \qquad \widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^n (Y_i - \overline{Y})^2.$$

The fact that the estimator of the theoretical mean μ is the sample mean is fairly intuitive and one can show the estimator is unbiased for μ. The (unbiased) sample variance estimator,

$$S^2 = \frac{1}{n-1}\sum_{i=1}^n (Y_i - \overline{Y})^2$$

Since $\widehat{\sigma}^2 = (n-1)/nS^2$, it follows that the maximum likelihood estimator of σ^2 is biased, but both estimators are consistent and will thus get arbitrarily close to the true value σ^2 for n sufficiently large.

Proposition 3.1 (Invariance of maximum likelihood estimators)**.** *If $g(\boldsymbol{\theta}) : \mathbb{R}^p \mapsto \mathbb{R}^k$ for $k \leq p$ is a function of the parameter vector, then $g(\widehat{\boldsymbol{\theta}})$ is the maximum likelihood estimator of the function.*

The invariance property explains the widespread use of maximum likelihood estimation. For example, having estimated the parameter λ, we can now use the model to derive other quantities of interest and get the "best" estimates for free. For example, we could compute the maximum likelihood estimate of the probability of waiting more than one minute, $\Pr(T > 60) = \exp(-60/\widehat{\lambda}) = 0.126$, or using **R** built-in distribution function `pexp`.

```r
# Note: default R parametrization for the exponential is
# in terms of rate, i.e., the inverse scale parameter
pexp(q = 60, rate = 1/mean(waiting), lower.tail = FALSE)
#> [1] 0.126
```

Another appeal of the invariance property is the possibility to compute the MLE in the most suitable parametrization, which is convenient if the support is restricted. If g is a one-to-one function of $\boldsymbol{\theta}$, for example if $\theta > 0$, taking $g(\theta) = \ln \theta$ or, if $0 \leq \theta \leq 1$, by maximizing $g(\theta) = \ln(\theta) - \ln(1-\theta) \in \mathbb{R}$ removes the support constraints for the numerical optimization.

Definition 3.3 (Score and information matrix)**.** Let $\ell(\boldsymbol{\theta})$, $\boldsymbol{\theta} \in \boldsymbol{\Theta} \subseteq \mathbb{R}^p$, be the log likelihood function. The gradient of the log likelihood $U(\boldsymbol{\theta}) = \partial \ell(\boldsymbol{\theta}) / \partial \boldsymbol{\theta}$ is termed **score** function.

The **observed information matrix** is the hessian of the negative log likelihood

$$j(\boldsymbol{\theta}; \boldsymbol{y}) = -\frac{\partial^2 \ell(\boldsymbol{\theta}; \boldsymbol{y})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^\top},$$

evaluated at the maximum likelihood estimate $\widehat{\boldsymbol{\theta}}$, so $j(\widehat{\boldsymbol{\theta}})$. Under regularity conditions, the **expected information**, also called **Fisher information** matrix, is

$$i(\boldsymbol{\theta}) = \mathsf{E}\left\{U(\boldsymbol{\theta}; \boldsymbol{Y}) U(\boldsymbol{\theta}; \boldsymbol{Y})^\top\right\} = \mathsf{E}\left\{j(\boldsymbol{\theta}; \boldsymbol{Y})\right\}$$

Both the Fisher (or expected) and the observed information matrices are symmetric and encode the curvature of the log likelihood and provide information about the variability of $\widehat{\boldsymbol{\theta}}$.

Example 3.5 (Information for the exponential model)**.** The observed and expected information of the exponential model for a random sample $Y_1, \ldots, Y_n$, parametrized in terms of scale λ, are

$$\begin{aligned} j(\lambda; \boldsymbol{y}) &= -\frac{\partial^2 \ell(\lambda)}{\partial \lambda^2} = \frac{n}{\lambda^2} + \frac{2}{n\lambda^3} \sum_{i=1}^n y_i \\ i(\lambda) &= \frac{n}{\lambda^2} + \frac{2}{n\lambda^3} \sum_{i=1}^n \mathsf{E}(Y_i) = \frac{n}{\lambda^2} \end{aligned}$$

since $\mathsf{E}(Y_i) = \lambda$ and expectation is a linear operator.

We find $i(\widehat{\lambda}) = j(\widehat{\lambda}) = n/\overline{y}^2$.

The exponential model may be restrictive for our purposes, so we consider for the purpose of illustration and as a generalization a Weibull distribution.

Definition 3.4 (Weibull distribution)**.** The distribution function of a **Weibull** random variable with scale $\lambda > 0$ and shape $\alpha > 0$ is

$$F(x; \lambda, \alpha) = 1 - \exp\left\{-(x/\lambda)^\alpha\right\}, \qquad x \geq 0, \lambda > 0, \alpha > 0,$$

while the corresponding density is

$$f(x; \lambda, \alpha) = \frac{\alpha}{\lambda^\alpha} x^{\alpha-1} \exp\left\{-(x/\lambda)^\alpha\right\}, \qquad x \geq 0, \lambda > 0, \alpha > 0.$$

The quantile function, the inverse of the distribution function, is $Q(p) = \lambda\{-\ln(1-p)\}^{1/\alpha}$. The Weibull distribution includes the exponential as special case when $\alpha = 1$. The expected value of $Y \sim \mathsf{Weibull}(\lambda, \alpha)$ is $\mathsf{E}(Y) = \lambda\Gamma(1 + 1/\alpha)$.

Example 3.6 (Score and information of the Weibull distribution)**.** The log likelihood for a simple random sample whose realizations are $y_1, \ldots, y_n$ of size n from a $\mathsf{Weibull}(\lambda, \alpha)$ model is

$$\ell(\lambda, \alpha) = n \ln(\alpha) - n\alpha \ln(\lambda) + (\alpha - 1) \sum_{i=1}^n \ln y_i - \lambda^{-\alpha} \sum_{i=1}^n y_i^\alpha.$$

The score, which is the gradient of the log likelihood, is easily obtained by differentiation[3]

$$U(\lambda, \alpha) = \begin{pmatrix} \frac{\partial \ell(\lambda,\alpha)}{\partial \lambda} \\ \frac{\partial \ell(\lambda,\alpha)}{\partial \alpha} \end{pmatrix} = \begin{pmatrix} -\frac{n\alpha}{\lambda} + \alpha\lambda^{-\alpha-1} \sum_{i=1}^n y_i^\alpha \\ \frac{n}{\alpha} - n\ln(\lambda) + \sum_{i=1}^n \ln y_i - \sum_{i=1}^n \left(\frac{y_i}{\lambda}\right)^\alpha \times \ln\left(\frac{y_i}{\lambda}\right). \end{pmatrix}$$

and the observed information is the 2×2 matrix-valued function

$$\begin{aligned} j(\lambda, \alpha) &= -\begin{pmatrix} \frac{\partial^2 \ell(\lambda,\alpha)}{\partial \lambda^2} & \frac{\partial^2 \ell(\lambda,\alpha)}{\partial \lambda \partial \alpha} \\ \frac{\partial^2 \ell(\lambda,\alpha)}{\partial \alpha \partial \lambda} & \frac{\partial^2 \ell(\lambda,\alpha)}{\partial \alpha^2} \end{pmatrix} \\ &= \begin{pmatrix} \lambda^{-2}\left\{-n\alpha + \alpha(\alpha+1)\sum_{i=1}^n (y_i/\lambda)^2\right\} & \lambda^{-1}\sum_{i=1}^n [1 - (y_i/\lambda)^\alpha\{1 + \alpha\ln(y_i/\lambda)\}] \\ \lambda^{-1}\sum_{i=1}^n [1 - (y_i/\lambda)^\alpha\{1 + \alpha\ln(y_i/\lambda)\}] & n\alpha^{-2} + \sum_{i=1}^n (y_i/\lambda)^\alpha\{\ln(y_i/\theta)\}^2 \end{pmatrix} \end{aligned}$$

[3] Using for example a symbolic calculator.

Proposition 3.2 (Gradient-based optimization). *To obtain the maximum likelihood estimator, we will typically find the value of the vector $\boldsymbol{\theta}$ that solves the score vector, meaning $U(\widehat{\boldsymbol{\theta}}) = \mathbf{0}_p$. This amounts to solving simultaneously a p-system of equations by setting the derivative with respect to each element of $\boldsymbol{\theta}$ to zero. If $j(\widehat{\boldsymbol{\theta}})$ is a positive definite matrix (i.e., all of it's eigenvalues are positive), then the vector $\widehat{\boldsymbol{\theta}}$ is the maximum likelihood estimator.*

We can use a variant of Newton–Raphson algorithm if the likelihood is thrice differentiable and the maximum likelihood estimator does not lie on the boundary of the parameter space. If we consider an initial value $\boldsymbol{\theta}^\dagger$, then a first order Taylor series expansion of the score likelihood in a neighborhood $\boldsymbol{\theta}^\dagger$ of the MLE $\widehat{\boldsymbol{\theta}}$ gives

$$\begin{aligned}\mathbf{0}_p = U(\widehat{\boldsymbol{\theta}}) &\stackrel{\cdot}{\simeq} \left.\frac{\partial \ell(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}\right|_{\boldsymbol{\theta}=\boldsymbol{\theta}^\dagger} + \left.\frac{\partial^2 \ell(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}\partial \boldsymbol{\theta}^\top}\right|_{\boldsymbol{\theta}=\boldsymbol{\theta}^\dagger} (\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^\dagger)\\ &= U(\boldsymbol{\theta}^\dagger) - j(\boldsymbol{\theta}^\dagger)(\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^\dagger)\end{aligned}$$

and solving this for $\widehat{\boldsymbol{\theta}}$ (provided the $p \times p$ matrix $j(\widehat{\boldsymbol{\theta}})$ is invertible), we get

$$\widehat{\boldsymbol{\theta}} \stackrel{\cdot}{\simeq} \boldsymbol{\theta}^\dagger + j^{-1}(\boldsymbol{\theta}^\dagger)U(\boldsymbol{\theta}^\dagger),$$

*which suggests an iterative procedure from a starting value $\boldsymbol{\theta}^\dagger$ in the vicinity of the mode until the gradient is approximately zero. If the value is far from the mode, then the algorithm may diverge to infinity. To avoid this, we may multiply the term $j^{-1}(\boldsymbol{\theta}^\dagger)U(\boldsymbol{\theta}^\dagger)$ by a damping factor $c < 1$. A variant of the algorithm, termed Fisher scoring, uses the expected or Fisher information $i(\boldsymbol{\theta})$ in place of the observed information, $j(\boldsymbol{\theta})$, for numerical stability and to avoid situations where the latter is not positive definite. This is the optimization routine used in the `glm` function in **R**.*

Example 3.7 (Maximum likelihood of a Weibull sample). We turn to numerical optimization to obtain the maximum likelihood estimate of the Weibull distribution, in the absence of closed-form expression for the MLE. To this end, we create functions that encode the log likelihood, here taken as the sum of log density contributions. The function `nll_weibull` below takes as argument the vector of parameters, `pars`, and returns the negative of the log likelihood which we wish to minimize[4] We also code the gradient, although we can resort to numerical differentiation at little additional costs. We then use `optim`, the default optimization routine in **R**, to minimize `nll_weibull`. The function returns a list containing a convergence code (`0` indicating convergence), the MLE in `par`, the log likelihood $\ell(\widehat{\boldsymbol{\theta}})$ and the Hessian matrix, which is the matrix of second derivatives of the negative log likelihood evaluated at $\widehat{\boldsymbol{\theta}}$. The log likelihood surface, for pairs of scale and shape vectors $\boldsymbol{\theta} = (\lambda, \alpha)$,

[4] Most optimization algorithms minimize functions with respect to their arguments, so we minimize the negative log likelihood, which is equivalent to maximizing the log likelihood.

are displayed in Figure 3.3. We can see that the maximum likelihood value has converged, and check that the score satisfies $U(\widehat{\boldsymbol{\theta}}) = 0$ at the returned optimum value.

```r
# Load data vector
data(waiting, package = "hecstatmod")
# Negative log likelihood for a Weibull sample
nll_weibull <- function(pars, y){
  # Handle the case of negative parameter values
  if(isTRUE(any(pars <= 0))){ # parameters must be positive
    return(1e10) # large value (not infinite, to avoid warning messages)
  }
  - sum(dweibull(x = y, scale = pars[1], shape = pars[2], log = TRUE))
}
# Gradient of the negative Weibull log likelihood
gr_nll_weibull <- function(pars, y){
  scale <- pars[1]
  shape <- pars[2]
  n <- length(y)
  grad_ll <- c(scale = -n*shape/scale + shape*scale^(-shape-1)*sum(y^shape),
               shape = n/shape - n*log(scale) + sum(log(y)) -
                 sum(log(y/scale)*(y/scale)^shape))
  return(- grad_ll)
}
# Use exponential submodel MLE as starting parameters
start <- c(mean(waiting), 1)
# Check gradient function is correctly coded!
# Returns TRUE if numerically equal to tolerance
isTRUE(all.equal(numDeriv::grad(nll_weibull, x = start, y = waiting),
                 gr_nll_weibull(pars = start, y = waiting),
                 check.attributes = FALSE))
#> [1] TRUE
# Numerical minimization using optim
opt_weibull <- optim(
  par = start,  # starting values
  fn = nll_weibull,  # pass function, whose first argument is the parameter vector
  gr = gr_nll_weibull, # optional (if missing, numerical derivative)
  method = "BFGS", # gradient-based algorithm, common alternative is "Nelder"
  y = waiting, # vector of observations, passed as additional argument to fn
  hessian = TRUE) # return matrix of second derivatives evaluated at MLE
# Alternative using pure Newton
# nlm(f = nll_weibull, p = start, hessian = TRUE, y = waiting)
# Parameter estimates - MLE
(mle_weibull <- opt_weibull$par)
#> [1] 32.6  2.6
# Check gradient for convergence
gr_nll_weibull(mle_weibull, y = waiting)
#>     scale     shape
#> 0.0000142 0.0001136
# Is the Hessian of the negative positive definite (all eigenvalues are positive)
# If so, we found a maximum and the matrix is invertible
isTRUE(all(eigen(opt_weibull$hessian)$values > 0))
#> [1] TRUE
```

3.2 Sampling distribution

The **sampling distribution** of an estimator $\widehat{\boldsymbol{\theta}}$ is the probability distribution induced by the underlying data, given that the latter inputs are random.

For simplicity, suppose we have a simple random sample, so the log likelihood is a sum of n terms and information accumulates linearly with the sample size: the data carry more information about the unknown parameter vector, whose true value we denote $\boldsymbol{\theta}_0$. Under suitable regularity conditions, cf. Section 4.4.2 of Davison (2003), for large sample size n, we can perform a Taylor series of the score vector and apply the central limit theorem. Since $U(\boldsymbol{\theta})$ and $i(\boldsymbol{\theta})$ are the sum of n independent random variables, and that $\mathsf{E}\{U(\boldsymbol{\theta})\} = \mathbf{0}_p$, and $\mathsf{Var}\{U(\boldsymbol{\theta})\} = i(\boldsymbol{\theta})$, application of the central limit theorem yields

$$i(\boldsymbol{\theta}_0)^{-1/2}U(\boldsymbol{\theta}_0) \stackrel{\cdot}{\sim} \mathsf{normal}_p(\mathbf{0}, \mathbf{I}_p).$$

We can use this to obtain approximations to the sampling distribution of $\widehat{\boldsymbol{\theta}}$, given that

$$\widehat{\boldsymbol{\theta}} \stackrel{\cdot}{\sim} \mathsf{normal}_p\{\boldsymbol{\theta}_0, i^{-1}(\boldsymbol{\theta})\}$$

where the covariance matrix is the inverse of the Fisher information. In practice, since the true parameter value $\boldsymbol{\theta}_0$ is unknown, we replace it with either $i^{-1}(\widehat{\boldsymbol{\theta}})$ or the inverse of the observed information $j^{-1}(\widehat{\boldsymbol{\theta}})$, as both of these converge to the true value.

As the sample size grows, the $\widehat{\boldsymbol{\theta}}$ becomes centered around the value $\boldsymbol{\theta}_0$ that minimizes the discrepancy between the model and the true data generating process. In large samples, the sampling distribution of the maximum likelihood estimator is approximately quadratic.

Example 3.8 (Covariance matrix and standard errors for the Weibull distribution)**.** We use the output of our optimization procedure to get the observed information matrix and the standard errors for the parameters of the Weibull model. The latter are simply the square root of the diagonal entries of the inverse Hessian matrix, $[\mathrm{diag}\{j^{-1}(\widehat{\boldsymbol{\theta}})\}]^{1/2}$.

```
# The Hessian matrix of the negative log likelihood
# evaluated at the MLE (observed information matrix)
obsinfo_weibull <- opt_weibull$hessian
vmat_weibull <- solve(obsinfo_weibull)
# Standard errors
se_weibull <- sqrt(diag(vmat_weibull))
```

From these, one can readily Wald-based confidence intervals for parameters from $\boldsymbol{\theta}$.

Proposition 3.3 (Asymptotic normality and transformations)**.** *The asymptotic normality result can be used to derive standard errors for other quantities of interest. If $\phi = g(\boldsymbol{\theta})$ is a differentiable function of $\boldsymbol{\theta}$ whose gradient does not vanish at $\widehat{\boldsymbol{\theta}}$ then $\widehat{\phi} \stackrel{\cdot}{\sim} \mathsf{normal}(\phi_0, \mathrm{V}_\phi)$, with $\mathrm{V}_\phi = \nabla\phi^\top \mathbf{V}_{\boldsymbol{\theta}} \nabla\phi$, where $\nabla\phi = [\partial\phi/\partial\theta_1, \ldots, \partial\phi/\partial\theta_p]^\top$. The variance matrix and the gradient are evaluated at the maximum likelihood estimate $\widehat{\boldsymbol{\theta}}$. This result readily extends to vector $\boldsymbol{\phi} \in \mathbb{R}^k$ for $k \leq p$, where $\mathrm{V}_\phi$is the Jacobian matrix of the transformation.*

Example 3.9 (Probability of waiting for exponential model.)**.** To illustrate the difference between likelihood ratio and Wald tests (and their respective confidence intervals), we consider the metro waiting time data and consider the probability of waiting more than one minute, $\phi = g(\lambda) = \exp(-60/\lambda)$. The maximum likelihood estimate is, by invariance, 0.126 and the gradient of g with respect to the scale parameter is $\nabla\phi = \partial\phi/\partial\lambda = 60\exp(-60/\lambda)/\lambda^2$.

```
lambda_hat <- mean(waiting)
phi_hat <- exp(-60/lambda_hat)
dphi <- function(lambda){60*exp(-60/lambda)/(lambda^2)}
V_lambda <- lambda_hat^2/length(waiting)
V_phi <- dphi(lambda_hat)^2 * V_lambda
(se_phi <- sqrt(V_phi))
#> [1] 0.0331
```

3.3 Likelihood-based tests

We consider a null hypothesis $\mathscr{H}_0$ that imposes restrictions on the possible values of $\boldsymbol{\theta}$ can take, relative to an unconstrained alternative $\mathscr{H}_1$. We need two **nested** models: a *full* model, and a *reduced* model that is a subset of the full model where we impose q restrictions. For example, the exponential distribution is a special case of the Weibull one if $\alpha = 1$. The testing procedure involves fitting the two models and obtaining the maximum likelihood estimators of each of $\mathscr{H}_1$ and $\mathscr{H}_0$, respectively $\widehat{\boldsymbol{\theta}}$ and $\widehat{\boldsymbol{\theta}}_0$ for the parameters under $\mathscr{H}_0$. The null hypothesis $\mathscr{H}_0$ tested is: 'the reduced model is an **adequate simplification** of the full model' and the likelihood provides three main classes of statistics for testing this hypothesis: these are

- likelihood ratio tests statistics, denoted R, which measure the drop in log likelihood (vertical distance) from $\ell(\widehat{\boldsymbol{\theta}})$ and $\ell(\widehat{\boldsymbol{\theta}}_0)$.
- Wald tests statistics, denoted W, which consider the standardized horizontal distance between $\widehat{\boldsymbol{\theta}}$ and $\widehat{\boldsymbol{\theta}}_0$.
- score tests statistics, denoted S, which looks at the scaled slope of ℓ, evaluated *only* at $\widehat{\boldsymbol{\theta}}_0$ (derivative of ℓ).

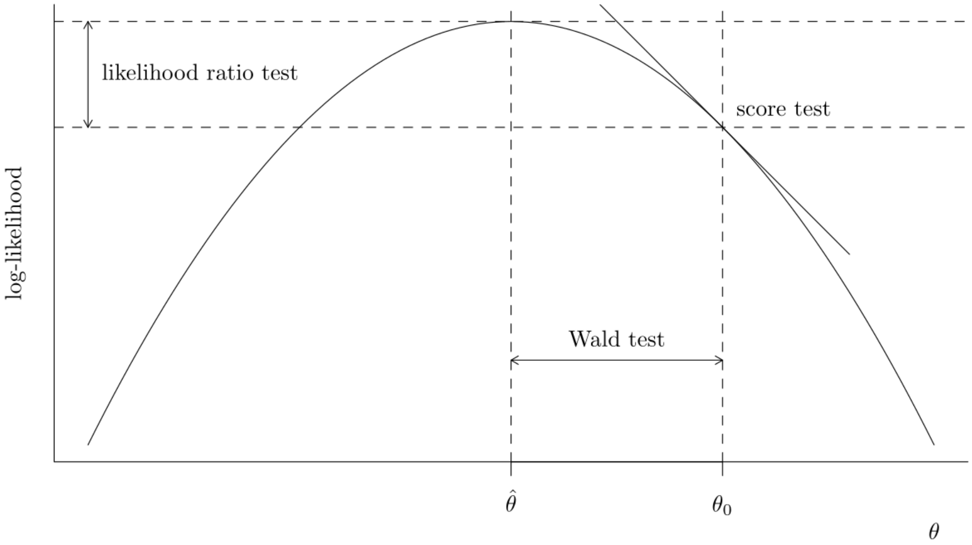


Figure 3.2: Log-likelihood curve: the three likelihood-based tests, namely Wald, likelihood ratio and score tests, are shown on the curve. The tests use different information about the function.

The three main classes of statistics for testing a simple null hypothesis $\mathscr{H}_0 : \boldsymbol{\theta} = \boldsymbol{\theta}_0$ against the alternative $\mathscr{H}_a : \boldsymbol{\theta} \neq \boldsymbol{\theta}_0$ are the Wald, likelihood ratio, and the score test statistics, defined respectively as

$$\begin{aligned} W = (\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}_0)^\top j(\widehat{\boldsymbol{\theta}})(\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}_0), R &= 2\left\{\ell(\widehat{\boldsymbol{\theta}}) - \ell(\boldsymbol{\theta}_0)\right\}, \\ S = U^\top(\boldsymbol{\theta}_0) i^{-1}(\boldsymbol{\theta}_0) U(\boldsymbol{\theta}_0), \end{aligned}$$

where $\widehat{\boldsymbol{\theta}}$ is the maximum likelihood estimate under the alternative and $\boldsymbol{\theta}_0$ is the null value of the parameter vector. Asymptotically, all the test statistics are equivalent (in the sense that they lead to the same conclusions about $\mathscr{H}_0$). If $\mathscr{H}_0$ is true, the three test statistics follow asymptotically a χ^2_q distribution under a null hypothesis $\mathscr{H}_0$, where the degrees of freedom q are the number of restrictions.

$$\begin{aligned} w(\theta_0) &= (\widehat{\theta} - \theta_0)/\mathsf{se}(\widehat{\theta}) \\ r(\theta_0) = \mathrm{sign}(\widehat{\theta} - \theta)\left[2\left\{\ell(\widehat{\theta}) - \ell(\theta)\right\}\right]^{1/2} \\ s(\theta_0) &= j^{-1/2}(\theta_0) U(\theta_0) \end{aligned}$$

We call $r(\theta_0)$ the directed likelihood root.

The likelihood ratio test statistic is normally the most powerful of the three likelihood tests. The score statistic S only requires calculation of the score and information under $\mathscr{H}_0$ (because by definition $U(\widehat{\theta}) = 0$), so it can be useful in problems where calculations of the maximum likelihood estimator under the alternative is costly or impossible.

The Wald statistic W is the most widely encountered statistic and two-sided 95% confidence intervals for a single parameter θ are of the form

$$\widehat{\theta} \pm \mathfrak{z}_{1-\alpha/2} \mathrm{se}(\widehat{\theta}),$$

where $\mathfrak{z}_{1-\alpha/2}$ is the $1-\alpha/2$ quantile of the standard normal distribution; for a 95% confidence interval, the 0.975 quantile of the normal distribution is $\mathfrak{z}_{0.975} = 1.96$. The Wald-based confidence intervals are by construction **symmetric**: they may include implausible values (e.g., negative values for if the parameter of interest θ is positive, such as variances).

Example 3.10 (Wald test to compare exponential and Weibull models)**.** We can test whether the exponential model is an adequate simplification of the Weibull distribution by imposing the restriction $\mathscr{H}_0 : \alpha = 1$. This imposes a single restriction to the model, so we compare the square statistic to a χ^2_1. Since α is directly a parameter of the distribution, we have the standard errors for free.

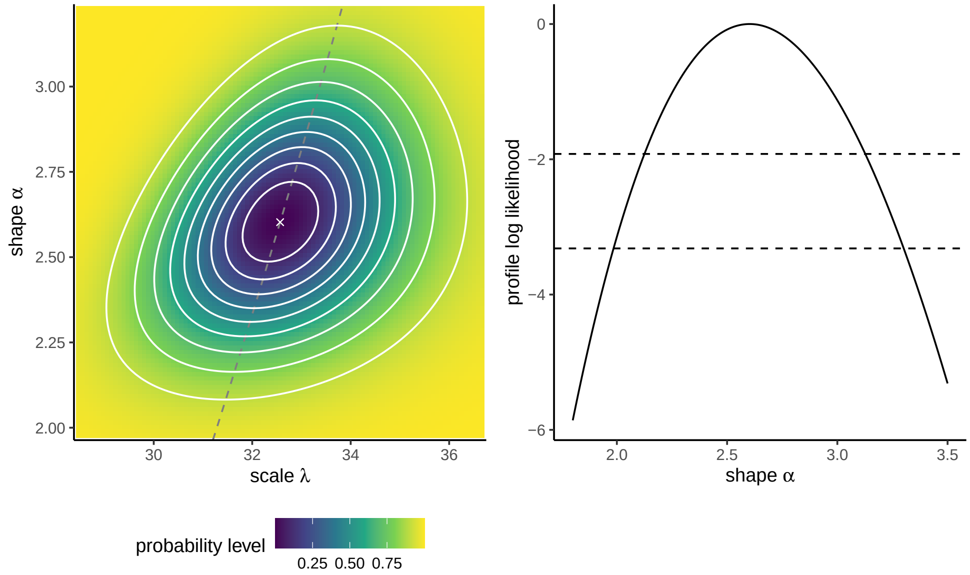


Figure 3.3: Profile log likelihood for α, shown as a dashed gray line (left) and as a transect (right). The left panel shows the log likelihood surface for the Weibull model applied to the `waiting` data with 10%, 20%, ..., 90% likelihood ratio confidence regions (white contour curves). Higher log likelihood values are indicated by darker colors. The cross indicates the maximum likelihood estimate. The profile on the right hand panel has been shifted vertically to be zero at the MLE; the dashed horizontal lines denote the cutoff points for the 95% and 99% confidence intervals.

```r
# Calculate Wald statistic
wald_exp <- (mle_weibull[2] - 1)/se_weibull[2]
# Compute p-value
pchisq(wald_exp^2, df = 1, lower.tail = FALSE)
#> [1] 3.61e-10
# p-value less than 5%, reject null
# Obtain 95% confidence intervals
mle_weibull[2] + qnorm(c(0.025, 0.975))*se_weibull[2]
#> [1] 2.1 3.1
# 1 is not inside the confidence interval, reject null
```

We reject the null hypothesis, meaning the exponential submodel is not an adequate simplification of the Weibull.

We can also check the goodness-of-fit of both models by drawing a quantile-quantile plot (cf. Definition 1.16). It is apparent from Figure 3.4 that the exponential model is overestimating the largest waiting times, whose dispersion in the sample is less than that implied by the model. By contrast, the near perfect straight line for the Weibull model in the right panel of Figure 3.4 suggests that the model fit is adequate.

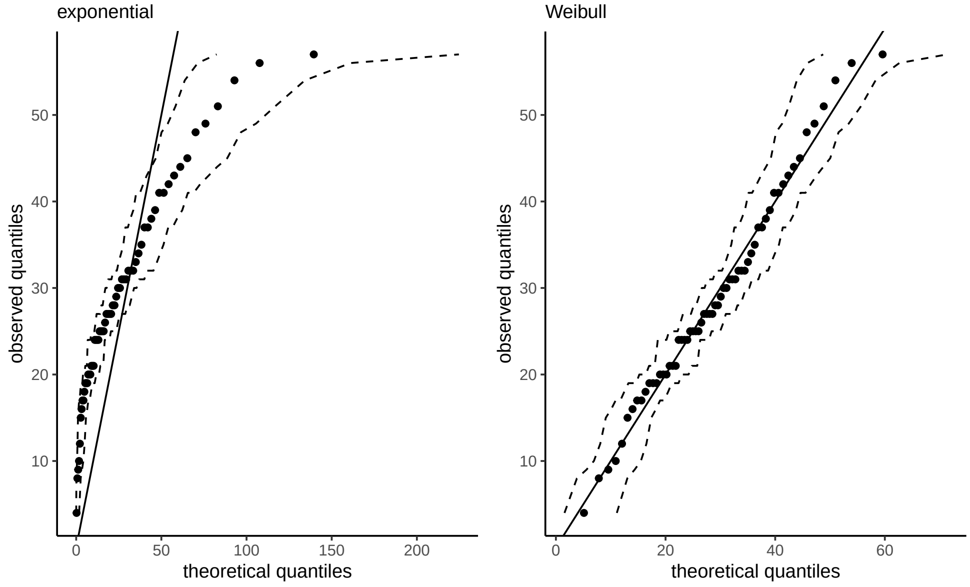


Figure 3.4: Quantile-quantile plots for exponential (left) and Weibull (right) models, with 95% pointwise simulation intervals.

Remark 3.1 (Lack of invariance of Wald-based confidence intervals). The Wald-based confidence intervals are not parametrization invariant: if we want intervals for a nonlinear continuous function $g(\theta)$, then in general $\mathsf{CI}_W\{g(\theta)\} \neq g\{\mathsf{CI}_W(\theta)\}$.

For example, consider the exponential submodel. We can invert the Wald test statistic to get a symmetric 95% confidence interval for ϕ, $[0.061, 0.191]$. If we were to naively transform the confidence interval for λ into one for ϕ, we would get $[0.063, 0.19]$, which highlights the invariance although the difference here is subtle. The Gaussian approximation underlying the Wald test is reliable if the sampling distribution of the likelihood is near quadratic, which happens when the likelihood function is roughly symmetric on either side of the maximum likelihood estimator.

The likelihood ratio test is invariant to interest-preserving reparametrizations, so the test statistic for $\mathscr{H}_0 : \phi = \phi_0$ and $\mathscr{H}_0 : \lambda = -60/\ln(\phi_0)$ are the same. The Wald confidence regions can be contrasted with the (better) ones derived using the likelihood ratio test: these are found through a numerical search to find the limits of

$$\left\{\theta : 2\{\ell(\widehat{\boldsymbol{\theta}}) - \ell(\boldsymbol{\theta})\} \leq \chi^2_p(1-\alpha)\right\},$$

where $\chi^2_p(1-\alpha)$ is the $(1-\alpha)$ quantile of the χ^2_p distribution. Such intervals, for $\alpha = 0.1, \ldots, 0.9$, appear in Figure 3.3 as contour curves. If $\boldsymbol{\theta}$ is multidimensional, confidence intervals for θ_i are derived using the profile likelihood, discussed in the sequel. Likelihood ratio-based confidence intervals are **parametrization invariant**, so $\mathsf{CI}_R\{g(\theta)\} = g\{\mathsf{CI}_R(\theta)\}$. Because the likelihood is zero if a parameter value falls outside the range of possible values for the parameter, the intervals only include plausible values of θ. In general, the intervals are asymmetric and have better coverage properties.

```r
# Exponential log likelihood
ll_exp <- function(lambda){
  sum(dexp(waiting, rate = 1/lambda, log = TRUE))
}
# MLE of the scale parameter
lambda_hat <- mean(waiting)
# Root search for the limits of the confidence interval
lrt_lb <- uniroot( # lower bound, using values below MLE
  f = function(r){
     2*(ll_exp(lambda_hat) - ll_exp(r)) - qchisq(0.95, 1)},
  interval = c(0.5 * min(waiting), lambda_hat))$root
lrt_ub <- uniroot( # upper bound,
  f = function(r){
     2*(ll_exp(lambda_hat) - ll_exp(r)) - qchisq(0.95, 1)},
  interval = c(lambda_hat, 2 * max(waiting)))$root
```

The likelihood ratio statistic 95% confidence interval for ϕ can be found by using a root finding algorithm: the 95% confidence interval for λ is $\mathsf{CI}_R(\lambda)[22.784, 37.515]$. By invariance, the 95% confidence interval for ϕ is $\mathsf{CI}_R(\phi) = [0.072, 0.202] = g\{\mathsf{CI}_R(\lambda)\}$.

3.4 Profile likelihood

Sometimes, we may want to perform hypothesis test or derive confidence intervals for selected components of the model. In this case, the null hypothesis only restricts part of the space and the other parameters, termed nuisance, are left unspecified — the question then is what values to use for comparison with the full model. It turns out that the values that maximize the constrained log likelihood are what one should use for the test, and the particular function in which these nuisance parameters are integrated out is termed a profile likelihood.

Definition 3.5 (Profile log likelihood)**.** Consider a parametric model with log likelihood function $\ell(\boldsymbol{\theta})$ whose p-dimensional parameter vector $\boldsymbol{\theta} = (\boldsymbol{\psi}, \boldsymbol{\varphi})$ can be decomposed into a q-dimensional parameter of interest $\boldsymbol{\psi}$ and a $(p-q)$-dimensional nuisance vector $\boldsymbol{\varphi}$.

The profile likelihood ℓ_{p}, a function of $\boldsymbol{\psi}$ alone, is obtained by maximizing the likelihood pointwise at each fixed value $\boldsymbol{\psi}_0$ over the nuisance vector $\boldsymbol{\varphi}_{\psi_0}$,

$$\ell_{\mathsf{p}}(\boldsymbol{\psi}) = \max_{\boldsymbol{\varphi}} \ell(\boldsymbol{\psi}, \boldsymbol{\varphi}) = \ell(\boldsymbol{\psi}, \widehat{\boldsymbol{\varphi}}_{\boldsymbol{\psi}}).$$

Example 3.11 (Profile log likelihood for the Weibull shape parameter)**.** Consider the shape parameter $\psi \equiv \alpha$ as parameter of interest, and the scale $\varphi \equiv \lambda$ as nuisance parameter. Using the gradients derived in Example 3.7, we find that the value of the scale that maximizes the log likelihood for given α is

$$\widehat{\lambda}_\alpha = \left(\frac{1}{n} \sum_{i=1}^{n} y_i^\alpha \right)^{1/\alpha}.$$

and plugging in this value gives a function of α alone, thereby also reducing the optimization problem for the Weibull to a line search along $\ell_{\mathsf{p}}(\alpha)$. The left hand panel of Figure 3.3 shows the ridge along the direction of α corresponding to the log likelihood surface. If one thinks of these contours lines as those of a topographic map, the profile likelihood corresponds in this case to walking along the ridge of both mountains along the ψ direction, with the right panel showing the elevation gain/loss. The corresponding elevation profile on the right of Figure 3.3 with cutoff values. We would need to obtain numerically using a root finding algorithm the limits of the confidence interval on either side of $\widehat{\alpha}$, but it's clear that $\alpha = 1$ is not inside the 99% interval.

```r
lambda_alpha <- function(alpha, y = waiting){
  (mean(y^alpha))^(1/alpha)
}
# Profile likelihood for alpha
prof_alpha_weibull <- function(par, y = waiting){
  sapply(par, function(a){
   nll_weibull(pars = c(lambda_alpha(a), a), y = y)
  })
}
```

Example 3.12 (Profile log likelihood for the Weibull mean)**.** As an alternative, we can use numerical optimization to compute the profile for another function. Suppose we are interested in the expected waiting time, which according to the model is $\mu = \mathsf{E}(Y) = \lambda\Gamma(1+1/\alpha)$. To this effect, we reparametrize the model in terms of (μ, α), where $\lambda = \mu/\Gamma(1+1/\alpha)$. We then make a wrapper function that optimizes the log likelihood for fixed value of μ, then returns $\widehat{\alpha}_{\mu}$, μ and $\ell_{\mathrm{p}}(\mu)$.

To get the confidence intervals for a scalar parameter, there is a trick that helps with the derivation. We compute the signed likelihood root $r(\psi) = \mathrm{sign}(\psi - \widehat{\psi})\{2\ell_{\mathrm{p}}(\widehat{\psi}) - 2\ell_{\mathrm{p}}(\psi)\}^{1/2}$ over a fine grid of ψ, then fit a smoothing spline to the equation flipping the axis (thus, the model has response $y = \psi$ and $x = r(\psi)$). We then predict the curve at the standard normal quantiles $\mathfrak{z}_{\alpha/2}$ and $\mathfrak{z}_{1-\alpha/2}$, and return these values as confidence interval. Figure 3.5 shows how these value correspond to the cutoff points on the log likelihood ratio scale, where the vertical line is given by $-\mathfrak{c}(1-\alpha)/2$ where $\mathfrak{c}$ denotes the quantile of a χ^2_1 random variable.

```
# Compute the MLE for the expected value via plug-in
mu_hat <- mle_weibull[1]*gamma(1+1/mle_weibull[2])
# Create a profile function
prof_weibull_mu <- function(mu){
  # For given value of mu
  alpha_mu <- function(mu){
  # Find the profile by optimizing (line search) for fixed mu and the best alpha
     opt <- optimize(f = function(alpha, mu){
     # minimize the negative log likelihood
      nll_weibull(c(mu/gamma(1+1/alpha), alpha), y = waiting)},
   mu = mu,
  interval = c(0.1,10) #search region
  )
  # Return the value of the negative log likelihood and alpha_mu
  return(c(nll = opt$objective, alpha = opt$minimum))
  }
  # Create a data frame with mu and the other parameters
  data.frame(mu = mu, t(sapply(mu, function(m){alpha_mu(m)})))
}
```

```
# Create a data frame with the profile
prof <- prof_weibull_mu(seq(22, 35, length.out = 101L))
# Compute signed likelihood root r
prof$r <- sign(prof$mu - mu_hat)*sqrt(2*(prof$nll - opt_weibull$value))

# Trick: fit a spline to obtain the predictions with mu as a function of r
# Then use this to predict the value at which we intersect the normal quantiles
fit.r <- stats::smooth.spline(x = cbind(prof$r, prof$mu), cv = FALSE)
pr <- predict(fit.r, qnorm(c(0.025, 0.975)))$y
# Plot the signed likelihood root - near linear indicates quadratic
g1 <- ggplot(data = prof,
     mapping = aes(x = mu, y = r)) +
  geom_abline(intercept = 0, slope = 1) +
  geom_line() +
  geom_hline(yintercept = qnorm(0.025, 0.975),
            linetype = "dashed") +
  labs(x = expression(paste("expectation ", mu)),
       y = "signed likelihood root")
# Create a plot of the profile
g2 <- ggplot(data = prof,
       mapping = aes(x = mu, y = opt_weibull$value - nll)) +
  geom_line() +
  geom_hline(yintercept = -qchisq(c(0.95), df = 1)/2,
             linetype = "dashed") +
  geom_vline(linetype = "dotted",
  xintercept = pr) +
  labs(x = expression(paste("expectation ", mu)),
       y = "profile log likelihood")

g1 + g2
```

The maximum profile likelihood estimator behaves like a regular likelihood for most quantities of interest and we can derive test statistics and confidence intervals in the usual way. One famous example of profile likelihood is the Cox proportional hazard covered in Chapter 7.

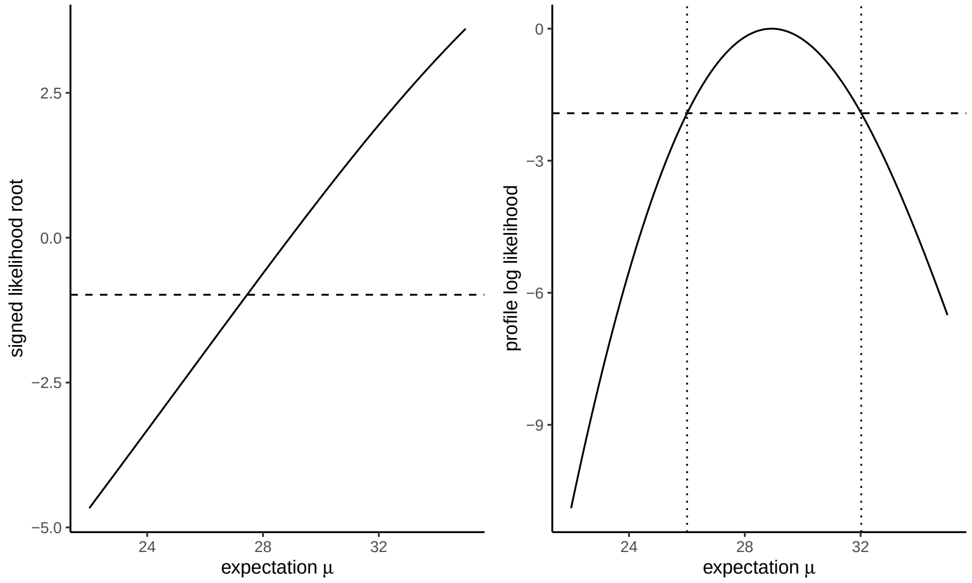


Figure 3.5: Signed likelihood root (left) and shifted profile log likelihood (right) as a function of the expected value μ in the Weibull model.

3.5 Information criteria

The likelihood can also serve as building block for model comparison: the larger $\ell(\widehat{\boldsymbol{\theta}})$, the better the fit. However, the likelihood doesn't account for model complexity in the sense that more complex models with more parameters lead to higher likelihood. This is not a problem for comparison of nested models using the likelihood ratio test because we look only at relative improvement in fit. There is a danger of **overfitting** if we only consider the likelihood of a model.

AIC and BIC are information criteria measuring how well the model fits the data, while penalizing models with more parameters,

$$\begin{aligned}\mathsf{AIC} &= -2\ell(\widehat{\boldsymbol{\theta}}) + 2p\\ \mathsf{BIC} &= -2\ell(\widehat{\boldsymbol{\theta}}) + p\ln(n),\end{aligned}$$

where p is the number of parameters in the model. The smaller the value of AIC (or of BIC), the better the model fit.

Note that information criteria do not constitute formal hypothesis tests on the parameters, but they can be used to compare models that are not nested. Such tools work under regularity conditions, and the estimated information criteria are quite noisy, so comparison for non-nested models are hazardous although popular among practitioners. If we want to compare likelihood from different probability models, we need to make sure they include normalizing constant. The BIC is more stringent than AIC, as its penalty increases with the sample size, so it selects models with fewer parameters. The BIC is **consistent**, meaning that it will pick the true correct model from an ensemble of models with probability one as $n \to \infty$. In practice, this is of little interest if one assumes that all models are approximation of reality (it is unlikely that the true model is included in the ones we consider). AIC often selects overly complicated models in large samples, whereas BIC chooses models that are overly simple.

A cautionary warning: while you can compare regression models that are not nested using information criteria, they can only be used when the response variable is the same. You could compare a Poisson regression with a linear regression for some response Y using information criteria provided you include all normalizing constants in your model. Software often drops constant terms; this has no impact when you compare models with the same constant factors, but it matters when these differ. However, **you cannot** compare them to a log-linear model with response $\ln(Y)$. Comparisons for log-linear and linear models are valid only if you use the Box–Cox likelihood, as it includes the Jacobian of the transformation.

4 Linear regression models

4.1 Introduction

The linear regression model, or linear model, is one of the most versatile workhorse for statistical inference. Linear regression is used primarily to evaluate the effects of explanatory variables (oftentimes treatment in an experimental setting) on the mean response of a continuous response, or for prediction. It combines a formulation for the mean of a **response variable** Y_i of a random sample of size n as a **linear function** of observed **explanatories** (also called predictors or covariates) $X_1, \ldots, X_p$,

$$\underset{\text{conditional mean}}{\mathsf{E}(Y_i \mid \boldsymbol{X}_i = \boldsymbol{x}_i)} = \mu_i = \underset{\text{linear combination of explanatories}}{\beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}} \equiv \mathbf{x}_i \boldsymbol{\beta}. \tag{4.1}$$

where $\mathbf{x}_i = (1, x_{i1}, \ldots, x_{ip})$ is a $(p+1)$ row vector containing a constant and the explanatories of observation i, and $\boldsymbol{\beta} = (\beta_0, \ldots, \beta_p)^\top$ is a $p+1$ column vector of coefficients for the mean. The model formulation is conditional on the values of the observed explanatories; this amounts to treating the p explanatory variables $X_1, \ldots, X_p$ as non-random quantities, or known in advance. The regression coefficients $\boldsymbol{\beta}$ is the same for all observations, but the vector of explanatories $\mathbf{x}_i$ may change from one observation to the next. The model is **linear** in the coefficients $\beta_0, \ldots, \beta_p$.

To simplify the notation, we aggregate observations into an n-vector $\boldsymbol{Y}$ and the explanatories into an $n \times (p+1)$ matrix $\mathbf{X}$ by concatenating a column of ones and the p column vectors $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_p$, each containing the n observations of the respective explanatories. The matrix $\mathbf{X}$ is termed **model matrix** (or sometimes design matrix in experimental settings), and it's ith row is $\mathbf{x}_i$.

We suppose, in addition to the mean specification, that the response variables are independent and identically distributed, drawn from a mean-zero distribution with constant variance σ^2. Assuming that the distribution are drawn from a location family, we may rewrite the linear model in terms of the mean plus an error term,

$$\underset{\text{observation}}{Y_i} = \underset{\text{mean } \mu_i}{\mathbf{x}_i \boldsymbol{\beta}} + \underset{\text{error term}}{\varepsilon_i}.$$

where ε_i is the error term specific to observation i, and we assume that the errors $\varepsilon_1, \ldots, \varepsilon_n$ are independent and identically distributed. We fix the expectation or theoretical mean of ε_i to zero to encode the fact we do not believe the model is systematically off, so $\mathsf{E}(\varepsilon_i \mid \boldsymbol{X}_i = \boldsymbol{x}_i) = 0$ $(i = 1, \ldots, n)$. The variance term σ^2 is included to take into account the fact that no exact linear relationship links $\boldsymbol{X}_i$ and Y_i, or that measurements of Y_i are subject to error.

The normal or Gaussian linear model specifies that responses follow a normal distribution, with $Y_i \mid \boldsymbol{X}_i = \boldsymbol{x}_i \sim \mathsf{normal}(\mathbf{x}_i\boldsymbol{\beta}, \sigma^2)$. The normal distribution is a location-scale family, so $Y \sim \mathsf{normal}(\mu, \sigma^2)$ is equal in distribution with $\mu + \varepsilon$ for $\varepsilon \sim \mathsf{normal}(0, \sigma^2)$.

4.1.1 Motivating examples

We present some motivating examples that are discussed in the sequel.

Example 4.1 (Consistency of product description)**.** Study 1 of Lee and Choi (2019) considered descriptors and the impact on the perception of a product on the discrepancy between the text description and the image. In their first experience, a set of six toothbrushes is sold, but the image shows either a pack of six, or a single one). The authors also measured the prior familiarity with the brand of the item. Participants were recruited using an online panel, and the data in `LC19_S1` includes the results of the $n = 96$ participants who passed the attention check (one additional participant response was outlying and removed). We could fit a linear model for the average product evaluation score, `prodeval`, as a function of the familiarity of the brand `familiarity`, an integer ranging from 1 to 7, and a dummy variable for the experimental factor `consistency`, coded `0` for consistent image/text descriptions and `1` if inconsistent. The resulting model matrix is then 96×3. The `prodeval` response is heavily discretized, with only 19 unique values ranging between 2.33 and 9.

```r
data(LC19_S1, package = "hecedsm")
# Fit a linear model using "lm"
# The first argument is a formula of the form y ~ x1 + x2
# where y is the response and x's are explanatories,
# separated by a plus (+) sign
modmat <- model.matrix(
     ~ familiarity + consistency,
     data = LC19_S1)
# Extract the model matrix
tail(modmat, n = 5L) # first five lines
```

```
#>    (Intercept) familiarity consistencyinconsistent
#> 92           1           6                       1
#> 93           1           4                       1
#> 94           1           7                       1
#> 95           1           7                       1
#> 96           1           7                       1
dim(modmat) # dimension of the model matrix
#> [1] 96  3
```

Example 4.2 (Gender discrimination in a US college)**.** To make concepts and theoretical notions more concrete, we will use observational data collected in a college in the United States. The goal of the administration was to investigate potential gender inequality in the salary of faculty members. The data contains the following variables:

- `salary`: nine-month salary of professors during the 2008–2009 academic year (in thousands USD).
- `rank`: academic rank of the professor (`assistant`, `associate` or `full`).
- `field`: categorical variable for the field of expertise of the professor, one of `applied` or `theoretical`.
- `sex`: binary indicator for sex, either `man` or `woman`.
- `service`: number of years of service in the college.
- `years`: number of years since PhD.

Before drafting a model, it is useful to perform an exploratory data analysis. If salary increases with year, there is more heterogeneity in the salary of higher ranked professors: logically, assistant professors are either promoted or kicked out after at most 6 years according to the data. The limited number of years prevents large variability for their salaries.

Salary increases over years of service, but its variability also increases with rank. Note the much smaller number of women in the sample: this will impact our power to detect differences between sex. A contingency table of sex and academic rank can be useful to see if the proportion of women is the same in each rank: women represent 16% of assistant professors and 16% of associate profs, but only 7% of full professors and these are better paid on average.

Table 4.1: Contingency table of the number of prof in the college by sex and academic rank.

	assistant	associate	full
man	56	54	248
woman	11	10	18

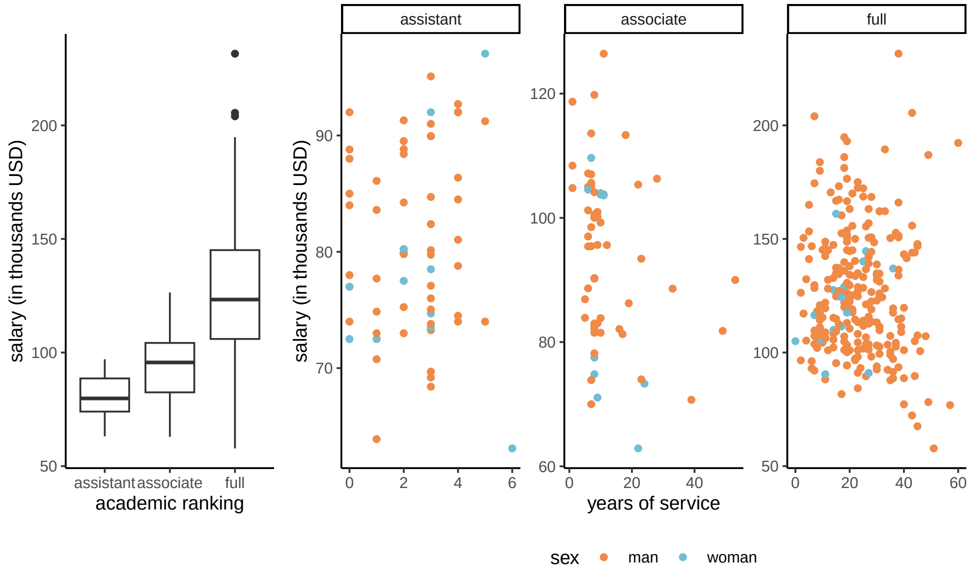


Figure 4.1: Exploratory data analysis of `college` data: salaries of professors as a function of the number of years of service and the academic ranking

Some of the potential explanatory variables of the `college` data are categorical (`rank`, `sex`, `field`), the latter two being binary. The other two continuous variables, `years` and `service`, are strongly correlated with a correlation of 0.91.

Example 4.3 (Teaching to read and pre-post experiments)**.** The `BSJ92` data in package `hecedsm` contains the results of an experimental study by Baumann, Seifert-Kessell, and Jones (1992) on the effectiveness of different reading strategies on understanding of children. These are described in the abstract

> Sixty-six fourth-grade students were randomly assigned to one of three experimental groups: (a) a Think-Aloud (TA) group, in which students were taught various comprehension monitoring strategies for reading stories (e.g., self-questioning, prediction, retelling, rereading) through the medium of thinking aloud; (b) a Directed Reading-Thinking Activity (DRTA) group, in which students were taught a predict-verify strategy for reading and responding to stories; or (c) a Directed Reading Activity (DRA) group, an instructed control, in which students engaged in a noninteractive, guided reading of stories.

The data are balanced, as there are 22 observations in each of the three subgroups, of which `DR` is the control. The researchers applied a series of three tests (an error detection task for test 1, a comprehension monitoring questionnaire for test 2, and the *Degrees of Reading Power* cloze test labelled test 3). Tests 1 and 2 were administered both before and after the intervention: this gives us a change to establish the average *improvement* in student by adding `pretest1` as covariate for a regression of `posttest`, for example. The tests 1 were out of 16, but the one administered after the experiment was made more difficult to avoid cases of students getting near full scores. The correlation between pre-test and post-test 1 is ($\widehat{\rho}_1 = 0.57$), much stronger than that for the second test ($\widehat{\rho}_2 = 0.21$).

4.2 Mean model specification

This section covers the mean model specification, starting with parametrization of models with factors (i.e., categorical explanatories).

4.2.1 What explanatories?

The first step of an analysis is deciding which explanatory variables should be added to the mean model specification, and under what form. Models are but approximations of reality; Section 2.1 of Venables (2000) argues that, if we believe the true mean function linking explanatories $\boldsymbol{X}$ and the response Y is of the form $\mathsf{E}(Y \mid \boldsymbol{X}) = f(\boldsymbol{X})$ for f sufficiently smooth, then the linear model is a first-order approximation. For interpretation purposes, it makes sense to mean-center any continuous explanatory, as this facilitates interpretation.

In an experimental setting, where the experimental group or condition is randomly allocated, we can directly compare the different treatments and draw causal conclusions (since all other things are constant, any detectable difference is due on average to our manipulation). Although we usually refrain from including any other explanatory to keep the design simple, it may be nevertheless helpful to consider some concomitant variables that explain part of the variability to filter background noise and increase power. For example, for the Baumann, Seifert-Kessell, and Jones (1992) data, our interest is in comparing the average scores as a function of the teaching method, we would include `group`. In this example, it would also make sense to include the `pretest1` result as an explanatory. This way, we will model the average difference in improvement from pre-test to post-test rather than the average score.

In an observational setting, people self-select in different groups, so we need to account for differences. Linear models in economics and finance often add control variables to the model to account for potential differences due to socio-demographic variables (age, revenue, etc.) that would be correlated to the group. Any test for coefficients would capture only correlation between the outcome Y and the postulated explanatory factor of interest.

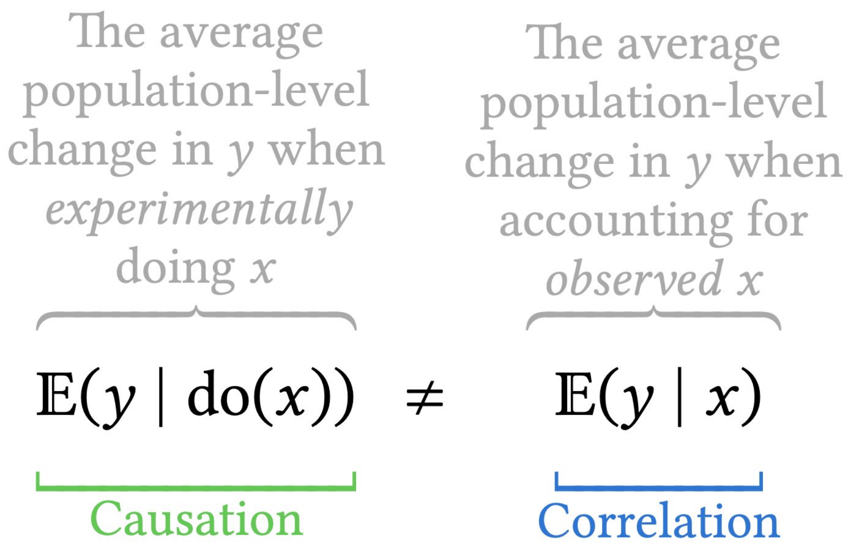

The average population-level change in *y* when *experimentally* doing *x*
The average population-level change in *y* when accounting for *observed x*
$\mathbb{E}(y \mid \mathrm{do}(x)) \neq \mathbb{E}(y \mid x)$
Causation
Correlation

Figure 4.2: Difference between experimental and observational studies by Andrew Heiss CC-BY 4.0

4.2.2 Continuous explanatories

Continuous explanatories are typically specified by including a single linear term, leading to the simple linear regression of the form $Y \mid X = x \sim \mathsf{normal}(\beta_0 + \beta x, \sigma^2)$. In this situation β_0 is the intercept (the mean value of Y when $x = 0$) and β_1 is the slope, i.e., the average increase of Y when x increases by one unit. Figure 4.3 shows such an example of a model with a single explanatory. As revealed by the exploratory data analysis of Example 4.2, this model is simplistic and clearly insufficient to explain differences in salary.

The **intercept** β_0 is the value when all of $x_1, \ldots, x_p$ are zero. The interpretation of the other mean parameters in the model depends crucially on the parametrization and on potential interactions or higher order terms.

Rather, a more interesting perspective considers the effect of an increase of an explanatory variable. If $\mu = \mathbf{x}\boldsymbol{\beta}$ and each, then a one unit increase of the j component $(j = 1, \ldots, p)$ leads to a change of $\partial\mu/\partial x_j$.

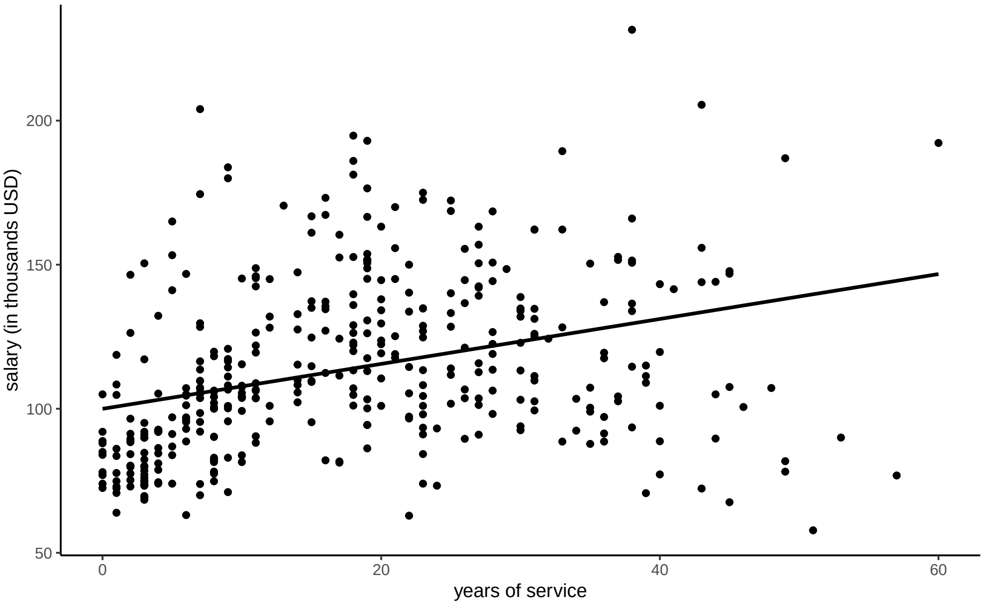


Figure 4.3: Simple linear regression model for the salary of professors as a function of the number of years of service.

Generally, we can increase X_j by one unit and compare the increase in the mean, here for X_j

$$\mathsf{E}(Y \mid X_j = x_j + 1, \boldsymbol{X}_{-j} = \boldsymbol{x}_{-j}) - \mathsf{E}(Y \mid X_j = x_j, \boldsymbol{X}_{-j} = \boldsymbol{x}_{-j}) = \beta_j.$$

If the relationship between explanatory X and response Y, as assessed from a scatterplot, is not linear, we may consider more complicated function of the explanatories, as Example 4.4 shows.

Example 4.4 (Quadratic curve for the automobile data)**.** We consider a linear regression model for the fuel autonomy of cars as a function of the power of their motor (measured in horsepower) from the `auto` dataset. The postulated model,

$$\texttt{mpg}_i = \beta_0 + \beta_1\texttt{horsepower}_i + \beta_2\texttt{horsepower}_i^2 + \varepsilon_i,$$

includes a quadratic term. Figure 4.4 shows the scatterplot with the fitted regression line, above which the line for the simple linear regression for horsepower is added. The marginal effect of an increase of one unit in `horsepower` is $\beta_1 + 2\beta_2\texttt{horsepower}$, which depends on the value of the explanatory.

To fit higher order polynomials, we use the `poly` as the latter leads to more numerical stability. For general transformations, the `I` function tells the software interpret the input "as is". Thus, `lm(y~x+I(x^2))`, would fit a linear model with design matrix $[\mathbf{1}_n \, \mathbf{x} \, \mathbf{x}^2]$.

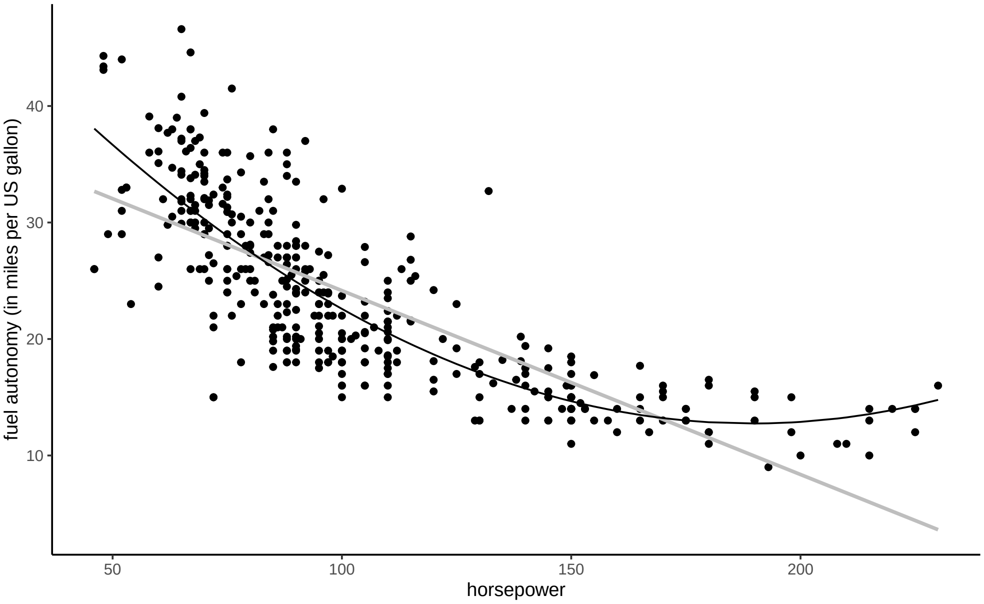


Figure 4.4: Linear regression models for the fuel autonomy of cars as a function of motor power.

It appears graphically that the quadratic model fits better than the simple linear alternative: we will assess this hypothesis formally later. For the degree two polynomial, Figure 4.4 show that fuel autonomy decreases rapidly when power increases between 50 to 100, then more slow until 189.35 hp. After that, the model postulates that autonomy increases again as evidenced by the scatterplot, but beware of extrapolating (weird things can happen beyond the range of the data, as exemplified by Hassett's cubic model for the number of daily cases of Covid19 in the USA).

The representation in Figure 4.4 may seem counter-intuitive given that we fit a linear model, but it is a 2D projection of 3D coordinates for the equation $\beta_0 + \beta_1 x - y + \beta_2 z = 0$, where $x =$ `horsepower`, $z =$ `horsepower`^{2} and $y =$ `mpg`. Physics and common sense force $z = x^2$, and so the fitted values lie on a curve in a 2D subspace of the fitted plan, as shown in grey in the three-dimensional Figure 4.5.

Remark 4.1 (Discretization of continuous covariates). Another option is to transform a continuous variable X into a categorical variable by discretizing into bins and fitting a piecewise-linear function of X. The prime example of such option is treating a Likert scale

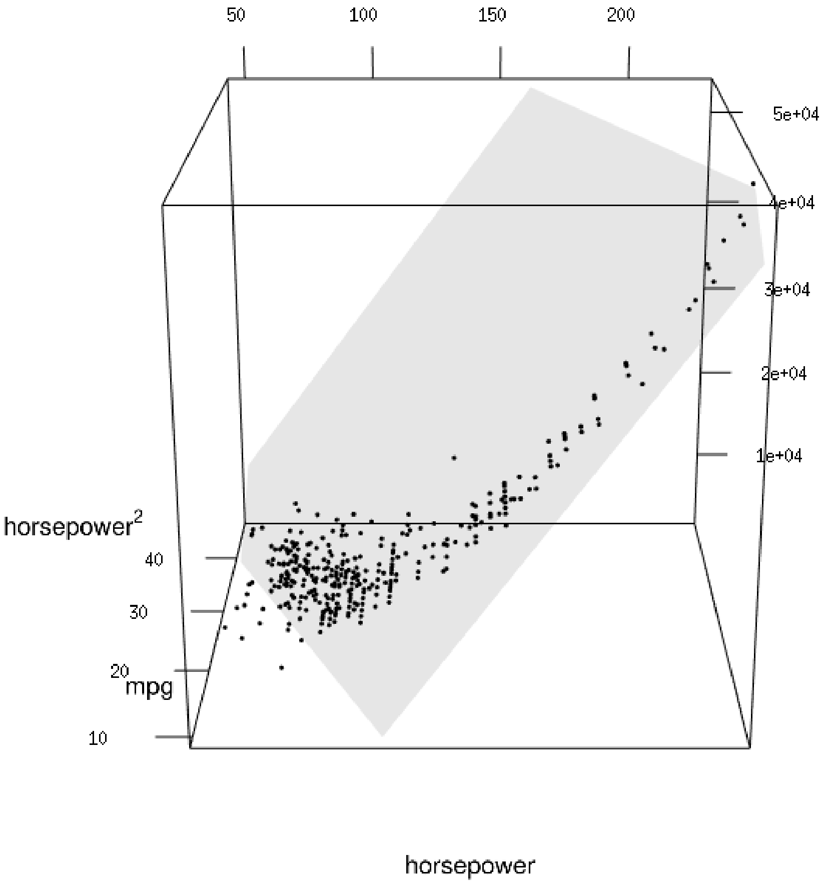


Figure 4.5: 3D graphical representation of the linear regression model for the `auto` data.

as a categorical variable. While this allows one to fit more flexible functional relations between X and Y, this comes at the cost of additional coefficients for the same estimation budget (fewer observations to estimate the effect of X results in lower precision of the coefficients).

4.2.3 Categorical covariates

Dummies are variables (columns of explanatories from the model matrix) which only include -1, 0 and 1 to give indicator of the level of groups. For a binary outcome, we can create a column that has entries 1 for the treatment and 0 for the control group.

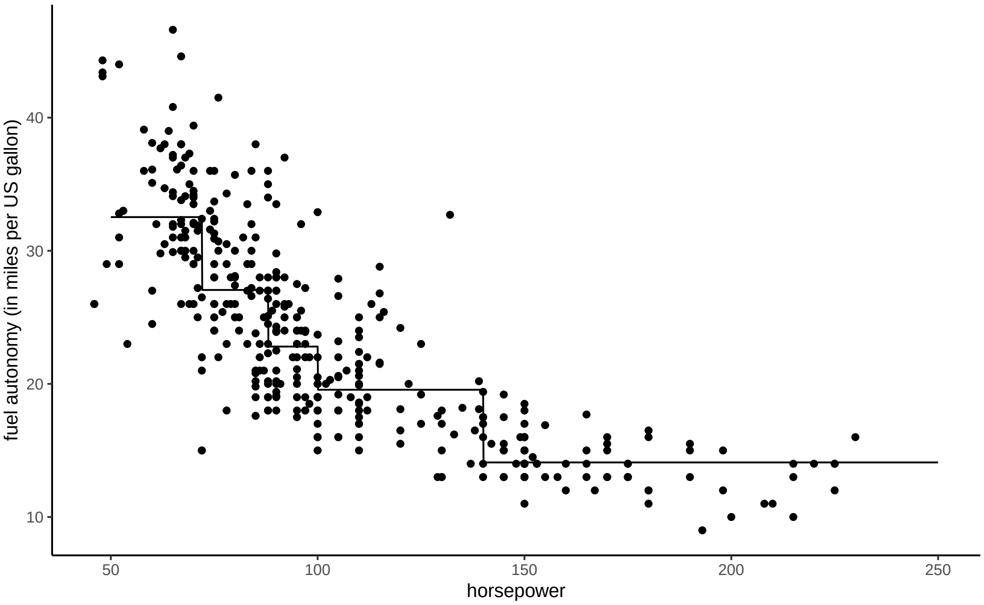


Figure 4.6: Piecewise-linear model for the fuel autonomy of cars as a function of motor power.

Example 4.5 (Linear models with a single binary variable). Moon and VanEpps (2023) consider the impact of providing suggested amounts for donations to a charity (as opposed to an open-ended request). In Study 1, participants were given the chance of winning 25$ and giving part of this amount to charity.

Consider for example a linear model that includes the `amount` (in dollars, from 0 for people who did not donate, up to 25 dollars) as a function of

$$\texttt{condition} = \begin{cases} 0, & \text{open-ended,} \\ 1, & \text{suggested quantity} \end{cases}$$

The equation of the simple linear model that includes the binary variable `condition` is

$$\begin{aligned} \mathsf{E}(\texttt{amount} \mid \texttt{condition}) &= \beta_0 + \beta_1 \mathbf{1}_{\texttt{condition}=\texttt{quantity}}. \\ &= \begin{cases} \beta_0, & \texttt{condition} = 0, \\ \beta_0 + \beta_1 & \texttt{condition} = 1. \end{cases} \end{aligned}$$

Let μ_0 denote the theoretical average amount for the open-ended amount and μ_1 that of participants of the treatment `quantity` group. A linear model that only contains a binary variable X as regressor amounts to specifying a different mean for each of two groups: the average of the treatment group is $\beta_0 + \beta_1 = \mu_1$ and $\beta_1 = \mu_1 - \mu_0$ represents the difference between the average donation amount of people given `open-ended` amounts and those who are offered suggested amounts (`quantity`), including zeros for the amount of people who did not donate. The parametrization of the linear model with β_0 and β_1 is in terms of pairwise differences relative to the baseline category and is particularly useful if we want to test for mean difference between the groups, as this amounts to testing $\mathscr{H}_0 : \beta_1 = 0$.

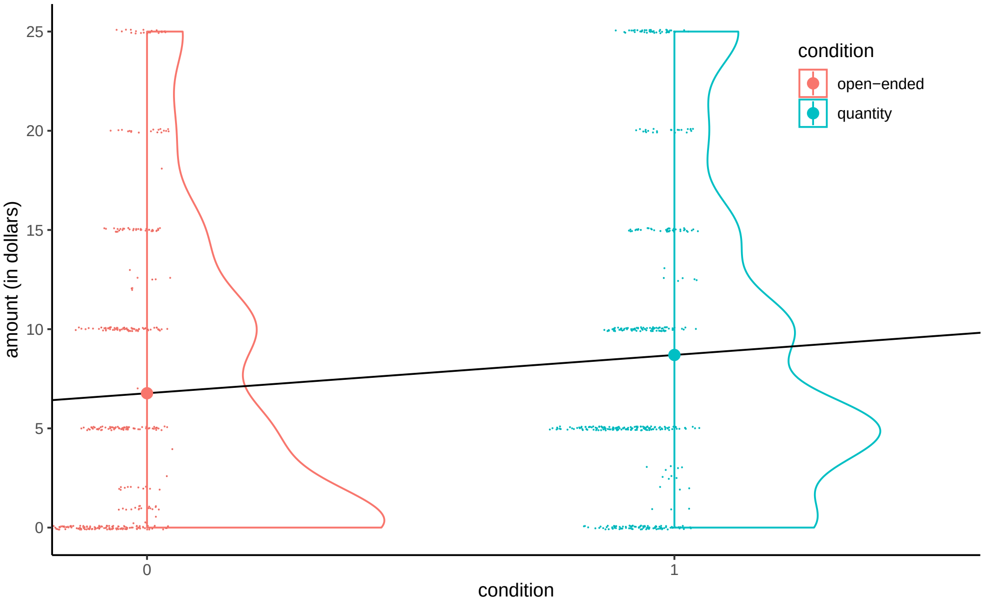


Figure 4.7: Simple linear model for the `MV23_S1` data using the binary variable `condition` as explanatory even if the equation defines a line, only its values in $0/1$ are realistic.

Even if the linear model defines a line, the latter is only meaningful when evaluated at 0 or 1; Figure 4.7 shows it in addition to sample observations (jittered horizontally) and a density estimate for each condition. The colored dot represents the mean, which will coincide with the estimates.

It is clear that the data are heavily discretized, with lots of ties and zeros. However, given the sample size of 869 observations, we can easily draw conclusions in each group.

Let us consider categorical variables with $K > 2$ levels, which in **R** are of class `factor`. The default parametrization for factors are in terms of treatment contrast: the reference level of the factor (by default, the first value in alphanumerical order) will be treated as the reference category and assimilated to the intercept. The software will then create a set of $K-1$ dummy variables for a factor with K levels, each of which will have ones for the relevant value and zero otherwise.

Example 4.6 (Dummy coding for categorical variables)**.** Consider the Baumann, Seifert-Kessell, and Jones (1992) study and the sole inclusion of the `group` variable. The data are ordered by group: the first 22 observations are for group `DR`, the 22 next ones for group `DRTA` and the last 22 for `TA`. If we fit a model with `group` as categorical variables

```
class(BSJ92$group) # Check that group is a factor
#> [1] "factor"
levels(BSJ92$group) # First level shown is reference
#> [1] "DR"   "DRTA" "TA"
# Print part of the model matrix
# (three individuals from different groups)
model.matrix(~ group, data = BSJ92)[c(1,23,47),]
#>    (Intercept) groupDRTA groupTA
#> 1            1         0       0
#> 23           1         1       0
#> 47           1         0       1
# Compare with levels of factors recorded
BSJ92$group[c(1,23,47)]
#> [1] DR   DRTA TA
#> Levels: DR DRTA TA
```

The mean model specification is

$$\mathsf{E}(Y \mid \text{group}) = \beta_0 + \beta_1 \mathbf{1}_{\text{group}=\texttt{DRTA}} + \beta_2 \mathbf{1}_{\text{group}=\texttt{TA}}.$$

Since the variable `group` is categorical with $K=3$ levels, we need $K-1=2$ dummy explanatories to include the effect and obtain one average per group. With the default parametrization, we obtain

- $\mathbf{1}_{\text{group}=\texttt{DRTA}} = 1$ if `group=DRTA` and zero otherwise.
- $\mathbf{1}_{\text{group}=\texttt{TA}} = 1$ if `group=TA` and zero otherwise.

Because the model includes an intercept and the model ultimately describes three group averages, we only need two additional variables. With the treatment parametrization, the group mean of the reference group equals the intercept coefficient, $\mu_{\texttt{DR}} = \beta_0$,

Table 4.2: Parametrization of dummies for a categorical variable with the default treatment contrasts.

	(Intercept)	groupDRTA	groupTA
DR	1	0	0
DRTA	1	1	0
TA	1	0	1

When `group=DR` (baseline), both indicator variables `groupDRTA` and `groupTA` are zero. The average in each group is $\mu_{\texttt{DR}} = \beta_0$, $\mu_{\texttt{DRTA}} = \beta_0 + \beta_1$ and $\mu_{\texttt{TA}} = \beta_0 + \beta_2$. We thus find that β_1 is the difference in mean between group `DRTA` and group `DR`, and similarly $\beta_2 = \mu_{\texttt{TA}} - \mu_{\texttt{DR}}$.

Remark 4.2 (Sum-to-zero constraints). The parametrization discussed above, which is the default for the `lm` function, isn't the only one available. We consider an alternative ones: rather than comparing each group mean with that of a baseline category, the default parametrization for analysis of variance models is in terms of sum-to-zero constraints, whereby the intercept is the equiweighted average of every group, and the parameters $\beta_1, \ldots, \beta_{K-1}$ are differences to this average.

```r
model.matrix(
    ~ group,
    data = BSJ92,
    contrasts.arg = list(group = "contr.sum"))
```

Table 4.3: Parametrization of dummies for the sum-to-zero constraints for a categorical variable.

	(Intercept)	group1	group2
DR	1	1	0
DRTA	1	0	1
TA	1	-1	-1

In the sum-to-zero constraint, we again only get two dummy variables, labelled `group1` and `group2`, along with the intercept. The value of `group1` is 1 if `group=DR`, 0 if `group=DRTA` and -1 if `group=TA`. Using the invariance property, we find $\mu_{\texttt{DR}} = \beta_0 + \beta_1$, $\mu_{\texttt{DRTA}} = \beta_0 + \beta_2\beta_1$ and $\mu_{\texttt{TA}} = \beta_0 - \beta_1 - \beta_2$ (more generally, the intercept minus the sum of all the other mean coefficients). Some algebraic manipulation reveals that $\beta_0 = (\mu_{\texttt{DR}} + \mu_{\texttt{DRTA}} + \mu_{\texttt{TA}})/3$.

If we removed the intercept, then we could include three dummies for each treatment group and each parameter would correspond to the average. This isn't recommended in **R** because the software treats models without the intercept differently and some output will be nonsensical (e.g., the coefficient of determination will be wrong).

Example 4.7 (Parameter interpretation for analysis of covariance)**.** We consider a pre-post model for the error detection task test of Baumann, Seifert-Kessell, and Jones (1992). We fit a linear model with the pre-test score and the experimental condition.

```
data(BSJ92, package = "hecedsm") #load data
str(BSJ92) # Check that categorical variables are factors
#> tibble [66 x 6] (S3: tbl_df/tbl/data.frame)
#>  $ group    : Factor w/ 3 levels "DR","DRTA","TA": 1 1 1 1 1 1 1 1 1 1 ...
#>  $ pretest1 : int [1:66] 4 6 9 12 16 15 14 12 12 8 ...
#>  $ pretest2 : int [1:66] 3 5 4 6 5 13 8 7 3 8 ...
#>  $ posttest1: int [1:66] 5 9 5 8 10 9 12 5 8 7 ...
#>  $ posttest2: int [1:66] 4 5 3 5 9 8 5 5 7 7 ...
#>  $ posttest3: int [1:66] 41 41 43 46 46 45 45 32 33 39 ...
# Check summary statistics for posttest1
BSJ92 |> # compute group average
   group_by(group) |>
   summarize(mean_pre = mean(pretest1),
             mean_post = mean(posttest1),
             diff_impr = mean_post - mean_pre)
#> # A tibble: 3 x 4
#>   group mean_pre mean_post diff_impr
#>   <fct>    <dbl>     <dbl>     <dbl>
#> 1 DR       10.5       6.68   -3.82
#> 2 DRTA      9.73      9.77    0.0455
#> 3 TA        9.14      7.77   -1.36
# Fit the ANOVA for the difference
linmod1 <- lm(
   posttest1 - pretest1 ~ group,
   data = BSJ92)
coef(linmod1) # Mean model coefficients
#> (Intercept)   groupDRTA     groupTA
#>       -3.82        3.86        2.45
# Fit a linear regression
linmod2 <- lm(
   posttest1 ~ pretest1 + group,
   data = BSJ92 |>
      dplyr::mutate( # mean-center pretest result
        pretest1 = pretest1 - mean(pretest1)))
coef(linmod2) # Mean model coefficients
#> (Intercept)    pretest1   groupDRTA     groupTA
#>       6.188       0.693       3.627       2.036
```

With the ANOVA model for the group as a function of the improvement and using the default treatment parameterization,, the intercept is the average of post-test minus pre-test score for group DR, and the other two coefficients are the difference between groups DRTA and DR, and the difference between groups TA and DR. Thus, the higher average improvement is for DRTA, then TA, then the baseline DR.

Consider next a linear model in which we allow the post-test score to be a linear function of the pre-test. we find that, for each point score on the pre-test, the post-test score increases by 0.693 marks regardless of the group. The DRTA group (respectively TA) has an average, ceteris paribus, that is 3.627 (respectively 2.036) points higher than that of the baseline group DR for two people with the same pre-test score. Because we centered the continuous covariate pretest1, the intercept β_0 is the average post-test score of a person from the DR group who scored the overall average of all 66 students in the pre-test.

Example 4.8 (Wage inequality in an American college)**.** We consider a linear regression model for the college data that includes sex, academic rank, field of study and the number of years of service as explanatories.

The postulated model is

$$\begin{aligned}\texttt{salary} &= \beta_0 + \beta_1\texttt{sex}_{\texttt{woman}} + \beta_2\texttt{field}_{\texttt{theoretical}} \\ &\quad + \beta_3\texttt{rank}_{\texttt{associate}} + \beta_4\texttt{rank}_{\texttt{full}} + \beta_5\texttt{service} + \varepsilon.\end{aligned}$$

Table 4.4: Estimated coefficients of the linear model for the college (in USD, rounded to the nearest dollar).

$\widehat{\beta}_0$	$\widehat{\beta}_1$	$\widehat{\beta}_2$	$\widehat{\beta}_3$	$\widehat{\beta}_4$	$\widehat{\beta}_5$
86596	-4771	-13473	14560	49160	-89

The interpretation of the coefficients is as follows:

- The estimated intercept is $\widehat{\beta}_0 = 86596$ dollars; it corresponds to the mean salary of men assistant professors who just started the job and works in an applied domain.
- everything else being equal (same field, academic rank, and number of years of service), the estimated salary difference between a woman and is estimated at $\widehat{\beta}_1 = -4771$ dollars.
- *ceteris paribus*, the salary difference between a professor working in a theoretical field and one working in an applied field is β_2 dollars: our estimate of this difference is -13473 dollars, meaning applied pays more than theoretical.
- *ceteris paribus*, the estimated mean salary difference between associate and assistant professors is $\widehat{\beta}_3 = 14560$ dollars.
- *ceteris paribus*, the estimated mean salary difference between full and assistant professors is $\widehat{\beta}_4 = 49160$ dollars.
- within the same academic rank, every additional year of service leads to a mean salary increase of $\widehat{\beta}_5 = -89$ dollars.

4.3 Parameter estimation

The linear model includes $p+1$ mean parameters and a standard deviation σ, which is assumed constant for all observations.

4.3.1 Ordinary least squares estimator

Given a design or model matrix $\mathbf{X}$ and a linear model formulation $\mathsf{E}(Y_i) = \mathbf{x}_i\boldsymbol{\beta}$, we can try to find the parameter vector $\boldsymbol{\beta} \in \mathbb{R}^{p+1}$ that minimizes the mean squared error, i.e., the average squared vertical distance between the fitted values $\widehat{y}_i = \mathbf{x}_i\widehat{\boldsymbol{\beta}}$ and the observations y_i.

Proposition 4.1 (Ordinary least squares)**.** *Consider the optimization problem*

$$\begin{aligned}\widehat{\boldsymbol{\beta}} &= \mathrm{argmin}_{\boldsymbol{\beta} \in \mathbb{R}^{p+1}} \sum_{i=1}^{n} (y_i - \mathbf{x}_i\boldsymbol{\beta})^2 \\ &= (\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta}).\end{aligned}$$

We can compute the derivative of the right hand side with respect to $\boldsymbol{\beta}$, set it to zero and solve

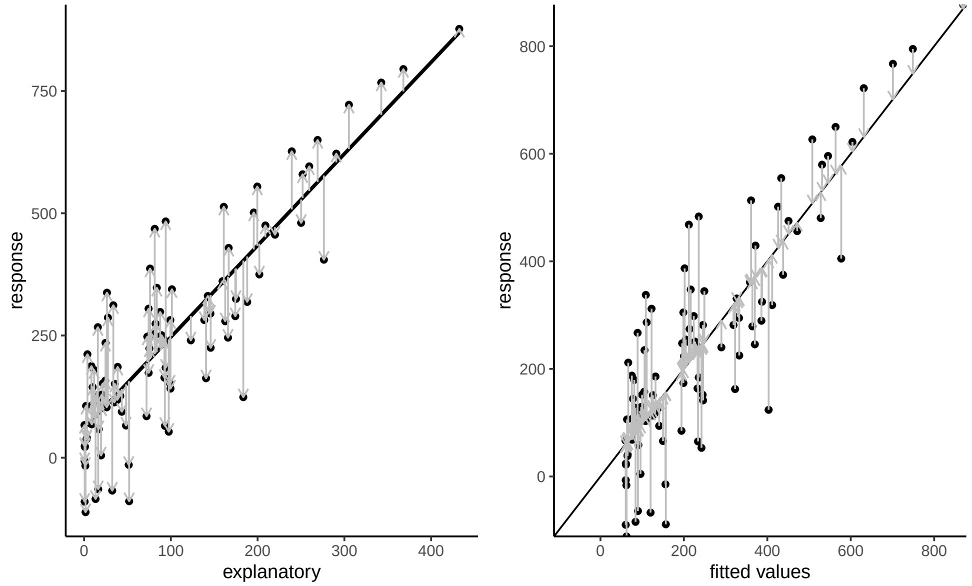


Figure 4.8: Ordinary residuals e_i (vertical vectors) added to the regression line in the scatter (x, y) (left) and the fit of response y_i against fitted values $\widehat{y}_i$. The ordinary least squares line minimizes the average squared length of the ordinary residuals.

for $\widehat{\boldsymbol{\beta}}$*,*

$$\begin{aligned}\mathbf{0}_n &= \frac{\partial}{\partial \boldsymbol{\beta}}(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta}) \\ &= \frac{\partial(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})}{\partial \boldsymbol{\beta}}\frac{\partial(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})}{\partial(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})} \\ &= 2\mathbf{X}^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})\end{aligned}$$

using the chain rule. Distributing the terms leads to the so-called normal equation

$$\mathbf{X}^\top\mathbf{X}\boldsymbol{\beta} = \mathbf{X}^\top\boldsymbol{y}.$$

If the $n \times p$ *matrix* $\mathbf{X}$ *is full-rank, meaning that it's columns are not linear combinations of one another, the quadratic form* $\mathbf{X}^\top\mathbf{X}$ *is invertible and we obtain the solution to the least square problems,*

$$\widehat{\boldsymbol{\beta}} = \left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\boldsymbol{y}. \tag{4.2}$$

*This is the **ordinary least squares estimator** (OLS). The explicit solution means that no numerical optimization is needed for linear models.*

We could also consider maximum likelihood estimation. Proposition 4.1 shows that, assuming normality of the errors, the least square estimators of $\boldsymbol{\beta}$ coincide with the maximum likelihood estimator of $\boldsymbol{\beta}$.

Proposition 4.2 (Maximum likelihood estimation of the normal linear model)**.** *The linear regression model specifies that the observations* $Y_i \sim \mathsf{normal}(\mathbf{x}_i\boldsymbol{\beta}, \sigma^2)$ *are independent. The linear model has* $p+2$ *parameters (β and* σ^2*) and the log likelihood is, abstracting from constant terms,*

$$\ell(\boldsymbol{\beta}, \sigma) \propto -\frac{n}{2}\ln(\sigma^2) - \frac{1}{2\sigma^2}\left\{(\boldsymbol{y}-\mathbf{X}\boldsymbol{\beta})^\top(\boldsymbol{y}-\mathbf{X}\boldsymbol{\beta})\right\}^2.$$

Maximizing the log likelihood with respect to β is equivalent to minimizing the sum of squared errors $\sum_{i=1}^n (y_i - \mathbf{x}_i\boldsymbol{\beta})^2$*, regardless of the value of* σ*, and we recover the OLS estimator* $\widehat{\boldsymbol{\beta}}$*. The maximum likelihood estimator of the variance* $\widehat{\sigma}^2$ *is thus*

$$\widehat{\sigma}^2 = \mathrm{argmax}_{\sigma^2}\ell(\widehat{\boldsymbol{\beta}}, \sigma^2).$$

The profile log likelihood for σ^2*, excluding constant terms that don't depend on* σ^2*, is*

$$\ell_{\mathrm{p}}(\sigma^2) \propto -\frac{1}{2}\left\{n\ln\sigma^2 + \frac{1}{\sigma^2}(\boldsymbol{y}-\mathbf{X}\hat{\boldsymbol{\beta}})^\top(\boldsymbol{y}-\mathbf{X}\hat{\boldsymbol{\beta}})\right\}.$$

Differentiating each term with respect to σ^2 *and setting the gradient equal to zero yields the maximum likelihood estimator*

$$\begin{aligned}\widehat{\sigma}^2 &= \frac{1}{n}(\boldsymbol{Y}-\mathbf{X}\hat{\boldsymbol{\beta}})^\top(\boldsymbol{Y}-\mathbf{X}\hat{\boldsymbol{\beta}})\\ &= \frac{1}{n}\sum_{i=1}^n (y_i - \mathbf{x}_i\widehat{\boldsymbol{\beta}})^2\\ &= \frac{\mathsf{SS}_e}{n};\end{aligned}$$

where SS_e *is the sum of squared residuals. The usual unbiased estimator of* σ^2 *calculated by software is* $S^2 = \mathsf{SS}_e/(n-p-1)$*, where the denominator is the sample size* n *minus the number of mean parameters* $\boldsymbol{\beta}$*,* $p+1$*.*

Remark 4.3 (Invariance)*.* One direct consequence of likelihood estimation is that the fitted values $\widehat{y}_i$ for two model matrices $\mathbf{X}_a$ and $\mathbf{X}_b$, are the same if they generate the same linear span, as in Example 4.6. The interpretation of the coefficients will however change. If we include an intercept term, then we get the same output if the columns of explanatory are mean-centered.

The value of $\boldsymbol{\beta}$ is such that it will maximize the correlation between Y and $\widehat{Y}$. In the case of a single categorical variable, we will obtain fitted values $\widehat{y}$ that correspond to the sample mean of each group.

Remark 4.4 (Geometry). The vector of fitted values $\widehat{\boldsymbol{y}} = \mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{H}_{\mathbf{X}}\boldsymbol{y}$ is the projection of the response vector $\boldsymbol{y}$ on the linear span generated by the columns of $\mathbf{X}$. The matrix $\mathbf{H}_{\mathbf{X}} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top$, often called hat matrix, is an orthogonal projection matrix, so $\mathbf{H}_{\mathbf{X}} = \mathbf{H}_{\mathbf{X}}^\top$ and $\mathbf{H}_{\mathbf{X}}\mathbf{H}_{\mathbf{X}} = \mathbf{H}_{\mathbf{X}}$ and $\mathbf{H}_{\mathbf{X}}\mathbf{X} = \mathbf{X}$. Since the vector of residuals $\boldsymbol{e} = (e_1, \ldots, e_n)^\top$, which appear in the sum of squared errors, is defined as $\boldsymbol{y} - \widehat{\boldsymbol{y}}$ and $\widehat{\boldsymbol{y}} = \mathbf{X}\boldsymbol{\beta}$, simple algebraic manipulations show that the inner product between ordinary residuals and fitted values is zero, since

$$\begin{aligned}
\widehat{\boldsymbol{y}}^\top \boldsymbol{e} &= \widehat{\boldsymbol{\beta}}^\top \mathbf{X}^\top (\boldsymbol{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}) \\
&= \boldsymbol{y}^\top \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top(\boldsymbol{y} - \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\boldsymbol{y}) \\
&= \boldsymbol{y}^\top \mathbf{H}_{\mathbf{X}}\boldsymbol{y} - \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\boldsymbol{y} \\
&= 0
\end{aligned}$$

where we use the definition of $\widehat{\boldsymbol{y}}$ and $\boldsymbol{e} = \boldsymbol{y} - \widehat{\boldsymbol{y}}$ on the first line, then substitute the OLS estimator $\widehat{\boldsymbol{\beta}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\boldsymbol{y}$ and distribute terms. Similarly, $\mathbf{X}^\top\boldsymbol{e} = \mathbf{0}_{p+1}$. The ordinary residuals are thus orthogonal to both the model matrix $\mathbf{X}$ and to the fitted values.

A direct consequence of this fact is that the sample linear correlation between $\boldsymbol{e}$ and $\widehat{\boldsymbol{y}}$ is zero; we will use this property to build graphical diagnostics.

Since the inner product is zero, the mean of $\boldsymbol{e}$ must be zero provided that $\mathbf{1}_n$ is in the linear span of $\mathbf{X}$.

Proposition 4.3 (Information matrix for normal linear regression models)**.** *The entries of the observed information matrix of the normal linear model are*

$$\begin{aligned}
-\frac{\partial^2 \ell(\boldsymbol{\beta}, \sigma^2)}{\partial\boldsymbol{\beta}\partial\boldsymbol{\beta}^\top} &= \frac{1}{\sigma^2}\frac{\partial \mathbf{X}^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})}{\partial\boldsymbol{\beta}^\top} = \frac{\mathbf{X}^\top\mathbf{X}}{\sigma^2} \\
-\frac{\partial^2 \ell(\boldsymbol{\beta}, \sigma^2)}{\partial\boldsymbol{\beta}\partial\sigma^2} &= -\frac{\mathbf{X}^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})}{\sigma^4} \\
-\frac{\partial^2 \ell(\boldsymbol{\beta}, \sigma^2)}{\partial(\sigma^2)^2} &= -\frac{n}{2\sigma^4} + \frac{(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})^\top(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})}{\sigma^6}.
\end{aligned}$$

If we evaluate the observed information at the MLE, we get

$$j(\widehat{\boldsymbol{\beta}}, \widehat{\sigma^2}) = \begin{pmatrix} \frac{\mathbf{X}^\top\mathbf{X}}{\widehat{\sigma^2}} & \mathbf{0}_{p+1} \\ \mathbf{0}_{p+1}^\top & \frac{n}{2\widehat{\sigma^4}} \end{pmatrix}$$

since $\widehat{\sigma}^2 = \mathsf{SS}_e/n$ and the residuals are orthogonal to the model matrix. Since $\mathsf{E}(Y \mid \mathbf{X}) = \mathbf{X}\boldsymbol{\beta}$, the Fisher information is

$$i(\boldsymbol{\beta}, \sigma^2) = \begin{pmatrix} \frac{\mathbf{X}^\top\mathbf{X}}{\sigma^2} & \mathbf{0}_{p+1} \\ \mathbf{0}_{p+1}^\top & \frac{n}{2\sigma^4} \end{pmatrix}$$

Since zero off-correlations in normal models amount to independence, the MLE for σ^2 and $\boldsymbol{\beta}$ are independent. Provided the $(p+1)$ square matrix $\mathbf{X}^\top\mathbf{X}$ is invertible, the large-sample variance of the ordinary least squares estimator is $\sigma^2(\mathbf{X}^\top\mathbf{X})^{-1}$ and that of the MLE of the variance is $2\sigma^4/n$.

4.3.2 Fitting linear models with software

Although we could build the model matrix ourselves and use the least square formula of Equation 4.2, the numerical routines implemented in software are typically better behaved. The `lm` function in **R** fits **linear models**, as does `glm` with the default arguments. Objects of class `lm` have multiple methods allow you to extract specific objects from `lm` objects. For example, the functions `coef`, `resid`, `fitted`, `model.matrix` will return the coefficients $\widehat{\boldsymbol{\beta}}$, the ordinary residuals $\boldsymbol{e}$, the fitted values $\widehat{\boldsymbol{y}}$ and the model matrix $\mathbf{X}$.

```
data(BSJ92, package = "hecedsm") #load data
str(BSJ92) # Check that categorical variables are factors
# Fit the linear regression
linmod <- lm(posttest1 ~ pretest1 + group,
             data = BSJ92)
beta_hat <- coef(linmod) # beta coefficients
vcov_beta <- vcov(linmod) # Covariance matrix of betas
summary(linmod) # summary table
beta_ci <- confint(linmod) # Wald confidence intervals for betas
yhat <- fitted(linmod) # fitted values
e <- resid(linmod) # ordinary residuals

# Check OLS formula
X <- model.matrix(linmod) # model matrix
y <- college$salary
isTRUE(all.equal(
  c(solve(t(X) %*% X) %*% t(X) %*% y),
  as.numeric(coef(linmod))
))
```

The `summary` method is arguably the most useful: it will print mean parameter estimates along with standard errors, t values for the Wald test of the hypothesis $\mathscr{H}_0 : \beta_i = 0$ and the associated P-values. Other statistics and information about the sample size, the degrees of freedom, etc., are given at the bottom of the table. Note that the `lm` function uses the unbiased estimator of the variance σ^2.

Remark 4.5 (Linearity). The model is linear in the coefficients β, so the quadratic curve $\beta_0 + \beta_1 x + \beta_2 x^2$ is a linear model because it is a sum of coefficients times functions of explanatories. By contrast, the model $\beta_0 + \beta_1 x^{\beta_2}$ is nonlinear in $\boldsymbol{\beta}$.

4.4 Coefficient of determination

When we specify a model, the error term ε accounts for the fact no perfect linear relationship characterizes the data (if it did, we wouldn't need statistic to begin with). Once we have fitted a model, we estimate the variance σ^2; one may then wonder which share of the total variance in the sample is explained by the model.

The total sum of squares, defined as the sum of squared residuals from the intercept-only model, serves as comparison — the simplest model we could come up with would involving every observation by the sample mean of the response and so this gives (up to scale) the variance of the response, $\mathsf{SS}_c = \sum_{i=1}^n (y_i - \overline{y})^2$. We can then compare the variance of the original data with that of the residuals from the model with covariate matrix $\mathbf{X}$, defined as $\mathsf{SS}_e = \sum_{i=1}^n e_i^2$ with $e_i = y_i - \widehat{\beta}_0 - \sum_{j=1}^p \widehat{\beta}_j X_j$. We define the coefficient of determination, or squared multiple correlation coefficient of the model, R^2, as

$$R^2 = 1 - \frac{\mathsf{SS}_e}{\mathsf{SS}_c} = \frac{\sum_{i=1}^n (y_i - \overline{y})^2 - \sum_{i=1}^n e_i^2}{\sum_{i=1}^n (y_i - \overline{y})^2}.$$

An alternative decomposition shows that $R^2 = \mathsf{cor}^2(\boldsymbol{y}, \widehat{\boldsymbol{y}})$, i.e., the coefficient of determination can be interpreted as the square of Pearson's linear correlation between the response $\boldsymbol{y}$ and the fitted values $\widehat{\boldsymbol{y}}$.

Its important to note that R^2 is not a goodness-of-fit criterion, like the log likelihood: some phenomena are inherently noisy and even a good model will fail to account for much of the response's variability. Moreover, one can inflate the value of R^2 by including more explanatory variables and making the model more complex, thereby improving the likelihood and R^2. Indeed, the coefficient is non-decreasing in the dimension of $\mathbf{X}$, so a model with $p+1$ covariate will necessarily have a higher R^2 values than only p of the explanatories. For model comparisons, it is better to employ information criteria or else rely on the predictive performance if this is the purpose of the regression. Lastly, a model with a high R^2 may imply high correlation, but the relation may be spurious: linear regression does not yield causal models!

4.5 Model assumptions

So far, we have fit models and tested significance of the parameters without checking the model assumptions. The correctness of statements about the p-values and confidence intervals depend on the (approximate) validity of the model assumptions, which all stem from the distributional assumption for the error, assumed to be independent and identically distributed with $\varepsilon_i \stackrel{\cdot}{\sim} \mathsf{normal}(0, \sigma^2)$. This compact mathematical description can be broken down into four assumptions.

- linearity: the mean of Y is $\beta_0 + \beta_1 \mathrm{X}_1 + \cdots + \beta_p \mathrm{X}_p$.
- homoscedasticity: the error variance is constant
- independence of the errors/observations conditional on covariates.
- normality of the errors

This section reviews the assumptions made in order to allow statistical inference using the linear model and different residuals that serve as building blocks for graphical diagnostics. We investigate the consequences of violation of these assumptions and outline potential mitigation strategies, many of which are undertaken in other chapters.

When we perform an hypothesis test, we merely fail to reject the null hypothesis, either because the latter is true or else due to lack of evidence. The same goes for checking the validity of model assumptions: scientific reasoning dictates that we cannot know for certain whether these hold true. Our strategy is therefore to use implications of the linear model assumptions to create graphical diagnostic tools, so as to ensure that there is no gross violation of these hypothesis. However, it is important to beware of over-interpreting diagnostic plots: the human eye is very good at finding spurious patterns.

Other good references for the material in this section is:

- Forecasting: Principles and Practice, section 5.3

4.5.1 Residuals

Residuals are predictions of the errors ε and represent the difference between the observed value Y_i and the estimated value on the line. The ordinary residuals are

$$e_i = Y_i - \widehat{Y}_i, \qquad i = 1, \ldots, n.$$

The sum of the ordinary residuals is always zero by construction if the model includes an intercept, meaning $\overline{e} = 0$.

Not all observations contribute equally to the adjustment of the fitted hyperplane. The geometry of least squares shows that the residuals are orthogonal to the fitted values, and $\boldsymbol{e} = (\mathbf{I}_n - \mathbf{H}_{\mathbf{X}})\boldsymbol{Y}$, where $\mathbf{H}_{\mathbf{X}} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top$ is an $n \times n$ projection matrix that spans the p-dimensional linear combination of the columns of $\mathbf{X}$, $\mathscr{S}(\mathbf{X})$. If $\mathsf{Va}(\boldsymbol{Y}) = \sigma^2\mathbf{I}_n$, it follows that $\mathsf{Va}(\boldsymbol{e}) = \sigma^2(\mathbf{I}_n - \mathbf{H}_{\mathbf{X}})$ because $(\mathbf{I}_n - \mathbf{H}_{\mathbf{X}})$ is a projection matrix, therefore idempotent and symmetric. Because the matrix has rank $n-p$, the ordinary residuals cannot be independent from one another.

If the errors are independent and homoscedastic, the ordinary residual e_i has variance $\sigma^2(1-h_i)$, where the leverage term $h_i = (\mathbf{H}_{\mathbf{X}})_{ii} = \mathbf{x}_i(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{x}_i$ is the ith diagonal entry of the projection matrix $(\mathbf{H}_{\mathbf{X}})$ and $\mathbf{x}_i$ is the ith row of the model matrix corresponding to observation i.

We thus conclude that ordinary residuals do not all have the same standard deviation and they are not independent. This is problematic, as we cannot make meaningful comparisons: points with low leverage are bound to deviate more from the fitted model than others. To palliate to this, we can standardize the residuals so each has the same variance under the null of independent homoscedastic errors — the leverage terms h_i are readily calculated from the model matrix $\mathbf{X}$. The only remaining question is how to estimate the variance. If we use the ith observation to estimate both the residual and the variance, we introduce additional dependence. A better way is remove the ith observation and refit the model with the $n-1$ remaining observations to get of $s^2_{(-i)}$ (there are tricks and closed-form expressions for these, so one doesn't need to fit n different linear models). The jacknife studentized residual $r_i = e_i/\{s_{(-i)}(1-h_i)\}$, also termed externally studentized residuals, are not independent, but they are identically distributed and follow a Student distribution with $n-p-2$ degrees of freedom. These can be obtained in **R** with the command `rstudent`.

When to use which residuals? By construction, the vector of ordinary residuals $\boldsymbol{e}$ is orthogonal to the fitted values $\widehat{\boldsymbol{y}}$ and also to each column of the model matrix $\mathbf{X}$: this means a simple linear regression of $\boldsymbol{e}$ with any of these as covariate gives zero intercept and zero slope. However, residual patterns due to forgotten interactions, nonlinear terms, etc. could be picked up from pair plots of ordinary residuals against the explanatories.

While the jackknife studentized residuals r_i are not orthogonal, they are not very different. Use jackknife residuals $\boldsymbol{r}$ to check for equality of variance and distributional assumptions (e.g., using quantile-quantile plots).

One thus typically uses ordinary residuals $\boldsymbol{e}$ for plots of fitted values/explanatories against residuals and otherwise jackknife studentized residuals for any other graphical diagnostic plot.

4.5.2 Collinearity

The linearity assumption can be interpreted broadly to mean that all relevant covariates have been included and that their effect is correctly specified in the equation of the mean. Adding superfluous covariates to a model has limited impact: if the (partial) correlation between a column vector $\mathbf{X}_k$ and the response variable $\boldsymbol{Y}$ is zero, then $\beta_k = 0$ and the estimated coefficient $\widehat{\beta}_k \approx 0$ because the least square estimators are unbiased. If we include many useless variables, say k, the lack of parsimony can however make interpretation more difficult. The price to pay for including the k additional covariates is an increase in the variance of the estimators $\widehat{\boldsymbol{\beta}}$.

It is nevertheless preferable to include more variables than to forget key predictors: if we omit an important predictor, their effect may be picked up by other regressors (termed **confounders**) in the model with are correlated with the omitted variable. The interpretation of the other effects can be severely affected by confounders. For example, the simple linear model (or two-sample t-test) for salary as a function of sex for the `college` data is invalid because sex is a confounder for rank. Since there are more men than women full professor, the mean salary difference between men and women is higher than it truly is. One way to account for this is to include control variables (such as rank), whose effect we need not be interested in, but that are necessary for the model to be adequate. We could also have used stratification, i.e., tested for wage discrimination within each academic rank. This is the reason why sociodemographic variables (sex, age, education level, etc.) are collected as part of studies.

A linear model is not a causal model: all it does is capture the linear correlation between an explanatory variable and the response. When there are more than one explanatory, the effect of X_j given what has not already been explained by $\mathbf{X}_{-j}$. Thus, if we fail to reject $\mathscr{H}_0 : \beta_j = 0$ in favor of the alternative $\mathscr{H}_1 : \beta_j \neq 0$, we can only say that there is no significant *linear* association between X_j and Y once the effect of other variables included in the model has been accounted for. There are thus two scenarios: either the response is uncorrelated with X_j (uninteresting case, but easy to pick up by plotting both or computing linear correlation), or else there is a strong correlation between X_j and both the response Y as well as (some) of the other explanatory variables $\mathrm{X}_1, \ldots, \mathrm{X}_p$. This problem is termed (multi)collinearity.

One potential harm of collinearity is a decrease in the precision of parameter estimators. With collinear explanatories, many linear combinations of the covariates represent the response nearly as well. Due to the (near) lack of identifiability, the estimated coefficients become numerically unstable and this causes an increase of the standard errors of the parameters. The predicted or fitted values are unaffected. Generally, collinearity leads to high estimated standard errors and the regression coefficients can change drastically when new observations are included in the model, or when we include or remove explanatories.

The individual β coefficients may not be statistically significant, but the global F-test will indicate that some covariates are relevant for explaining the response. This however would also be the case if there are predictors with strong signal, so neither is likely to be useful to detect issues.

The added-variable plot shows the relation between the response Y and an explanatory X_j after accounting for other variables: the slope $\widehat{\beta}_j$ of the simple linear regression is the same of the full model. A similar idea can be used to see how much of X_j is already explained by the other variables. For a given explanatory variable X_j, we define its **variance inflation factor** as $\mathsf{VIF}(j) = (1 - R^2(j))^{-1}$, where $R^2(j)$ is the coefficient of determination of the model obtained by regressing X_j on all the other explanatory variables, i.e.,

$$\mathrm{X}_j = \beta_0^\star + \beta_1^\star \mathrm{X}_1 + \cdots + \beta_{j-1}^\star \mathrm{X}_{j-1} + \beta_{j+1}^\star \mathrm{X}_{j+1} + \cdots + \beta_p^\star \mathrm{X}_p + \varepsilon^\star$$

By definition, $R^2(j)$ represents the proportion of the variance of X_j that is explained by all the other predictor variables. Large variance inflation factors are indicative of problems (typically covariates with $\mathsf{VIF} > 10$ require scrutinity, and values in the hundreds or more indicate serious problems).

Added-variable plots can also serve as diagnostics, by means of comparison of the partial residuals with a scatterplot of the pair (Y, X_j); if the latter shows very strong linear relation, but the slope is nearly zero in the added-variable plot, this hints that collinearity is an issue.

What can one do about collinearity? If the goal of the study is to develop a predictive model and we're not interested in the parameters themselves, then we don't need to do anything. Collinearity is not a problem for the overall model: it's only a problem for the individual effects of the variables. Their joint effect is still present in the model, regardless of how the individual effects are combined.

If we are interested in individual parameter estimates, for example, to see how (and to what extent) the predictor variables explain the behaviour of Y, then things get more complicated. Collinearity only affects the variables that are strongly correlated with one another, so we only care if it affects one or more of the variables of interest. There sadly is no good solution to the problem. One could

- try to obtain more data, so as to reduce the effects of collinearity appearing in specific samples or that are due to small sample size.
- create a composite score by somehow combining the variables showing collinearity.
- remove one or more of the collinear variables. You need to be careful when doing this not to end up with a misspecified model.
- use penalized regression. If $\mathbf{X}^\top\mathbf{X}$ is (nearly) not invertible, this may restore the uniqueness of the solution. Penalties introduce bias, but can reduce the variance of

the estimators $\boldsymbol{\beta}$. Popular choices include ridge regression (with an l_2 penalty), lasso (l_1 penalty), but these require adjustment in order to get valid inference.

Whatever the method, it's important to understand that it can be very difficult (and sometimes impossible) to isolate the individual effect of a predictor variable strongly correlated with other predictors.

Example 4.9 (Collinearity in the `college` data)**.** We consider the `college` data analysis and include all the covariates in the database, including `years`, the number of years since PhD. One can suspect that, unless a professor started his or her career elsewhere before moving to the college, they will have nearly the same years of service. In fact, the correlation between the two variables, `service` and `years` is 0.91. The variance inflation factor for the five covariates

For categorical variables, the variance inflation factor definition would normally yield for each level a different value; an alternative is the generalized variance inflation factor (Fox and Monette 1992). Here, we are interested in gender disparities, so the fact that both service and field are strongly correlated is not problematic, since the VIF for `sex` is not high and the other variables are there to act as control and avoid confounders.

Table 4.5: (Generalized) variance inflation factor for the `college` data.

service	years	rank	sex	field
5.92	7.52	2.01	1.03	1.06

4.5.3 Leverage and outliers

The leverage h_i of observation i measures its impact on the least square fit, since we can write $h_i = \partial \widehat{y}_i / \partial y_i$. Leverage values tell us how much each point impacts the fit: they are strictly positive, are bounded below by $1/n$ and above by 1. The sum of the leverage values is $\sum_{i=1}^n h_i = p + 1$: in a good design, each point has approximately the same contribution, with average weight $(p+1)/n$.

Points with high leverage are those that have unusual combinations of explanatories. An influential observation ($h_i \approx 1$) pulls the fitted hyperplane towards itself so that $\hat{y}_i \approx y_i$. As a rule of thumb, points with $h_i > 2(p+1)/n$ should be scrutinized.

It is important to distinguish betwen **influential** observations (which have unusual $\mathbf{x}$ value, i.e., far from the overall mean) and **outliers** (unusual value of the response y). If an observation is both an outlier and has a high leverage, it is problematic.

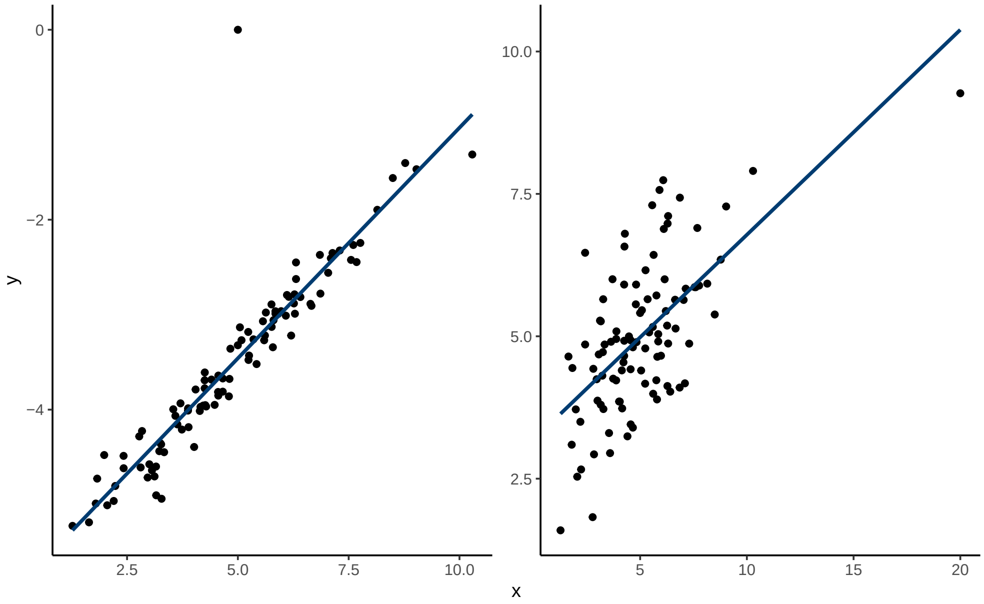


Figure 4.9: Outlier and influential observation. The left panel shows an outlier, whereas the right panel shows an influential variable (rightmost x value).

If influential observations can be detected by inspecting the leverage of each observation, outliers are more difficult to diagnose.

An outlier stands out from the rest of the observations, either because it has an usual response value, or because it falls far from the regression surface. Loosely speaking, an outlier is an unusual values of Y for a given combination of $\mathbf{X}$ that stands out from the rest. Outliers can be detected during the exploratory data analysis or picked-up in residual plots (large values of $|e_i|$ in plots of fitted versus residuals) or added-variable plots. One could potentially test whether an jackknife studentized residual is an outlier (adjusting for the fact we would consider only largest values). One can also consider Cook's distance, C_j, a statistic giving the scaled distance between the fitted values $\hat{\boldsymbol{y}}$ and the fitted values for the model with all but the jth observation, $\hat{\boldsymbol{y}}^{(-j)}$,

$$C_j = \frac{1}{(p+1)S^2}\sum_{i=1}^n \left\{\hat{y}_i - \hat{y}_i^{(-j)}\right\}^2$$

Large values of C_j indicate that its residual e_j is large relative to other observations or else its leverage h_j is high. A rule of thumb is to consider points for which $C_j > 4/(n-p-1)$. In practice, if two observations are outlying and lie in the same region, their Cook distance will be halved.

Outliers and influential observations should not be disregarded because they don't comply with the model, but require further investigation. They may motivate further modelling for features not accounted for. It is also useful to check for registration errors in the data (which can be safely discarded).

Except in obvious scenarios, unusual observations should not be discarded. In very large samples, the impact of a single outlier is hopefully limited. Transformations of the response may help reduce outlyingness. Otherwise, alternative objective functions (as those employed in robust regression) can be used; these downweight extreme observations, at the cost of efficiency.

4.6 Diagnostic plots

We review the assumptions in turn and discuss what happens when the assumptions fail to hold.

4.6.1 Independence assumption

Usually, the independence of the observations follows directly from the type of sampling used — this assumption is implicitly true if the observations were taken from a *random sample* from the population. This is generally not the case for longitudinal data, which contains repeated measures from the same individuals across time. Likewise, time series are bound not to have independent observations. If we want to include all the time points in the analysis, we must take into account the possible dependence (correlation) between observations. If we ignore correlation, the estimated standard errors are too small relative to the truth, so the effective sample size is smaller than number of observations.

What is the impact of dependence between measurements? Heuristically, correlated measurements carry less information than independent ones. In the most extreme case, there is no additional information and measurements are identical, but adding them multiple times unduly inflates the statistic and leads to more frequent rejections.

The lack of independence can also have drastic consequences on inference and lead to false conclusions: Figure 4.10 shows an example with correlated samples within group (or equivalently repeated measurements from individuals) with 25 observations per group. The y-axis shows the proportion of times the null is rejected when it shouldn't be. Here, since the data are generated from the null model (equal mean) with equal variance, the inflation in the number of spurious discoveries, false alarm or type I error is alarming and the inflation is substantial even with very limited correlation between measurements.

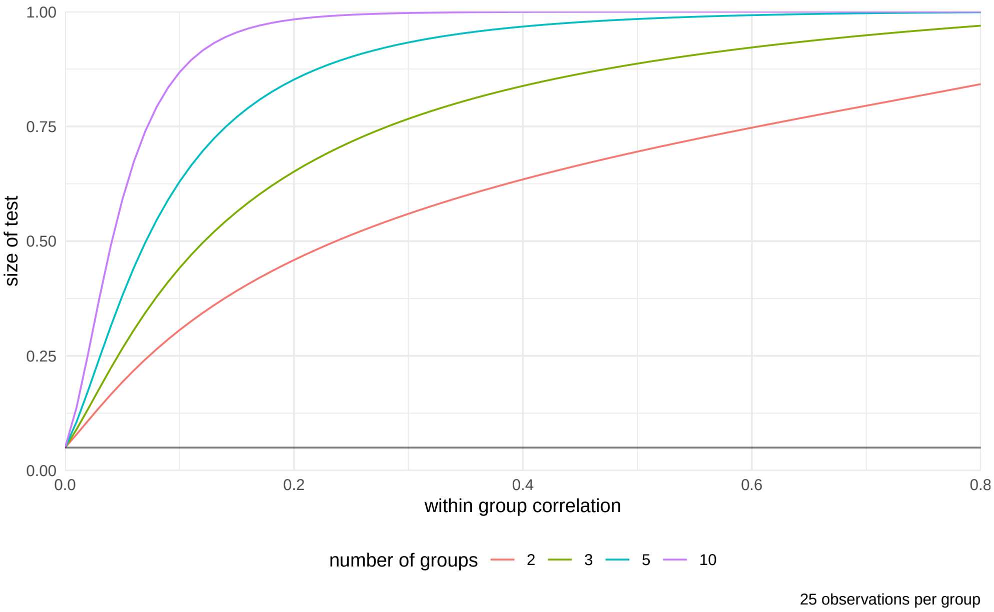


Figure 4.10: Percentage of rejection of the null hypothesis for the F-test of equality of means for the one way ANOVA with data generated with equal mean and variance from an equicorrelation model (within group observations are correlated, between group observations are independent). The nominal level of the test is 5%.

The first source of dependence is clustered data, meaning measurements taken from subjects that are not independent from one another (family, groups, etc.) More generally, correlation between observations can arises from space-time dependence, roughly categorized into

- longitudinal data: repeated measurements are taken from the same subjects (few time points)
- time series: observations observed at multiple time periods (many time points).

Time series require dedicated models not covered in this course. Because of autocorrelation, positive errors tend to be followed by positive errors, etc. We can plot the residuals as a function of time, and a scatterplot of lagged residuals e_i versus e_{i-1} $(i = 2, \ldots, n)$.

However, lagged residuals plots only show dependence at lag one between observations. For time series, we can look instead at a correlogram, i.e., a bar plot of the correlation between two observations h units apart as a function of the lag h (Brockwell and Davis 2016, Definition 1.4.4).

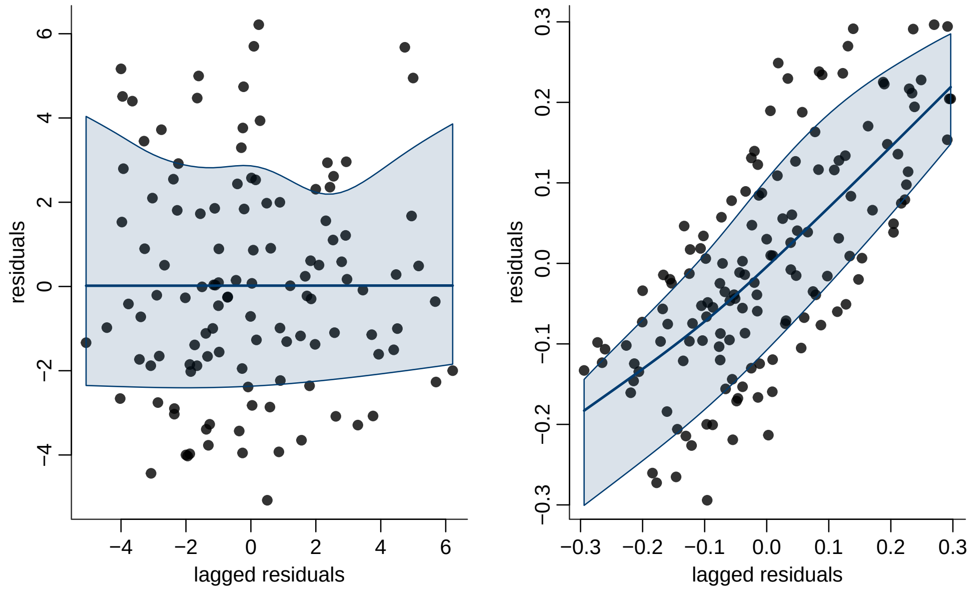


Figure 4.11: Lagged residual plots: there is no evidence against independence in the left panel, whereas the right panel shows positively correlated residuals.

For $y_1, \ldots, y_n$ and constant time lags $h = 0, 1, \ldots$ units, the autocorrelation at lag h is

$$r(h) = \frac{\gamma(h)}{\gamma(0)}, \qquad \gamma(h) = \frac{1}{n}\sum_{i=1}^{n-|h|}(y_i - \overline{y})(y_{i+h}) - \overline{y})$$

If the series is correlated, the sample autocorrelation will likely fall outside of the pointwise confidence intervals, as shown in Figure 4.12. Presence of autocorrelation requires modelling the correlation between observations explicitly using dedicated tools from the time series literature. We will however examine $\mathsf{AR}(1)$ models as part of the chapter on longitudinal data.

When observations are positively correlated, the estimated standard errors reported by the software are too small. This means we are overconfident and will reject the null hypothesis more often then we should if the null is true (inflated Type I error, or false positive).

4.6.2 Linearity assumption

The second assumption of the linear model is that of linearity, which means that the mean model is correctly specified, all relevant covariates have been included and their effect is

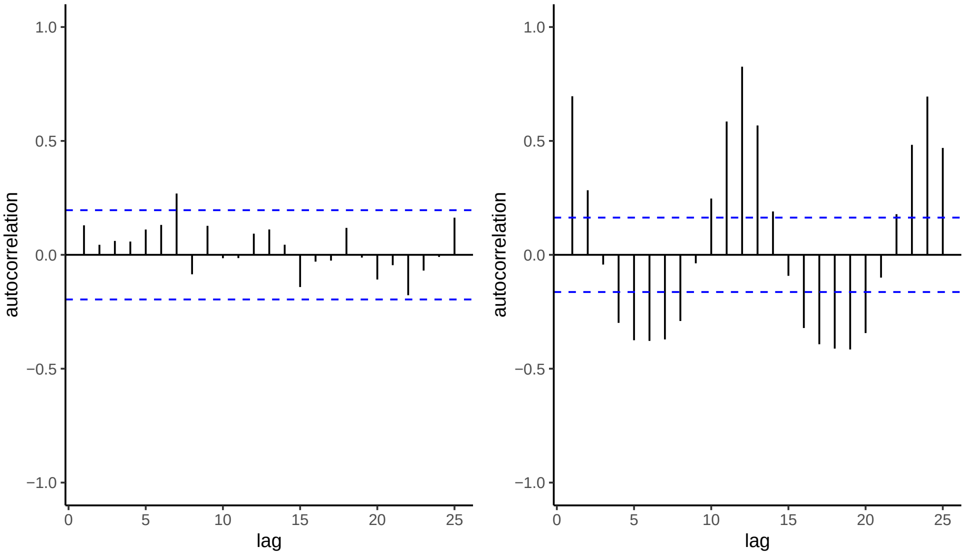


Figure 4.12: Correlogram of independent observations (left) and the ordinary residuals of the log-linear model fitted to the air passengers data (right). While the mean model of the latter is seemingly correctly specified, there is residual dependence between monthly observations and yearly (at lag 12). The blue lines give approximate pointwise 95% confidence intervals for white noise (uncorrelated observations).

correctly specified. To check that the response surface of the linear model is adequate, we plot e_i against $\widehat{y}_i$ or X_{ij} (for $j = 1, \ldots, p$). Since the linear correlation between $\boldsymbol{e}$ and $\widehat{\boldsymbol{y}}$ (or $\boldsymbol{e}$ and $\mathbf{X}_j$) is zero by construction, patterns (e.g., quadratic trend, cycles, changepoints) are indicative of misspecification of the mean model. One can add a smoother to detect patterns. Figure 4.13 shows three diagnostics plots, the second of which shows no pattern in the residuals, but skewed fitted values.

If there is residual structure in plots of ordinary residuals against either (a) the fitted values or (b) the explanatory variables, a more complex model can be adjusted including interactions, nonlinear functions, …If the effect of an explanatory variable is clearly nonlinear and complicated, smooth terms could be added (we won't cover generalized additive models in this course).

Plotting residuals against left-out explanatory variables can also serve to check that all of the explanatory power of the omitted covariate is already explained by the columns of $\mathbf{X}$.

If an important variable has been omitted and is not available in the dataset, then the

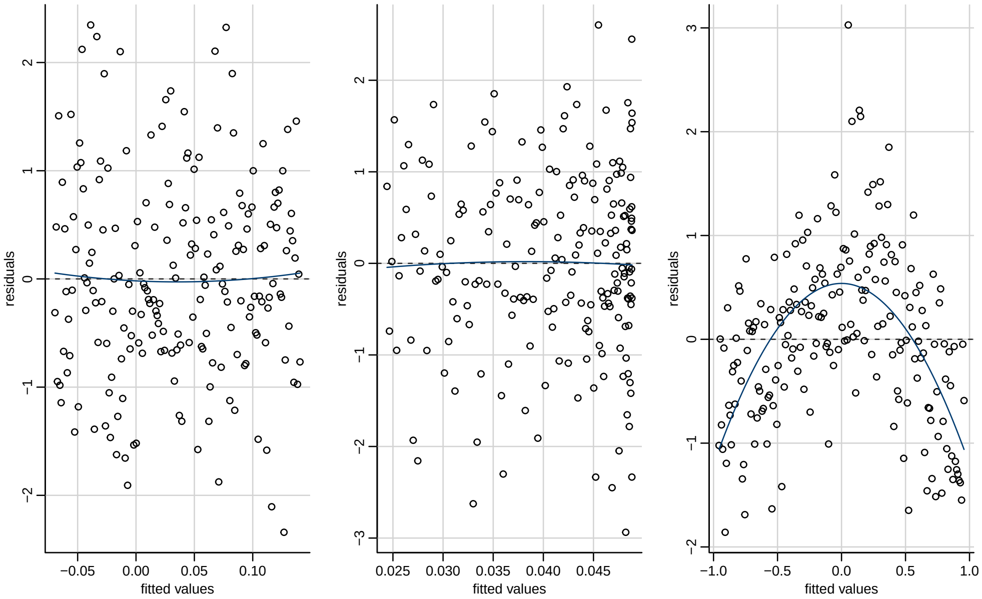


Figure 4.13: Scatterplots of residuals against fitted values. The first two plots show no departure from linearity (mean zero). The third plot shows a clear quadratic pattern, suggesting the mean model is misspecified. Note that the distribution of the fitted value need not be uniform, as in the second panel which shows more high fitted values.

effect of that variable is captured by both the errors (the portion orthogonal to the model matrix $\mathbf{X}$, i.e., unexplained by the covariates included in the model) and the remaining part is captured by other explanatories of the model that are correlated with the omitted variable. These variables can act as confounders. There is little that can be done in either case unless the data for the omitted variable are available, but subject-specific knowledge may help make sense of the results.

4.6.3 Constant variance assumption

If the variance of the errors is the same for all observations (homoscedasticity), that of the observations Y is also constant. The most common scenarios for heteroscedasticity are increases in variance with the response, or else variance that depends on explanatory variables $\mathbf{X}$, most notably categorical variables. For the former, a log-transform (or Box–Cox transformation) can help stabilize the variance, but we need the response to be positive. For the latter, we can explicitly model that variance and we will see how to include different variance per group later on. A popular strategy in the econometrics literature, is to use robust (inflated) estimators of the standard errors such as White's sandwich estimator of the variance.

If the residuals (or observations) are heteroscedastic (non constant variance), the estimated effects of the variables (the β parameters) are still valid in the sense that the ordinary least squares estimator $\widehat{\boldsymbol{\beta}}$ is unbiased. However, the estimated standard errors of the $\widehat{\beta}$ are no longer reliable and, consequently, the confidence intervals and the hypothesis tests for the model parameters will be incorrect. Indeed, if the variance of the errors differs from one observation to the next, we will estimate an average of the different variance terms. The standard errors of each term are incorrect (too small or too large) and the conclusions of the tests (p-values) will be off because the formulas of both t-test and F-test statistics include estimates of $\hat{\sigma}^2$.

Looking at the plot of jackknife studentized residuals against regressors (or fitted values) is instructive — for example, we often see a funnel pattern when there is an increase in variance in the plot of the jackknife studentized residuals against fitted value, or else in boxplots with a categorical variable as in Figure 4.15. However, if we want to fit a local smoother to observe trends, it is better to plot the absolute value of the jackknife studentized residuals against regressors or observation number.

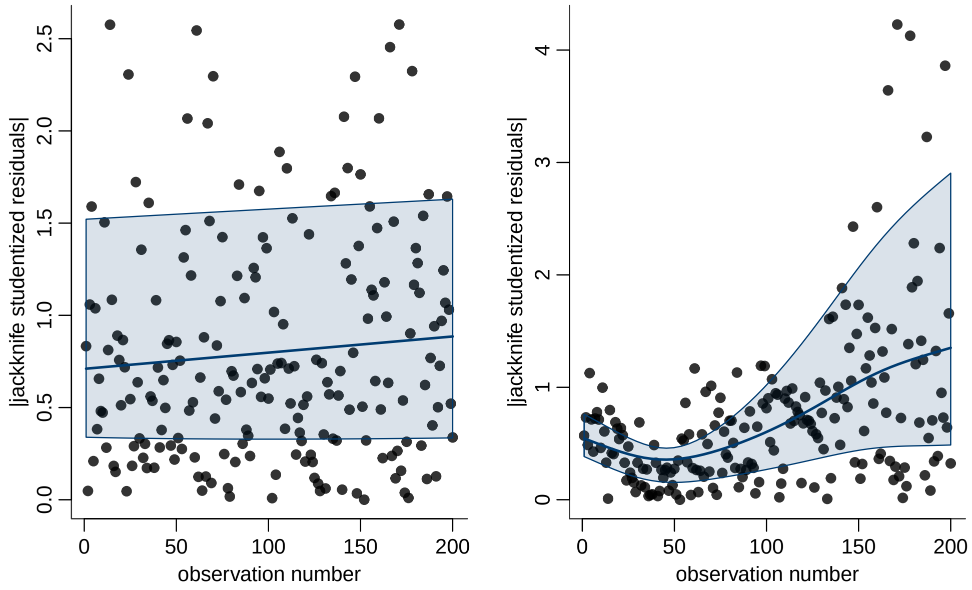


Figure 4.14: Plot of the absolute value of jackknife studentized residuals against observation number. The left panel is typical of homoscedastic data, whereas the right panel indicates an increase in the variance.

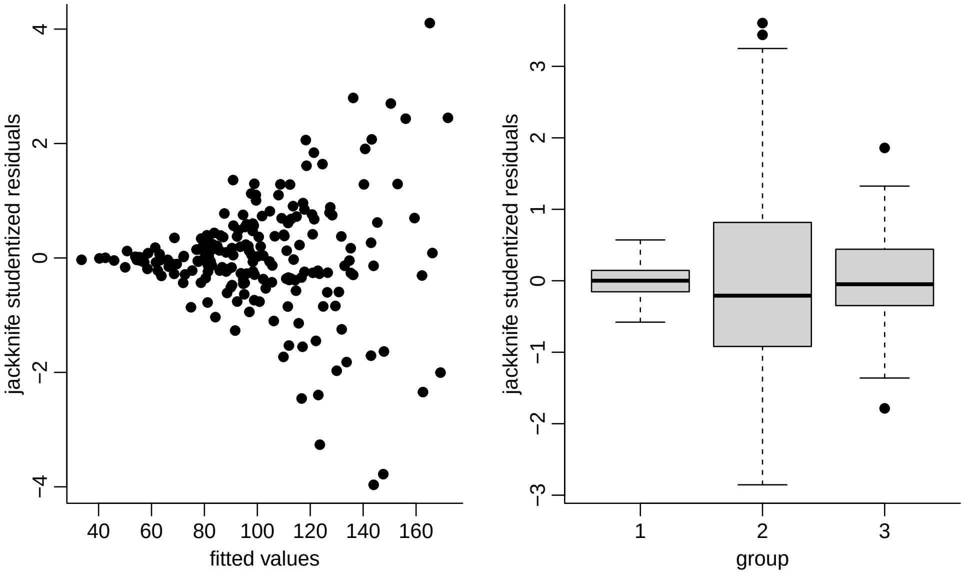


Figure 4.15: Plot of jackknife studentized residuals against fitted value (left) and categorical explanatory (right). Both clearly display heteroscedasticity.

An obvious extension of the linear model is to allow variance to vary according to explanatories, typically categorical covariates. In a likelihood framework, this is easy to do and we will cover this approach in more detail.

We can perform hypothesis tests for the homogeneity (equal) variance assumption. The most commonly used tests are Bartlett's test, the likelihood ratio test under the assumption of normally distributed data, with a Bartlett correction to improve the χ^2 approximation to the null distribution. The second most popular is Levene's test (a more robust alternative, less sensitive to outliers). For both tests, the null distribution is $\mathscr{H}_0 : \sigma_1^2 = \cdots = \sigma_K^2$ against the alternative that at least two differ. The Bartlett test statistic has a χ^2 null distribution with $K-1$ degrees of freedom, whereas Levene's test has an F-distribution with ($K-1$, $n-K$) degrees of freedom: it is equivalent to computing the one-way ANOVA F-statistic with the absolute value of the centered residuals, $|y_{ik} - \widehat{\mu}_k|$, as observations.

What are the impacts of unequal variance if we use the F-test instead? For one, the pooled variance will be based on a weighted average of the variance in each group, where the weight is a function of the sample size. This can lead to size distortion (meaning that the proportion of type I error is not the nominal level α as claimed) and potential loss of power. The following toy example illustrates this.

Example 4.10 (Violation of the null hypothesis of equal variance)**.**

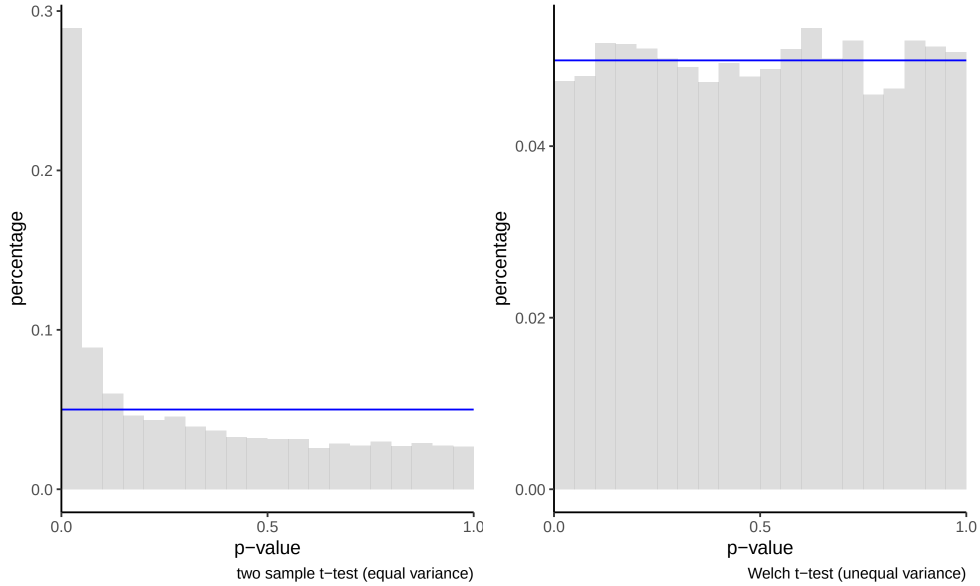


Figure 4.16: Histogram of the null distribution of p-values obtained through simulation using the classical analysis of variance F-test (left) and Welch's unequal variance alternative (right), based on 10 000 simulations. Each simulated sample consist of 50 observations from a $\mathsf{Normal}(0,1)$ distribution and 10 observations from $\mathsf{Normal}(0,9)$. The uniform distribution would have 5% in each of the 20 bins used for the display.

We consider for simplicity a problem with $K=2$ groups, which is the two-sample t-test. We simulated 50 observations from a $\mathsf{Normal}(0,1)$ distribution and 10 observations from $\mathsf{Normal}(0,9)$, comparing the distribution of the p-values for the Welch and the F-test statistics. Figure 4.16 shows the results. The percentage of p-values less than $\alpha=0.05$ based on 10 000 replicates is estimated to be 4.76% for the Welch statistic, not far from the level. By contrast, we reject 28.95% of the time with the one-way ANOVA global F-test: this is a large share of innocents sentenced to jail based on false premises! While the size distortion is not always as striking, heterogeneity should be accounted in the design by requiring sufficient sample sizes (whenever costs permits) in each group to be able to estimate the variance reliably and using an adequate statistic.

There are alternative graphical ways of checking the assumption of equal variance, many including the standardized residuals $r_{ik}=(y_{ik}-\widehat{\mu}_k)/\widehat{\sigma}$ against the fitted values $\widehat{\mu}_k$. We will cover these in later sections.

Oftentimes, unequal variance occurs because the model is not additive. You could use variance-stabilizing transformations (e.g., log for multiplicative effects) to ensure approximately equal variance in each group. Another option is to use a model that is suitable for the type of response you have (including count and binary data). Lastly, it may be necessary to explicitly model the variance in more complex design (including repeated measures) where there is a learning effect over time and variability decreases as a result. Consult an expert if needed.

4.6.4 Normality assumption

The normality assumption is mostly for convenience: if the errors are assumed normally distributed, then the least square and the maximum likelihood estimators of $\boldsymbol{\beta}$ coincide. The maximum likelihood estimators of $\boldsymbol{\beta}$ are asymptotically normal under mild conditions on the model matrix and t-tests are surprisingly robust and unaffected by departure from the normality assumption. This means that inference is valid in large samples, regardless of the distribution of the errors/residuals (even if the null distribution are not exact). It is important to keep in mind that, for categorical explanatory variables, the sample size in each group must be sufficiently large for the central limit theorem to kick in since coefficients represent group average.

Sometimes, transformations can improve normality: if the data is right-skewed and the response is strictly positive, a log-linear model may be more adequate Section 4.7.1. This can be assessed by looking at the quantile-quantile plot of the externally studentized residuals. If the response Y is not continuous (including binary, proportion or count data), linear models give misleading answers and generalized linear models are more suitable.

The inference will be valid for large samples even if the errors are not normally distributed by virtue of the central limit theorem. If the errors $\varepsilon_i \sim \mathsf{normal}(0, \sigma^2)$, then the jacknnife studentized residuals should follow a Student distribution, with $r_i \sim \mathsf{Student}(n-p-2)$, (identically distributed, but not independent). A Student quantile-quantile plot can thus be used to check the assumption (and for n large, the normal plotting positions could be used as approximation if $n-p > 50$). One can also plot a histogram of the residuals. Keep in mind that if the mean model is not correctly specified, some residuals may incorporate effect of leftover covariates.

Quantile-quantile plots are discussed in Definition 1.16 but their interpretation requires training. For example, Figure 4.18 shows many common scenarios that can be diagnosed using quantile-quantile plots: discrete data is responsible for staircase patterns, positively skewed data has too high low quantiles and too low high quantiles relative to the plotting positions, heavy tailed data have high observations in either tails and bimodal data leads to jumps in the plot.

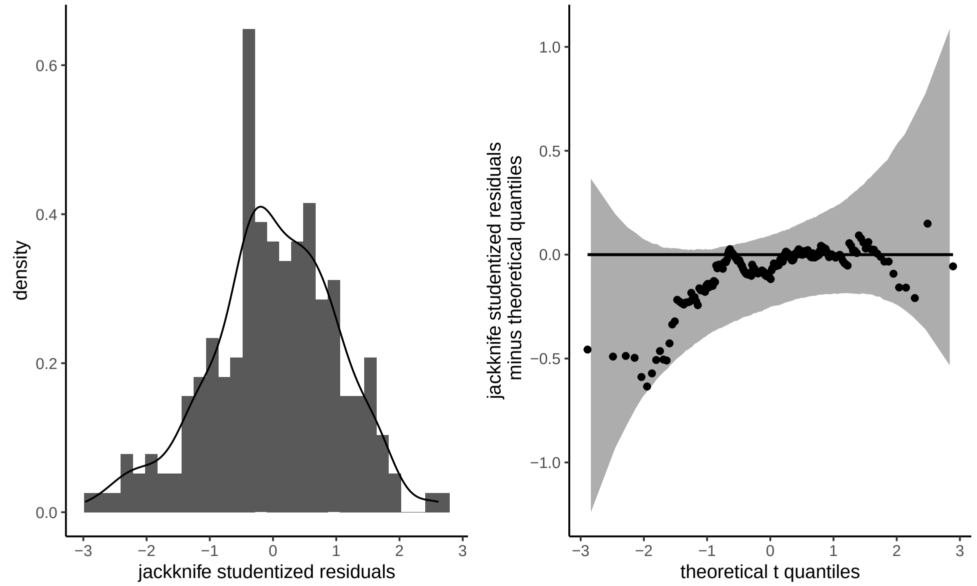


Figure 4.17: Histogram (left) and Student quantile-quantile plot (right) of the jackknife studentized residuals. The left panel includes a kernel density estimate (black), with the density of Student distribution (blue) superimposed. The right panel includes pointwise 95% confidence bands calculated using a bootstrap.

Example 4.11 (Diagnostic plots for the `college` data.)**.** We can look at the `college` data to see if the linear model assumptions hold.

Based on the plots of Figure 4.19, we find that there is residual heteroscedasticity, due to rank. Since the number of years in the first rank is limited and all assistant professors were hired in the last six years, there is less disparity in their income. It is important not to mistake the pattern on the x-axis for the fitted value (due to the large effect of rank and field, both categorical variable) with patterns in the residuals (none apparent). Fixing the heteroscedasticity would correct the residuals and improve the appearance of the quantile-quantile plot.

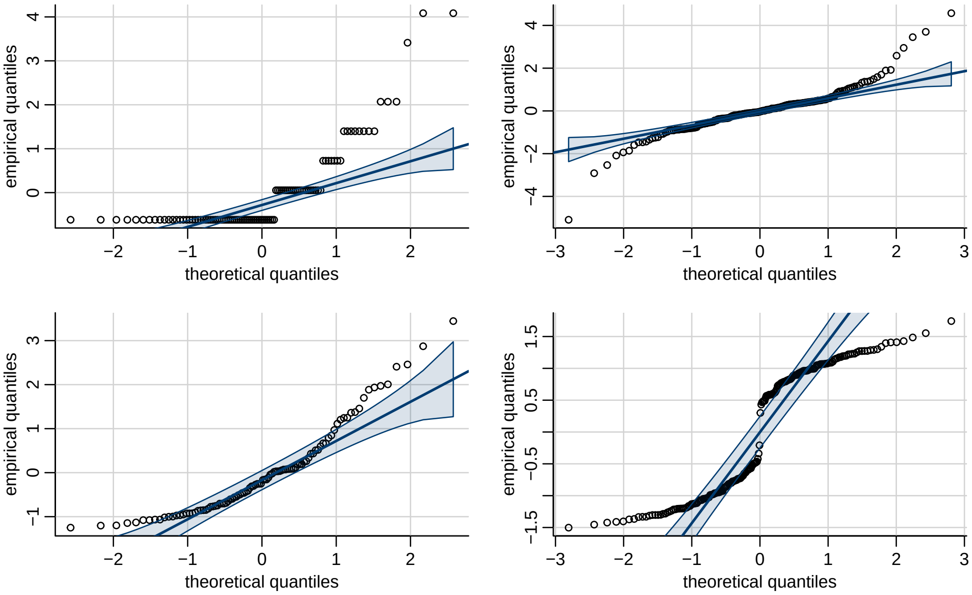


Figure 4.18: Quantile-quantile plots of non-normal data, showing typical look of behaviour of discrete (top left), heavy tailed (top right), skewed (bottom left) and bimodal data (bottom right).

4.7 Extensions of the model

4.7.1 Transformation of the response

If the response is strictly positive, there are some options that can alleviate lack of additivity, more specifically multiplicative mean-variance relationships.If the data is right-skewed and the response is strictly positive, a log-linear model may be more adequate and the parameters can be interpreted. Theory sometimes dictates a multiplicative model: for example, the Cobb–Douglas production function in economics is $P = \alpha L^{\beta_1} C^{\beta_2}$, where P stands for production, L for labor and C for capital; all inputs are positive, so taking a log-transform yields a model that is linear in β, with $\beta_0 = \ln(\alpha)$.

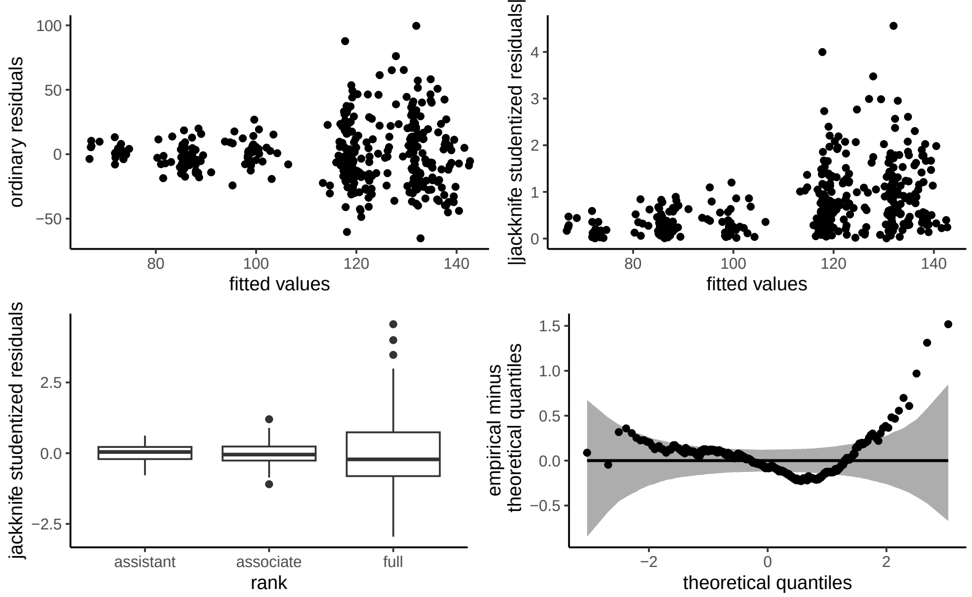


Figure 4.19: Diagnostic plots for the college data example: ordinary residuals against fitted values (top left), absolute value of the jacknnife studentized residuals against fitted values (top right), box and whiskers plot of jacknnife studentized residuals (bottom left) and detrended Student quantile-quantile plot (bottom right). There is clear group heteroscedasticity.

We can rewrite the log-linear model in the original response scale as

$$\begin{aligned} Y &= \exp\left(\beta_0 + \sum_{j=1}^{p} \beta_j X_j + \varepsilon\right) \\ &= \exp\left(\beta_0 + \sum_{j=1}^{p} \beta_j X_j\right) \cdot \exp(\varepsilon), \end{aligned}$$

and thus

$$\mathsf{E}(Y \mid \mathbf{X}) = \exp(\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p) \times \mathsf{E}\{\exp(\varepsilon) \mid \mathbf{X}\}.$$

If $\varepsilon \mid \mathbf{X} \sim \mathsf{normal}(\mu, \sigma^2)$, then $\mathsf{E}\{\exp(\varepsilon) \mid \mathbf{X}\} = \exp(\mu + \sigma^2/2)$ and $\exp(\varepsilon)$ follows a log-normal distribution.

An increase of one unit of X_j leads to a β_j increase of $\ln Y$ without interaction or nonlinear term for X_j, and this translates into a multiplicative increase of a factor $\exp(\beta_j)$ on the original data scale for Y. Indeed, we can compare the ratio of $\mathsf{E}(Y \mid X_1 = x+1)$ to $\mathsf{E}(Y \mid X_1 = x)$,

$$\frac{\mathsf{E}(Y \mid X_1 = x+1, X_2, \ldots, X_p)}{\mathsf{E}(Y \mid X_1 = x, X_2, \ldots, X_p)} = \frac{\exp\{\beta_1(x+1)\}}{\exp(\beta_1 x)} = \exp(\beta_1).$$

Thus, $\exp(\beta_1)$ represents the ratio of the mean of Y when $X_1 = x+1$ in comparison to that when $X_1 = x$, *ceteris paribus* (and provided this statement is meaningful). If $\beta_j = 0$, the multiplicative factor one is the identity, whereas negative values of the regression coefficient $\beta_j < 0$ leads to $\exp(\beta_j) < 1$. The percentage change is $1 - \exp(\beta_j)$ if $\beta_j < 0$ and $\exp(\beta_j) - 1$ if $\beta_j > 0$

Sometimes, we may wish to consider a log transformation of both the response and some of the continuous positive explanatories, when this make sense (a so-called log-log model). Consider the case where both Y and X_1 is log-transformed, so the equation for the mean on the original data scale reads

$$Y = X_1^{\beta_1}\exp(\beta_0 + \beta_2 X_2 + \cdots + \beta_p X_p + \varepsilon)$$

Taking the derivative of the left hand side with respect to $X_1 > 0$, we get

$$\begin{aligned}\frac{\partial Y}{\partial X_1} &= \beta_1 X_1^{\beta_1 - 1}\exp(\beta_0 + \beta_2 X_2 + \cdots + \beta_p X_p + \varepsilon)\\ &= \frac{\beta_1 Y}{X_1}\end{aligned}$$

and thus we can rearrange the expression so that

$$\frac{\partial X_1}{X_1}\beta_1 = \frac{\partial Y}{Y};$$

this is a partial **elasticity**, so β_1 is interpreted as a β_1 percentage change in Y for each percentage increase of X_1, *ceteris paribus*.

Example 4.12 (Log-log model)**.** Consider for example the Cobb–Douglas production function (Douglas 1976), which specifies that economic output Y is related to labour L and capital C via $\mathsf{E}(Y \mid L, C) = \beta_0 C^{\beta} L^{1-\beta}$ with $\beta \in (0,1)$. If we take logarithms on both sides (since all arguments are positive), then $\mathsf{E}(\ln Y \mid L, C) = \beta_0^* + \beta_1 \ln C + (1-\beta_1)\ln L$. We could fit a linear model with response $\ln Y - \ln L$ and explanatory variable $\ln C - \ln L$, to obtain an estimate of the coefficient β_1, while $\beta_0^* = \ln \beta_0$. A constrained optimization would be potentially necessary to estimate the model parameters of the resulting linear model if the estimates lie outside of the parameter space.

Proposition 4.4 (Box–Cox transformation)**.** *If the data are strictly positive, one can consider a Box–Cox transformation,*

$$y(\lambda) = \begin{cases} (y^\lambda - 1)/\lambda, & \lambda \neq 0 \\ \ln(y), & \lambda = 0. \end{cases}$$

The cases $\lambda = -1$ (inverse), $\lambda = 1$ (identity) and $\lambda = 0$ (log-linear model) are perhaps the most important because they yield interpretable models.

If we assume that $\boldsymbol{Y}(\lambda) \sim \mathsf{normal}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I}_n)$, then the likelihood is

$$L(\lambda, \boldsymbol{\beta}, \sigma; \boldsymbol{y}, \mathbf{X}) = (2\pi\sigma^2)^{-n/2} J(\lambda, \boldsymbol{y}) \times \\ \exp\left[-\frac{1}{2\sigma^2}\{\boldsymbol{y}(\lambda) - \mathbf{X}\boldsymbol{\beta}\}^\top\{\boldsymbol{y}(\lambda) - \mathbf{X}\boldsymbol{\beta}\}\right],$$

where J denotes the Jacobian of the Box–Cox transformation, $J(\lambda, \boldsymbol{y}) = \prod_{i=1}^n y_i^{\lambda-1}$. For each given value of λ, the maximum likelihood estimator is that of the usual regression model, with $\boldsymbol{y}$ replaced by $\boldsymbol{y}(\lambda)$, namely $\widehat{\boldsymbol{\beta}}_\lambda = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\boldsymbol{y}(\lambda)$ and $\widehat{\sigma}^2_\lambda = n^{-1}\{\boldsymbol{y}(\lambda) - \mathbf{X}\widehat{\boldsymbol{\beta}}_\lambda\}^\top\{\boldsymbol{y}(\lambda) - \mathbf{X}\widehat{\boldsymbol{\beta}}_\lambda\}$.

The profile log likelihood is

$$\ell_{\mathsf{p}}(\lambda) = -\frac{n}{2}\ln(2\pi\widehat{\sigma}^2_\lambda) - \frac{n}{2} + (\lambda - 1)\sum_{i=1}^n \ln(y_i)$$

The maximum profile likelihood estimator is the value λ minimizes the sum of squared residuals from the linear model with $\boldsymbol{y}(\lambda)$ as response.

The Box–Cox is not a panacea and should be reserved to cases where the transformation reduces heteroscedasticity (unequal variance) or creates a linear relation between explanatories and response: theory provides a cogent explanation of the data. Rather than an ad hoc *choice of transformation, one could choose a log transformation if the value 0 is included within the 95% confidence interval since this improves interpretability.*

Example 4.13 (Box–Cox transform for the `poison` data)**.** Box and Cox (1964) considered survival time for 48 animals based on a randomized trial; these data are analyzed in Example 8.25 of Davison (2003). Three poisons were administered with four treatments; each factor combination contained four animals, chosen at random. There is strong evidence that both the choice of poison and treatment affect survival time.

We could consider a two-way analysis of variance model for these data without interaction, given the few observations for each combination. The model would be of the form

$$Y = \beta_0 + \beta_1\texttt{poison}_2 + \beta_2\texttt{poison}_3 + \beta_3\texttt{treatment}_2 \\ + \beta_4\texttt{treatment}_3 + \beta_5\texttt{treatment}_4 + \varepsilon$$

The plot of fitted values against residuals shows that the model is not additive; there is also indications that the variance increases with the mean response. The model is inadequate: lowest survival times are underpredicted, meaning the residuals are positive and likewise the middle responses is positive. A formal test of non-additivity based on constructed variables further point towards non-additivity (Davison 2003, Example 8.24). Overall, the model fit is poor and any conclusion drawn from it dubious.

One could consider using a Box–Cox to find a suitable transformation of the residuals so as to improve normality. The profile log likelihood at the bottom left of Figure 4.20 suggests that $\lambda \approx -1$ would be a good choice. This has the benefit of being interpretable, as the reciprocal response Y^{-1} corresponds to the speed of action of the poison depending on both poison type and treatment. The diagnostics plots also indicate that the model for the reciprocal has no residual structure and the variance appears constant.

4.8 Concluding remarks

Linear regression is the most famous and the most widely used statistical model around. The name may appear reductive, but many tests statistics (t-tests, ANOVA, Wilcoxon, Kruskal–Wallis) can be formulated using a linear regression, while models as diverse as trees, principal components and deep neural networks are just linear regression model in disguise. What changes under the hood between one fancy model to the next are the optimization method (e.g., ordinary least squares, constrained optimization or stochastic gradient descent) and the choice of explanatory variables entering the model (spline basis for nonparametric regression, indicator variable selected via a greedy search for trees, activation functions for neural networks).

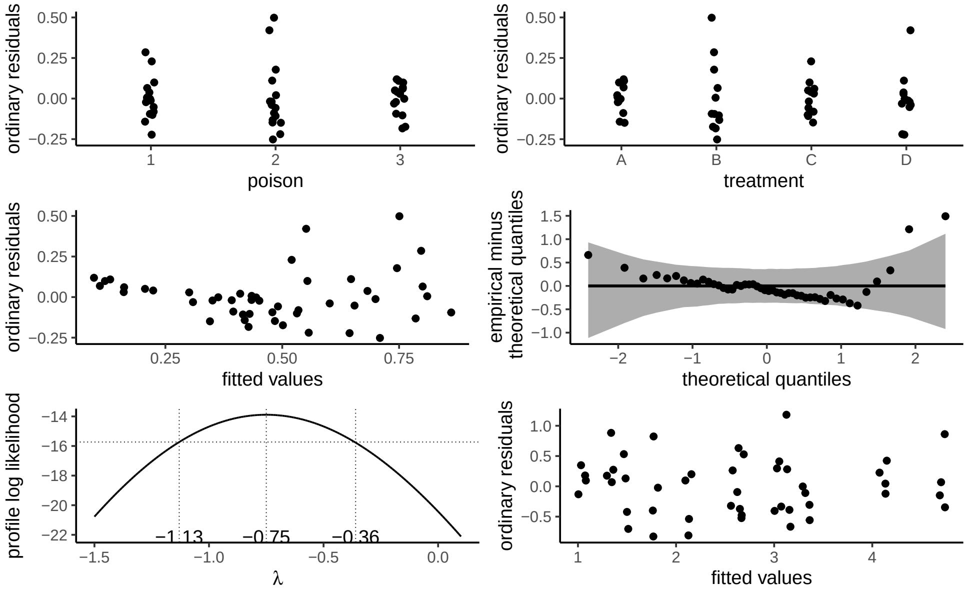


Figure 4.20: Diagnostic plots for the poison data. The top panel shows the ordinary residuals for the linear model for survival time as a function of poison and treatment, with jittered observations. The middle left plot shows the fitted values against residuals, which display evidence of trend and increase in variance with the survival time. The quantile-quantile plot in the middle right plot shows some evidence of departure from the normality, but the non-linearity and heteroscedasticity obscure this. The bottom panel shows the profile log likelihood for the Box–Cox transform, suggesting a value of -1 would be within the 95% confidence interval. After fitting the same additive model with main effect only to the reciprocal survival time, there is no more evidence of residual structure and unequal variance.

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