AN INTRODUCTION TO
INDUCTIVE STATISTICAL INFERENCE
FROM PARAMETER ESTIMATION TO DECISION-MAKING

Lecture notes for a quantitative–methodological module at the Master degree (M.Sc.) level

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at Karlshochschule
Abstract

These lecture notes aim at a post-Bachelor audience with a background at an introductory level in Applied Mathematics and Applied Statistics. They discuss the logic and methodology of the Bayes–Laplace approach to inductive statistical inference that places common sense and the guiding lines of the scientific method at the heart of systematic analyses of quantitative–empirical data. Following an exposition of exactly solvable cases of single- and two-parameter estimation, the main focus is laid on Markov Chain Monte Carlo (MCMC) simulations on the basis of Gibbs sampling and Hamiltonian Monte Carlo sampling of posterior joint probability distributions for regression parameters occurring in generalised linear models. The modelling of fixed as well as of varying effects (varying intercepts) is considered, and the simulation of posterior predictive distributions is outlined. The issues of model comparison with Bayes factors and the assessment of models’ relative posterior predictive accuracy with information entropy-based criteria DIC and WAIC are addressed. Concluding, a conceptual link to the behavioural subjective expected utility representation of a single decision-maker’s choice behaviour in static one-shot decision problems is established. Codes for MCMC simulations of multi-dimensional posterior joint probability distributions with the JAGS and Stan packages implemented in the statistical software R are provided. The lecture notes are fully hyperlinked. They direct the reader to original scientific research papers and to pertinent biographical information.

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Introductory remarks

Contemporaries of the 21st Century find themselves exposed to flows of information of unprecedented current strengths. In an incredibly diverse spectrum of walks of life, the volumes of data amassed as a consequence of the steadily progressing digital transformation have gradually attained astronomically huge dimensions. Given this state of affairs, a legitimate question arising to an enquiring mind is to whether or not, and, if answered in the affirmative, to what extent this societal process ought to have any bearings on one’s aspired academic training?

Though in view of present-day global developments in, foremost, business and communication it is quite plausible to question the future status of the English language as the world’s lingua franca in, say, five decades from now, it is with near certainty that the minimum level of statistical literacy required to keep up with the demands and expectations in one’s professional life will continue to rise. Moreover, the challenge of handling successfully the complexity of such pressing issues of humanity as planet Earth’s attested climate change and the need to maintain its habitability by practising a sustainable economic use of its natural resources makes systematic processing of information a valuable and much-sought intellectual skill. Not disregarding complementary methodological tools, conscientious and sense-inducing communal decision-making in information-heavy managerial contexts is likely to benefit from a sound technical training in the principles of statistical methods of data analysis of citizens aiming to assume positions with a certain degree of responsibility attached to them.

In the course of social interactions experienced by the generations of people living during the last few centuries and up to now, pursuing the scientific method has proven beyond doubt to be the most reliable human approach to satisfactory problem-solving. That is, given at hand a practical or theoretical problem of some urgency, forming one’s viewpoint on the basis of available factual information, and re-evaluating it in the light of relevant new evidence in order to draw conclusions as to reasonable subsequent action, defines a systematic inductive procedure of compelling resilience. As this technique constitutes a valid operationalisation of a notion of acting by common sense, it has the potential to increase both idealistic as well as overall economic value for the human community when transferred as a guiding principle for advancing matters to a wider field of socially important domains. There surely exists an obligation to hedge against a currently prevailing tendency of decision-making based on “alternative facts,” as the quality of the ensuing consequences and outcomes for the vast majority of people affected is self-evident.

Coles (2006) [12, p 3] paraphrases the prime objective of the scientific endeavour by reminiscing:

“When I started doing research it gradually dawned on me that if science is about anything at all, it is not about being certain but about dealing rigorously with uncertainty.”
The immediate implication of this viewpoint is that the actual issue one finds oneself confronted with when trying to make inferences from necessarily incomplete information is to have available a coherent and logically consistent framework for capturing and systematically processing fundamental uncertainty, which is interpreted in a scientific setting as representing the researcher’s state of knowledge concerning the problem of her/his interest.

It comes across as a somewhat irritating piece of historical irony in the evolution of the empirical sciences that the principles of such a calculus of “reasonable expectation” (according to Cox (1946) [13]) had been fully worked out halfway through the 20th Century, but were largely ignored by the majority of active empirical researchers until lately. Lasting contributions to its methodology emerged from the predominantly data-driven scientific disciplines of Physics, Astronomy, Anthropology, Biology, Economics, Psychology, Political Science and Statistics. For the sake of the uninitiated reader, a few brief historical comments are in order.

Arguably the history of the development of a framework of inductive statistical inference from past to present can be grouped into the following four periods:

- **pioneering period**: the foundations of the framework of inductive statistical inference were laid independently during the 18th Century by the English mathematician and Presbyterian minister Thomas Bayes (1702–1761) and the French mathematician and astronomer Marquis Pierre Simon de Laplace (1749–1827); see Bayes (1763) [6] and Laplace (1774) [62]. The latter of these two is credited for giving a full mathematical formulation of probability theory which presupposes prior information on the plausibilities of outcomes in a set of different possibilities, and how to update these plausibilities in the light of relevant new evidence.

- **conceptual period**: during the first half of the 20th Century the British economist John Maynard Keynes CB FBA (1883–1946), the British mathematician, statistician, geophysicist, and astronomer Sir Harold Jeffreys FRS (1891–1989), and the Italian probabilist statistician and actuary Bruno de Finetti (1906–1985) argued strongly that a concept of probability can only be meaningful when it relates to the states of knowledge of individuals, and so inherently bears a certain dimension of subjectivity. Their views are condensed in the classical monographs by Keynes (1921) [55] and Jeffreys (1939) [50], and the seminal paper by de Finetti (1937) [27]. The conceptual work of these authors was propagated in particular by the US-American physicist Edwin Thompson Jaynes (1922–1998) who supplemented it by a compelling interpretation of probability theory as extended logic; cf. Jaynes (2003) [48].

- **engineering period**: this period, which roughly started during the mid-1980ies, is characterised by the development of powerful algorithms for numerically simulating complicated multi-dimensional distribution functions using Markov Chain Monte Carlo (MCMC) and Hamiltonian Monte Carlo (HMC) techniques, and their stable and efficient implementation in standard statistical software; see, e.g., Geman and Geman (1984) [36], Duane et al (1987) [18], Gelfand and Smith (1990) [31], Lunn et al (2000) [66], or Plummer (2017) [84].

- **big data period**: the present period, when it has become commonplace to process large amounts of data, often in a machine learning context (see, e.g., Ng (2018) [76]).
Data sets, high-speed algorithms and other supporting material are shared by online communities such as the one active on the platform GitHub (github.com), or the Stan Development Team (mc-stan.org). A central objective of many efforts in this area is the performance of predictive analytics in a diverse field of applications. Associated with this focus is a continued interest in the possibilities of artificial intelligence; cf., e.g., Penrose (1989) [81].

Until quite recently, the dominant methodological paradigm for quantitative–empirical research work has been the frequentist approach to data analysis and statistical inference, the most prominent proponent of which was the English statistician, evolutionary biologist, eugenicist and geneticist Sir Ronald Aylmer Fisher FRS (1890–1962); cf. Fisher (1935) [28]. From the present perspective it appears as though Fisher had a rather strong influence on the sociology of the academic community in Statistics for most of the first half of the 20th Century; see, e.g., the insightful and revealing recount of statistics training in academic physics education by Jaynes(2003) [48, Sec. 10.2]. Fisher, having been a fierce opponent to the inductive statistical inference framework advocated by his contemporaries Jeffreys and Keynes, is generally assigned the authorship of the (originally intended as derogatory) term “Bayesian Statistics.” At the time, the leading figures of this framework referred to it instead as “inverse probability;” see Jeffreys (1939) [50, p 28] and Stigler (1986) [96, p 101]. The frequentist approach was outlined in the lecture notes [22].

The realisation for a need of a systematic rethinking of standard practices in statistical methodology has been heavily boosted during the last decade by recurrent problems of successfully reproducing published results in the research literature, foremost in the Social Sciences. Explicit examples are given, e.g., in Gill (1999) [38], who discusses the abundant but unreliable practice of null hypothesis significance testing in Political Science, in an article published by The Economist (2013) [19], in Nuzzo (2014) [77], and in some recent blog entries by, amongst others, Vasishth (2017) [104] or by Papineau (2018) [78]. Also Kruschke and Liddell (2017) [60] and Briggs (2012) [9] address this and other related conceptual difficulties with the frequentist approach. The worrisome fact of regularly failing reproduction attempts of proclaimed empirical effects has come to be known by the name of “replication crisis in science.”

In reflection of the massively increased interest in the Bayes–Laplace approach to data analysis and statistical inference since the last turn of the centuries, and in recognition of its undeniable track record of successes in all areas of quantitative–empirical investigation over the last few decades, there exists a plethora of recently published state-of-the-art textbooks. In chronological order, these comprise Sivia and Skilling (2006) [92], who focus on applications in Physics, Albert (2009) [2], Lee (2012) [63], Greenberg (2013) [41], who outlines uses in Econometrics, Gelman et al (2014) [35], which the community of applied statisticians considers to be the authoritative monograph in the field, Andreon and Weaver (2015) [4], giving explicit examples from statistical modelling in Astrophysics, Gill (2015) [39], who presents applications in the Social and Behavioural Sciences, Kruschke (2015) [58], with case studies from Biology, Psychology, Sociology and Sports, and McElreath (2016) [68], who establishes a link to interesting quantitative

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1In the context of recent developments in artificial intelligence, the video documentation of the conversion between Sir Roger Penrose and the advanced robot Sophia on YouTube provides some interesting insight. URL (cited on June 22, 2018): www.youtube.com/watch?v=YUt1FzQzZ0
Almost all of these textbooks provide an abundance of practical problems and exercises, generally in combination with fully operational codes implemented in the shareware statistical software packages R, JAGS and/or Stan.

The methods presented in these lecture notes are rooted in **Applied Statistics**. They address an audience at a post-Bachelor academic level, with a vested interest in acquainting themselves with standard pracitives of modern **statistical methods of data analysis**. The topics presented form a selection of the most frequently employed tools for building data-based **statistical models** for purposes of explanation and prediction of observable phenomena. These comprise in particular:

- **single-parameter estimation**, 
- fitting multi-dimensional **generalised linear models** employing MCMC simulations. 
- **model comparison**, and 
- elementary **decision-making** under conditions of uncertainty.

As implicitly hinted at above, we here deliberately assume an **interdisciplinary perspective**, being thoroughly convinced that the chances for successfully dealing with most kinds of modern-day problems of societal relevance will not be reasonably improved by confining one’s efforts to a possibly comfortable though narrow-minded intellectual niche.

There are **not** included in these lecture notes any explicit examples or exercises on the topics to be discussed. These are reserved for the lectures given throughout term time.

The present lecture notes are designed to be dynamical in character. On the one-hand side, this means that they will be updated on a regular basis. On the other, that its *.pdf version contains interactive features such as fully hyperlinked references to original publications at the websites [doi.org](http://doi.org), [jstor.org](http://jstor.org), or elsewhere, and also many active links to biographical information on scientists that have been influential in the historical development of **probability theory** and the **Bayes–Laplace approach to data analysis and statistical inference**, hosted by the websites [The MacTutor History of Mathematics archive](http://www-history.mcs.st-and.ac.uk) and [en.wikipedia.org](http://en.wikipedia.org).

Opting for the application of the **Bayes–Laplace approach to data analysis and statistical inference** entails the frequent performance of a large number of computations and numerical simulations, which, to ensure reliability, need to be meticulously checked for potential errors. However, these computations are an integral part of the fun of the research activity, and they are enormously facilitated by the provision of taylor-made software packages that are distributed as shareware on the internet. A widespread computational tool that we, too, will refer to in the course of these lecture notes is the statistical software package R. This can be obtained free of charge for many different operating systems from [cran.r-project.org](http:// cran.r-project.org). Useful and easily accessible introductory textbooks on the application of R for purposes of statistical data analysis are, e.g., Dalgaard (2008) [14], or Hatzinger et al (2014) [44]. Additional helpful information and assistance is available from the website [www.r-tutor.com](http://www.r-tutor.com). We strongly recommend the use of the convenient custom-made work environment **R Studio** provided at [www.rstudio.com](http://www.rstudio.com). Also, we point the

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2 Trotta’s (2008) [102] review discusses applications of the Bayes–Laplace approach in the cosmological context.
reader to an overview of R tools made available for Bayes–Laplace statistical inference which is maintained by Park; cf. Park (2018) [80]. Notation to be used follows the conventions of Refs. [22] and [23].
Chapter 1

Mathematical rules of probability theory

1.1 Probability and uncertainty

Jaynes (2003) [48], in his influential monograph, conceptualises probability theory as an extension of Aristotelian deductive logic. In the latter discipline, the objects of investigation are propositions. Propositions can be verbal statements that relate to some observable real-world phenomenon of a certain practical interest, or they can be suppositions in the context of an academic discourse. For instance, the assertions

\[ A: \text{The average travel time for human space missions from planet Earth to a like planet in the Andromeda Galaxy ranges between four and five hours.} \]

\[ B: \text{Prince Rogers Nelson was a US-American musician.} \]

\[ C: \text{The German team will win the next Cricket World Cup.} \]

are representative of simple kinds of propositions. In Aristotelian deductive logic, the truth content of a proposition can be exclusively either true or false, and so in this respect this specific logic is inherently two-valued in nature.

Employing Boolean algebra\(^2\), two propositions \( A \) and \( B \) can be combined to form a new proposition via

(i) the logical product (or mutual conjunction),

\[ AB : \text{“both of the propositions} \ A \ \text{and} \ B \ \text{are true”;} \quad (1.1) \]

note that naturally \( AB = BA \) applies, i.e., commutativity is a property of the product operation, and

(ii) the logical sum (or mutual disjunction),

\[ A + B : \text{“at least one of the propositions} \ A \ \text{and} \ B \ \text{is true”;} \quad (1.2) \]

again, naturally commutativity holds true for the sum operation, \( A + B = B + A \).

\(^1\)Named after the ancient Greek philosopher and scientist Aristotle (384 BC–322 BC).

\(^2\)Named after the English mathematician, educator, philosopher and logician George Boole (1815–1864).
More complex propositions still can be constructed by combining different propositions with both the logical product and the logical sum, and making use of bracketing sub-operations, i.e., inserting (…) where intended or needed.

With \( \overline{A} \) denoting the **logical complement** of some proposition \( A \) (referred to as “not \( A \)”), it follows that

\[
A \overline{A} \quad \text{is always false} \quad \text{(a contradiction)} \\
A + \overline{A} \quad \text{is always true} \quad \text{(a tautology)}
\]

Moreover, the logical identities

\[
AA = A \\
A + A = A
\]

apply. Of particular practical use are **De Morgan’s laws**\(^3\) which state that

\[
\overline{AB} = \overline{A} + \overline{B} \\
\overline{A + B} = \overline{A} \overline{B}
\]

Negating the latter relation yields

\[
A + B = \overline{AB}
\]

a result that is to be used later on.

Jaynes’ (2003) \(^{[48]}\) notion of an **extended logic** comes into effect by relaxing the strict demand for the binary truth content property of a proposition, but rather to assign to it a normalised **degree of plausibility**\(^4\) which depends on a researcher’s individual **state of knowledge** on the current matter of interest. This is to say that, subject to available background information collectively denoted by \( I \), a real number \( P(\ldots | I) \) from the interval \([0, 1]\) is assigned to a proposition which is referred to as its **probability**\(^5\). The \( I \)-proviso here serves to express the position that, by way of conception, a **probability** is always conditional on some form of **prior information**, see Jaynes (2003) \(^{[48]}\) p 87] and Sivia and Skilling (2006) \(^{[92]}\) p 5, or, as Keynes (1921) \(^{[55]}\) p 102] puts it, “relative to given premisses.”

To link back to the three example propositions introduced above, one may thus assign on the basis of presently available understanding the (prior) probabilities

\[
P(A|I_A) = 0, \text{ expressing a logical resp. practical impossibility},
\]

\[
P(B|I_B) = 1, \text{ expressing a logical resp. practical certainty}, \text{ and}
\]

\[
0 \leq P(C|I_C) \leq 1, \text{ expressing a logical resp. practical possibility of which the attributed degree of plausibility is considered limited.}
\]

---

3 Named after the British mathematician and logician [Augustus De Morgan (1806–1871)](https://en.wikipedia.org/wiki/Augustus_De_Morgan).

4 In decision theory, the “degree-of-belief” assigned by a rational agent to a certain outcome established itself as standard terminology.

5 The exploration of the psychological dimension underlying the assignment of probabilities to propositions was pioneered by Kahneman and Tversky (1972) \(^{[52]}\).
1.2. SUM AND PRODUCT RULES

In view of the interpretation of a probability as a researcher’s systematic way of handling practical situations with incomplete information (which, typically, is more often the case than not), it proves of little help to try to associate any physical reality with the corresponding numerical value from the interval \([0, 1]\). Rather, it constitutes a specific proposal for dealing with uncertainty within a logically consistent and coherent quantitative framework, the basic rules of which are to be described in the following. Indeed, it comes as a bit of a surprise, and a veritable manifestation of formal elegance, that the probabilistic calculus for plausible reasoning originated by Bayes and Laplace rests on the foundation of only a few rather simple first principles.

1.2 Sum and product rules

1.2.1 Sum rule

For probabilities assigned to a proposition \(A\) and its logical complement \(\overline{A}\), the **sum rule** states that

\[
P(A|I) + P(\overline{A}|I) = 1
\]  

must always be true.

1.2.2 Product rule

To calculate the probability of the logical product of two propositions, \(AB\), the **product rule** holds that

\[
P(AB|I) = P(A|BI)P(B|I) = P(B|AI)P(A|I) = P(BA|I),
\]

taking into account commutativity of the product operation, \(AB = BA\), in the second part of this rule.

Re-arranging, and assuming that \(P(A|I) > 0\) resp. \(P(B|I) > 0\) apply, alternative representations of the product rule are given by

\[
P(A|BI) = \frac{P(AB|I)}{P(B|I)}, \quad P(B|AI) = \frac{P(BA|I)}{P(A|I)}.
\]

The first variant is generally referred to as the **conditional probability** of proposition \(A\), given proposition \(B\) is true and relevant background information \(I\) is available. Analogously, the second variant expresses the **conditional probability** of proposition \(B\), given proposition \(A\) is true and \(I\) is known.

In preparation of concepts of importance in subsequent chapters, it is fitting at this stage to briefly raise the following point. The quantity \(P(AB|I)\) [or \(P(BA|I)\)] occurring in the product rule (1.11) represents the **joint probability** for propositions \(A\) and \(B\), given background information \(I\). It is instructive to formally supplement \(A\) and \(B\) by their logical complements, \(\overline{A}\) and \(\overline{B}\), and to represent the **joint probabilities** for all possible product combinations of these propositions, given \(I\),

\[\text{[Philosophical viewpoints opposing the idea of uncertainty being amenable to treatment within a quantitative framework have been put forward nearly a full century ago by Knight (1921) }^{[56]} \text{ and by Keynes (1921) }^{[55]}\]
Table 1.1: Representation of a discrete (prior) joint probability distribution and corresponding discrete marginal probability distributions for propositions $A$ and $B$ and their logical complements $\overline{A}$ and $\overline{B}$, given background information $I$, in terms of a $2 \times 2$ contingency table. The marginal cell entries are obtained by row-wise resp. column-wise summation over associated interior cell entries while respecting the sum rule (1.10).

| joint distribution (2-D) | proposition $B$ | proposition $\overline{B}$ | marginal distribution (1-D) |
|-------------------------|-----------------|---------------------------|-----------------------------|
| proposition $A$         | $P(AB|I)$       | $P(A\overline{B}|I)$      | $P(A|I)$                    |
| proposition $\overline{A}$ | $P(\overline{A}B|I)$ | $P(\overline{A}B|I)$      | $P(\overline{A}|I)$        |
| marginal distribution (1-D) | $P(B|I)$       | $P(\overline{B}|I)$       | 1                           |

in the form of a $2 \times 2$ contingency table. By way of summation, separately across row and column entries, while respecting the sum rule (1.10), the concept of a marginal probability for a proposition, given $I$, is introduced. The kind of $2 \times 2$ contingency table just outlined is depicted in Tab. 1.1.

1.2.3 Generalised sum rule

Starting from the negation of the second De Morgan’s law which was noted in Eq. (1.9), the derivation of a rule for calculating the probability of the logical sum of two propositions, $A + B$, is calculated. A string of algebraic manipulations leads to

$$P(A + B|I) \quad \text{Eq. (1.10)} = P(\overline{A}\overline{B}|I) \quad \text{Eq. (1.11)} = 1 - P(AB|I)$$

$$P(A|I) + P(\overline{A}B|I) \quad \text{Eq. (1.10)} = 1 - [1 - P(B|AI)]P(\overline{A}|I)$$

so that with one final application of Eq. (1.11) one obtains the generalised sum rule given by

$$P(A + B|I) = P(A|I) + P(B|I) - P(AB|I). \quad (1.14)$$

7There is a typo in the first line of Eq. (2.65) in Jaynes (2003) [48]. We here give the necessary correction in the expression following the second equality sign in Eq. (1.13).

8Re-arranging Eq. (1.14), to solve for $P(AB|I)$ instead, yields an alternative representation of the generalised sum rule, or “conjunction rule,” Eq. (1.11). By means of their famous “Linda the bank teller” example (amongst others), Tversky and Kahneman (1983) [103, p 297ff] were able to demonstrate the startling empirical fact that the conjunction rule is frequently violated in everyday (intuitive) decision-making. They termed this empirical phenomenon the “conjunction fallacy.” In their view, it can be explained as a consequence of decision-makers often resorting to a “representativeness heuristic” as an aid; see also Kahneman (2011) [51, Sec. 15].
1.3. BAYES’ THEOREM

At this point the list of elementary mathematical rules of probability theory has been completed. It comprises the sum rule (1.10), the product rule (1.11), and the generalised sum rule (1.14). We next turn to highlight a few important extensions of these rules when dealing with special kinds of sets of propositions.

1.2.4 Extensions to sets of propositions

Suppose given a finite set of \( k \in \mathbb{N} \) mutually exclusive and exhaustive propositions \( \{A_1, \ldots, A_k\} \), conditioned on some background information \( I \), so that
\[
P(A_i A_j | I) = 0 \quad \text{for} \quad i \neq j
\]  
(1.15)
is true. Then the sum rule (1.10) extends to the normalisation condition of probability theory, namely
\[
P(A_1 + \ldots + A_k | I) = P(A_1 | I) + \ldots + P(A_k | I) = \sum_{i=1}^{k} P(A_i | I) = 1.
\]  
(1.16)
This states that, when assigning probabilities across a closed set of exclusive possibilities, for reasons of overall consistency these must add up to 1.

Furthermore, on the basis of the normalisation condition (1.16) and the product rule (1.11), it holds that
\[
P(B | I) = \sum_{i=1}^{k} P(B A_i | I) = \sum_{i=1}^{k} P(B | A_i) P(A_i | I) > 0.
\]  
(1.17)
This is generally referred to as the marginalisation rule (see, e.g., Saha (2002) [88, p 5], Sivia and Skilling (2006) [92, p 7], or Andreon and Weaver [4, p 4]), and it possesses high practical value in the context of numerical simulations of probability distributions, a major topic in inductive statistical inference that is to be discussed later on. An immediate simple application of the marginalisation rule was illustrated in Tab. 1.1 above.

1.3 Bayes’ theorem

The core of the plausible reasoning framework developed as an efficient and reliable practical tool for inductive statistical inference is constituted by a result that is due to the English mathematician and Presbyterian minister Thomas Bayes (1702–1761); see the posthumous publication Bayes (1763) [6]. It states that for two propositions \( A \) and \( B \), given background information \( I \), it is always true that
\[
P(A | B I) = \frac{P(B | A I)}{P(B | I)} P(A | I),
\]  
(1.18)
On the face of it, Bayes’ theorem, as it has come to be known for a long time, is just a convenient re-arrangement of the product rule (1.11), provided \( P(B | I) > 0 \). However, its immense conceptual significance for plausible reasoning and inductive statistical inference was already glimpsed at by Bayes himself; cf. Stigler (1986) [96, pp 98–98].
In qualitative terms Bayes’ theorem is saying

\[
\text{(prior knowledge on proposition } A \text{) combined with (empirical evidence } B \text{ on proposition } A \text{) yields}
\]

\[
\text{(updated knowledge on proposition } A \text{)}
\]

According to Jaynes (2003) [48, p 112], in the clear-cut representation of Eq. (1.18), the theorem was first formulated by the French mathematician and astronomer Marquis Pierre Simon de Laplace (1749–1827); cf. Laplace (1774) [62].

To streamline communication, the different factors featuring in Bayes’ theorem (1.18) have been given names in their own right. These are:

- \( P(A | I) \) is referred to as the **prior probability** for proposition \( A \), subject to background information \( I \).
- \( P(B | A I) \) is the **likelihood** for a proposition \( B \), providing potentially relevant information for proposition \( A \), given background information \( I \).
- \( P(A | B I) \) is called the **posterior probability** for proposition \( A \) in light of the information pertaining to proposition \( B \) and background information \( I \), and, lastly,
- \( P(B | I) > 0 \) is usually known as the **evidence** relating to proposition \( B \).

By means of marginalisation, and on the basis of the sum rule (1.10) and the product rule (1.11), the evidence \( P(B | I) \) can be re-expressed as

\[
P(B | I) \overset{\text{Eq. (1.10)}}{=} P(B A | I) + P(B A^c | I) \]

\[
P(B | A I) P(A | I) + P(B | A^c I) P(A^c | I).
\]

(1.19)

In this form it is also referred to as the **average likelihood** or **marginal likelihood**; cf. McElreath (2016) [68, Sec. 2.3].

From Bayes’ theorem (1.18), one directly infers for the relation between the **prior probability** for proposition \( A \) and its **posterior probability** that

\[
\begin{cases}
\text{if } \frac{P(B | A I)}{P(B | I)} < 1 & \Rightarrow \ P(A | B I) < P(A | I) \\
\text{if } 0 < \frac{P(B | A I)}{P(B | I)} > 1 & \Rightarrow \ P(A | B I) > P(A | I)
\end{cases}
\]

\[
(1.20)
\]

\[9\text{Depicting the structure of Bayes’ theorem in this particular fashion ties in nicely with a famous quotation by the British economist John Maynard Keynes CB FBA (1883–1946), who is said to have once remarked: “When the facts change, I change my mind. What do you do, sir?” See URL (cited on July 8, 2018): www-history.mcs.st-and.ac.uk/Quotations/Keynes.html.}

\[10\text{Kahneman (2011) [51, p 147], in his stimulating popular book, refers to } P(A | I) \text{ as the “base rate” for proposition } A.\]
1.4. OUTLOOK ON INDUCTIVE DATA ANALYSIS AND MODEL BUILDING

depending on the evidence available through proposition \( B \), the probability for proposition \( A \) can potentially either decrease or increase.

For simple practical applications with only two propositions \( A \) and \( B \) involved, as is typically the case in situations analogous to drug testing, disease testing, or signal detection, it is helpful to rewrite Bayes’ theorem (1.13) by making use of the marginalisation rule (1.19). One thus obtains

\[
P(A|BI) = \frac{P(B|AI)}{P(B|AI)P(A|I) + P(B|\overline{A}I)P(\overline{A}|I)}P(A|I).
\]

(1.21)

The posterior probability for a proposition \( A \), in view of some evidence relating to a proposition \( B \) and background information \( I \), can then be easily computed provided the following three pieces of information are available; cf. Silver (2012) [91, p 244]:

(i) the prior probability for proposition \( A \) in the absence of evidence, \( P(A|I) \),

(ii) the “true positive rate,” \( P(B|AI) \), and

(iii) the “false positive rate,” \( P(B|\overline{A}I) \).

This last bit of discussion generalises to the case of a set of \( k \in \mathbb{N} \) mutually exclusive and exhaustive propositions \( \{A_1, \ldots, A_k\} \) in a straightforward fashion. Given prior probabilities \( P(A_i|I) \) for each proposition \( A_i \) in the set, and with the marginalisation rule (1.17) employed to express the average likelihood \( P(B|I) \) for some evidential proposition \( B \), one calculates posterior probabilities \( P(A_i|BI) \) for each proposition \( A_i \) in the set from Bayes’ theorem (1.18) according to

\[
P(A_i|BI) = \frac{P(B|A_iI)}{\sum_{j=1}^k P(B|A_jI)P(A_j|I)}P(A_i|I), \quad \text{for } i = 1, \ldots, k.
\]

(1.22)

In this specific form, Bayes’ theorem has high practical value as a computational basis for discretised numerical simulations of complicated high-dimensional probability distribution functions.

1.4 Outlook on inductive data analysis and model building

So why does the Bayes–Laplace approach to probability theory provide such a conceptually compelling basis for plausible reasoning and inductive statistical inference?

One of a number of strong arguments in its favour is that scientific objectivity is ensured by strict adherence to the requirements of logical consistency and fact-based reasoning. That is to say, on the basis of the rules of probability theory outlined in Sec. 1.2 two researching individuals that

(i) hold the same relevant background information \( I \) on a specific proposition \( A \) of scientific interest, and

(ii) have access to the same empirical evidence associated with a proposition \( B \),
must assign the same prior probability \( P(A|I) \) to proposition \( A \), and calculate the same posterior probability \( P(A|BI) \) for proposition \( A \) from the empirical evidence available. In practice, of course, different individuals typically have access to differing amounts of relevant background information and empirical evidence. The Bayes–Laplace approach, however, exposes itself deliberately to criticism in that it requires a researcher to state openly all of her/his assumptions that went into an inductive statistical inference process. There are no hidden agendas, which certainly facilitates to a novice the task of becoming acquainted with the specific rationale employed in this framework.[1]

Formally, Bayes’ theorem, for example in its variant (1.22), represents the fundamental principle according to which inductive statistical inference is to be performed, given prior information and empirical data of relevance to an actual research question. To begin with, the following specific substitutions need to be made:

\[
\text{proposition } A \leftarrow \text{model}(i), \text{ or hypothesis}(i), \text{ or set of parameter values}(i)
\]

\[
\text{proposition } B \leftarrow \text{data} ;
\]

here the concepts “model(i)” and “hypothesis(i)” can be interpreted as synonymous terms. In the Bayes–Laplace approach, data is considered fixed incomplete information, while the model, hypothesis, or set of parameter values of the researcher’s focus is the unknown entity about the plausibility of which inferences are to be made in light of available evidence. The unknown entity is to be described probabilistically by assigning a probability distribution to the range of possibilities it involves. One thus obtains

\[
P(\text{model}(i)|\text{data}, I) = \frac{P(\text{data} | \text{model}(i), I)}{P(\text{data} | I)} P(\text{model}(i) | I) . \tag{1.23}
\]

The nature of Bayes’ theorem hereby undergoes a qualitative change in that it transforms from a statement concerning four probability values (non-negative real numbers) to a functional relationship between entire probability distributions. The main statement is that the posterior probability distribution for the unknown entity of interest amounts to the product between the likelihood function for the data, given the unknown entity, and the prior probability distribution for the unknown entity, divided by a normalising constant (a positive real number, as the data is considered fixed) referred to as the average likelihood. Within the Bayes–Laplace approach, the posterior probability distribution is viewed as a “compromise” between the background information-driven prior probability distribution and the data-driven likelihood function; see, e.g., Kruschke (2015) [58, p 112].

11Jaynes (2003) [48, p 22] identifies as a dangerous pitfall for plausible reasoning what he refers to as the “mind projection fallacy.” He depicts this as the error of confusing epistemological statements (statements of knowledge of things) with ontological statements (statements of existence of things), and vice versa. Put differently, this describes a case where an individual confuses what they personally think exists with what actually (and, therefore, testably) does exist in reality.
At the heart of the activity of **inductive statistical inference** is the proposition of a **statistical model**, derived from comprehensible **theoretical considerations**. The general purpose of a **scientific theory** is to describe, explain and predict observable phenomena in its particular field of application. A **statistical model** is formulated in the concise language of **mathematics**. It typically comprises a certain finite number of **unobservable continuous parameters**, the values of which are to be estimated probabilistically via calculating a **posterior joint probability distribution** from (i) a discrete set of **measured data** for a finite number of relevant **statistical variables**, and (ii) a sensible **prior joint probability distribution** reflecting a given **state of knowledge**. In some rather special lower-dimensional cases it is possible to obtain posterior joint probability distributions as closed-form analytical solutions. In general, however, posterior joint probability distributions are in non-standard form due to inherent complexity, which often features already at the two-parameter level. The aim of **Markov Chain Monte Carlo** (MCMC) simulations is to generate **discretised approximations** to the continuous high-dimensional, multi-parameter posterior joint probability distributions to an accuracy that is reasonable for practical inference. Simulated **posterior joint probability distributions**, and even more so their associated **posterior marginal probability distributions**, can then be summarised by standard methods such as five number summaries, means, standard deviations and standard errors, skewnesses, kurtoses, and further tailor-made statistics of convenience.

To be recognised as meaningful and valuable by the scientific community, a proposed **statistical model** must cope well with two major challenges: (i) **retrodiction** of observed (and, therefore, known to the researcher) data, and (ii) **prediction** of new (and, therefore, unknown to the researcher) data. From a technical point of view this means engineering an acceptable balance between **under-fitting** and **over-fitting** when adapting a proposed **statistical model** to available empirical data. In this process, a researcher can resort to methods of **model comparison** by means of **information criteria**, and checks of a model’s **posterior predictive accuracy**. These techniques are to be addressed in these lecture notes in later chapters.

Input into the statistical model building process for explaining the variation of a **statistical variable** $Y$ in dependence on a set of $k \in \mathbb{N}$ predicting **independent variables** $\{X_1, \ldots, X_k\}$, given background information $I$, is a **prior joint probability distribution** $P(\theta_0, \ldots, \theta_k|I)$ for a set of typically $k + 1$ unknown **model parameters** $\{\theta_0, \ldots, \theta_k\}$. On the basis of relevant measured **data** $\{y_i\}_{i=1,\ldots,n}$ of sample size $n$ (which is thus given and fixed, and inherently amounts to incomplete information), the fundamental objective is to deduce a **posterior joint probability distribution** $P(\theta_0, \ldots, \theta_k|\{y_i\}_{i=1,\ldots,n}, I)$ for these model parameters, employing the logic of plausible reasoning according to the **Bayes–Laplace approach**. This activity leads to:

$$P(\theta_0, \ldots, \theta_k|\{y_i\}_{i=1,\ldots,n}, I) = \frac{P(\{y_i\}_{i=1,\ldots,n}|\theta_0, \ldots, \theta_k, I) \cdot P(\theta_0, \ldots, \theta_k|I)}{P(\{y_i\}_{i=1,\ldots,n}|I)} \quad (1.24)$$

and is referred to as the updating process; subject-specific information available to a researcher is being enlarged by learning from relevant empirical data. It is from the **posterior joint probability distribution** that the researcher draws all relevant inferences concerning her/his research question, while, in parallel, acknowledging overall **uncertainty** due to **incomplete information**.

---

\[^{12}\text{To avoid cluttering of notation, here and in the following we suppress conditioning on the (fixed) data for the } k \text{ independent variables } \{X_1, \ldots, X_k\}.\]
Multiple application of the product rule (1.11) transforms the prior joint probability distribution for the \( k + 1 \) unknown model parameters \( \{\theta_0, \ldots, \theta_k\} \) to the practically more convenient form

\[
P(\theta_0, \ldots, \theta_k | I) = P(\theta_0 | \theta_1, \ldots, \theta_k, I) \times P(\theta_1 | \theta_2, \ldots, \theta_k, I) \times \cdots \times P(\theta_k | I) . \tag{1.25}
\]

Frequently, in fact in particular in the context of numerical simulations, the simplifying assumption of separability is introduced for the prior joint probability distribution (reflecting the assumption of prior mutual logical independence of the model parameters), i.e., the product structure

\[
P(\theta_0, \ldots, \theta_k | I) = P(\theta_0 | I) \times \cdots \times P(\theta_k | I) \tag{1.26}
\]

is employed. Such a choice, however, disregards potential non-zero bivariate correlations between the model parameters which arise in generic situations. It can be justified, though, as expressing a researcher’s complete ignorance as to the existence and strengths of such interrelationships. The idea is that exactly the empirical data to be analysed will provide the clues necessary to make progress on the answer to this specific question.

We conclude this section by briefly reviewing two concepts that are used for assessing the quality of fit and the predictive accuracy of a statistical model. The so-called prior predictive probability distribution for a single datum \( y \), given a prior joint probability distribution for a set of continuous model parameters \( \{\theta_0, \ldots, \theta_k\} \) and the relevant single-datum likelihood function, is defined by (see, e.g., Gelman et al (2014) [35, Sec. 1.3], Andreon and Weaver [4, Sec. 8.10], or Gill (2015) [39, Sec. 6.4])

\[
P(y | I) := \int \cdots \int_{\theta_j \text{ ranges}} P(y, \theta_0, \ldots, \theta_k | I) \, d\theta_0 \cdots d\theta_k = \int \cdots \int_{\theta_j \text{ ranges}} \overbrace{P(y|\theta_0, \ldots, \theta_k, I)}^{\text{likelihood}} \overbrace{P(\theta_0, \ldots, \theta_k | I)}^{\text{prior}} \, d\theta_0 \cdots d\theta_k . \tag{1.27}
\]

Here, the single-datum likelihood function is weighted by the prior joint probability distribution for the model parameters and then integrated over the entire range of the various \( \theta_j \)-spectra. This operation amounts to averaging the single-datum likelihood function with the prior joint probability distribution over the \((k + 1)\)-dimensional parameter space.

The so-called posterior predictive probability distribution for a new datum \( y_{\text{new}} \), given a posterior joint probability distribution for a set of continuous model parameters \( \{\theta_0, \ldots, \theta_k\} \) and the relevant single-datum likelihood function, is defined by (see, e.g., Gelman et al (2014) [35, Sec. 1.3],
Andreon and Weaver [4, Sec. 8.10], or Gill (2015) [39, Sec. 6.4])

\[
P(\{y_i\}_{i=1,...,n}, \mathbf{I}) := \int \cdots \int_{\theta_j \text{ ranges}} P(\mathbf{y}_{\text{new}}|\theta_0, \ldots, \theta_k, \{\mathbf{y}_i\}_{i=1,...,n}, \mathbf{I}) \, d\theta_0 \cdots d\theta_k
\]

\[
= \int \cdots \int_{\theta_j \text{ ranges}} P(\mathbf{y}_{\text{new}}|\theta_0, \ldots, \theta_k, \{\mathbf{y}_i\}_{i=1,...,n}, \mathbf{I}) \times P(\theta_0, \ldots, \theta_k|\{\mathbf{y}_i\}_{i=1,...,n}, \mathbf{I}) \, d\theta_0 \cdots d\theta_k
\]

\[
= \int \cdots \int_{\theta_j \text{ ranges}} P(\mathbf{y}_{\text{new}}|\theta_0, \ldots, \theta_k, \mathbf{I}) \times P(\theta_0, \ldots, \theta_k|\{\mathbf{y}_i\}_{i=1,...,n}, \mathbf{I}) \, d\theta_0 \cdots d\theta_k,
\]

assuming in the final step conditional logical independence of the new datum \(y_{\text{new}}\) from the previous sample \(\{y_i\}_{i=1,...,n}\), given values for the model parameters. Here, the single-datum likelihood function is weighted by the posterior joint probability distribution for the model parameters and then integrated over the entire range of the various \(\theta_j\)-spectra. It thus represents the expectation of the conditional probability \(P(\mathbf{y}_{\text{new}}|\theta_0, \ldots, \theta_k, \mathbf{I})\) over the posterior joint probability distribution for \(\{\theta_0, \ldots, \theta_k\}\). Alternatively, this operation is viewed as averaging the single-datum likelihood function with the posterior joint probability distribution over the \((k + 1)\)-dimensional parameter space. Note that the posterior predictive probability distribution possesses a larger standard deviation than the posterior joint probability distribution, because it joins uncertainty inherent in both the empirical data and the model parameter estimation.

We now turn to describe ways of capturing in formal language different kinds of data-generating processes that are of importance for many practical applications.
Chapter 2

Likelihood functions and sampling distributions

In statistical modelling a first fundamental assumption is to suppose that every single measured datum $y_i$ for a particular statistical variable $Y$ of interest originates from a definite data-generating process. This data-generating process is to be described parametrically by means of a single-datum likelihood function, the specific form of which depends on the actual nature of the statistical variable $Y$ in question, e.g., its scale level of measurement. Conceptually, this single-datum likelihood function amounts to a probability distribution for the single measured datum $y_i$, given fixed values for the parameters of the data-generating process. A second fundamental assumption comprises the view that when taking measurements with respect to $Y$ from a total of $n$ sample units, then the order in which this data was obtained would not matter. This second assumption represents de Finetti’s (1930) [26] concept of exchangeability. This assumption is valid, if no particular chronological order is to be respected in the measurement process as, for instance, needs to be taken care of when gathering time series data. In technical language this is the requirement that the likelihood function for the entire data set for $Y$ be invariant under any permutation (re-ordering) of the measured values for $Y$. In practice, however, in most cases an even stronger assumption is built upon, namely that obtaining one value $y_i$ for $Y$ from some data-generating process may be considered logically independent from obtaining a second value $y_j$ from the same data-generating process, and vice versa, so that in consequence (as it is referred to) independently and identically distributed (iid) data arises; cf. Jaynes (2003) [48, p 62], Gilboa (2009) [37] p 42f, Greenberg (2013) [41] p 52f, Gelman et al (2014) [35] p 104f, and Gill (2015) [39, Sec. 12.4]. The iid assumption, which is practically convenient, may be justified as reflecting prior ignorance on the part of the researcher as regards potential autocorrelations amongst the different measured values of $Y$ [1] see McElreath (2016) [68, p 81].

We denote the single-datum likelihood function\(^2\) for a statistical variable $Y$ in a statistical model comprising $k + 1$ parameters $\{\theta_0, \ldots, \theta_k\}$ by $f(y_i|\theta_0, \ldots, \theta_k, I)$. As it happens, assuming fixed values for the set $\{\theta_0, \ldots, \theta_k\}$, for discretely varying $y_i$ this represents a normalised probability function, while for continuously varying $y_i$ this represents a normalised probability density func-

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1. Generally, data from convenience samples is plagued with a high degree of autocorrelation.
2. Alternatively: single-case likelihood function.
CHAPTER 2. LIKELIHOOD FUNCTIONS AND SAMPLING DISTRIBUTIONS

When the iid assumption appears sensible for describing a particular data-generating process for \( Y \), then given a total sample of measured values \( \{y_i\}_{i=1}^n \) of size \( n \), an immediate consequence for the total-data likelihood function is proportionality to the product of \( n \) single-datum likelihood functions \( f(y_i|\theta_0, \ldots, \theta_k, I) \), i.e.,

\[
P(\{y_i\}_{i=1}^n | \theta_0, \ldots, \theta_k, I) \propto \prod_{i=1}^n f(y_i|\theta_0, \ldots, \theta_k, I). \tag{2.1}
\]

In the following we will review some of the standard uni- and multivariate single-datum likelihood functions for both discretely and continuously varying statistical variables \( Y \). Most of the examples presented belong to the class of maximum entropy distributions that reflect for a specific context, and conditional on some set of definite constraints, maximum ignorance on the part of the researcher as to the unknown actual data-generating process; see, e.g., McElreath (2016) [68, p 282].

2.1 Univariate discrete data

The single-datum likelihood functions introduced in this section apply to univariate data \( y_i \) from a discrete one-dimensional statistical variable \( Y \). They depend on an unobservable and therefore unknown continuously varying parameter \( \theta \).

2.1.1 Bernoulli distributions

The one-parameter family of univariate Bernoulli distributions,

\[
y_i | \theta, I \sim \text{Bern}(\theta),
\]

was put forward by the Swiss mathematician Jakob Bernoulli (1654–1705). It can be used to model data-generating processes in which, in a single observation, \( y_i \) has two possible outcomes: “failure” (0) or “success” (1). This could be, for example,

- whether or not a student gets accepted for the degree programme she/he had applied for,
- whether or not a bank customer is granted the mortgage loan she/he had asked for,
- whether or not it will rain tomorrow at your present location, or
- whether or not your favourite football team will win their next league match.
2.1. \textit{Univariate Discrete Data}

$y_i$, here is a dimensionless quantity. Properties of \textbf{Bernoulli distributions} are (see, e.g., Rinne (2008) [86, Subsec. 3.8.2]):

Spectrum of values:

$$y_i \in \{0, 1\} .$$

(2.3)

Probability function:

$$P(y_i|\theta, I) = \theta^{y_i} (1-\theta)^{1-y_i}, \quad \text{with} \quad 0 \leq \theta \leq 1 ,$$

(2.4)

where the dimensionless parameter $\theta$ quantifies the \textbf{probability for “success,”} (1). The graph of a Bernoulli probability function is shown in Fig. \ref{fig:bernoulli} below for four different values of $\theta$.

Expectation value and variance:

$$E(y_i) = \theta \quad \text{(2.5)}$$

$$\text{Var}(y_i) = \theta(1-\theta) . \quad \text{(2.6)}$$

Note that under an exchange $\theta \leftrightarrow (1-\theta)$ one obtains a qualitatively identical distribution.

\textbf{Figure 2.1:} Some examples of Bernoulli sampling distributions for an uncertain dichotomous discrete quantity $y$.

\textbf{R:} dbinom($y_i$, 1, $\theta$), pbinom($y_i$, 1, $\theta$), qbinom($p$, 1, $\theta$), rbinom($n_{\text{simulations}}$, 1, $\theta$)

\textbf{JAGS:} dbern($\theta$) (sampling)

\textbf{Stan:} bernoulli($\theta$) (sampling)
2.1.2 Binomial distributions

The natural extension of Bernoulli distributions to situations with a finite number of repetitions under iid conditions of the underlying binary decision process was discussed by Bernoulli himself. He thus introduced the two-parameter family of univariate binomial distributions,

\[ y \mid n, \theta, I \sim \text{Bin}(n, \theta), \]

where \( n \in \mathbb{N} \) is the number of iid-repetitions, and \( \theta \) again denotes the probability for “success,” (1). The dimensionless non-negative integer quantity \( y \) is by its very nature varying discretely and represents a pure count with a known finite maximum. It could measure, for example,

- how many out of \( n \) students get accepted for the degree programme they had applied for,
- how many out of \( n \) bank customers are granted the mortgage loan they had asked for,
- on how many out of the next \( n \) days it will rain at your present location, or
- how many out of \( n \) upcoming matches in the league your favourite football team will win.

**Binomial distributions** are described by (see, e.g., Rinne (2008) [86, Subsec. 3.8.3]):

**Spectrum of values:**

\[ y \in \mathbb{N}_0. \] (2.8)

**Probability function:**

\[
P(y \mid n, \theta, I) = \binom{n}{y} \theta^y (1 - \theta)^{n-y}, \quad \text{with} \quad 0 \leq \theta \leq 1,
\] (2.9)

wherein the binomial coefficient is defined by

\[
\binom{n}{y} := \frac{n!}{y!(n-y)!},
\] (2.10)

for \( n \in \mathbb{N} \) and \( y \leq n \). Note that the binomial probability function is normalised with respect to the discrete variable \( y \) but not with respect to the continuous parameter \( \theta \). Its graph is shown in Fig. 2.2 below for four different values of \( \theta \) and \( n = 20 \).

Expectation value and variance:

\[
E(y) = n \theta \\
\text{Var}(y) = n \theta (1 - \theta).
\] (2.11)

A qualitatively identical distribution is obtained under the exchange \( \theta \leftrightarrow (1 - \theta) \).

**R:** `dbinom(y, n, theta), pbinom(y, n, theta), qbinom(p, n, theta), rbinom(n_simulations, n, theta)`

**JAGS:** `dbinomial(n, theta)` (sampling)

**Stan:** `binomial(n, theta)` (sampling)

It is of some practical interest that, by means of the logistic transformation \( \theta = \exp(u)/(1 + \exp(u)) \), binomial sampling distributions according to Eq. (2.9) can explicitly be shown to be members of the so-called **exponential family** of sampling distributions; see Sec. 2.4 below.

\(^3\text{We plot the graphs of probability functions with connecting lines to highlight shapes of envelopes. The probability functions are, of course, discrete by nature.}\)
2.1. Univariate discrete data

2.1.3 Poisson distributions

The one-parameter family of univariate Poisson distributions,

\[ y_i | \theta, I \sim \text{Pois}(\theta), \]

named after the French mathematician, engineer, and physicist Baron Siméon Denis Poisson FRSFor HFRSE MIF (1781–1840), is the most important tool in all of the empirical scientific disciplines for modelling count data. They can be considered to arise as special cases of binomial distributions when \( n \) is very large (\( n \gg 1 \)) and \( \theta \) is very small (\( 0 < \theta \ll 1 \)) (cf. Sivia and Skilling (2006) [92, Sec. 5.4]), and so typically describe instances of data-generating processes associated with (relatively) rare events. Examples for \( y_i \) as a pure count (i.e., a dimensionless non-negative integer) are

- the number of automobiles sold by a car vendor,
- the number of goals scored by a football team,
- the number of elephants living in certain parts of eastern or southern Africa, or
- the number of photons received from a faint distant luminous source by an astronomical telescope.

Figure 2.2: Some examples of binomial sampling distributions for an uncertain discrete quantity \( y \).
**Poisson distributions** have the properties (see, e.g., Rinne (2008) [86, Subsec. 3.9.2]):

**Spectrum of values:**

\[ y_i \in \mathbb{N}_0 \]  

(2.14)

**Probability function:**

\[
P(y_i | \theta, I) = \frac{\theta^{y_i}}{y_i!} \exp(-\theta), \quad \text{with} \quad \theta \in \mathbb{R}_{\geq 0},
\]

(2.15)

and \( \theta \) is the dimensionless **rate parameter** (also referred to as the intensity parameter). The Poisson probability function is normalised with respect to the discrete variable \( y_i \) but *not* with respect to the continuous parameter \( \theta \). Its graph is shown in Fig. 2.3 for four different values of \( \theta \).

**Expectation value and variance:**

\[
E(y_i) = \theta \quad \text{(2.16)}
\]

\[
\text{Var}(y_i) = \theta. \quad \text{(2.17)}
\]

Note that for **Poisson distributions** the (dimensionless) expectation value and variance *coincide*.

---

**Figure 2.3:** Some examples of Poisson sampling distributions for an uncertain discrete quantity \( y \).

**R:** `dpois(y_i, \theta), ppois(y_i, \theta), qpois(p, \theta), rpois(n\text{simulations}, \theta)`

**JAGS:** `dpois(\theta)` (sampling)

**Stan:** `poisson(\theta)` (sampling)
2.2. UNIVARIATE CONTINUOUS DATA

In many applications one finds the counts $y_i$ decomposed into a product of two dimensionful quantities,

$$\text{count} = \text{exposure} \times \text{rate} \quad \Rightarrow \quad \theta = \tau \times \lambda,$$

so that the rate parameter $\theta$ amounts to the product “length/size of interval/domain of observation, $\tau$, times number of events per unit interval/domain, $\lambda$.” In temporal contexts $\lambda$ represents counts per unit time, while in spatial contexts it stands for counts per unit length, counts per unit area, or counts per unit volume. In this view, the parameter $\tau$ is referred to as the exposure (of a sample unit to some data-generating influence) and carries the physical dimension of $[\text{time}], [\text{length}], [\text{area}], \text{or}[\text{volume}]$. The corresponding rate parameter $\lambda$ could represent, for example,

- the average number of automobiles sold by a car vendor per working day,
- the average number of goals scored by a football team per match,
- the average number of elephants living per ten-kilometres-squared of area in the Kruger National Park, or
- the average number of elliptical galaxies observed per megaparsec-cubed of comoving volume of space at a redshift of $z = 0.5$.

2.2 Univariate continuous data

The single-datum likelihood functions introduced in this section apply to univariate data $y_i$ from a continuous one-dimensional statistical variable $Y$. They depend on a certain number of unobservable and therefore unknown continuously varying parameters.

2.2.1 Gauß distributions

The two-parameter family of univariate Gauß distributions (or normal distributions),

$$y_i \mid \theta_1, \theta_2, \mathcal{I} \sim \mathcal{N}(\theta_1, \theta_2^2),$$

has gained its status as ranking amongst the best-known and most frequently applied continuous distributions foremost by the work of the German mathematician and astronomer Carl Friedrich Gauß (1777–1855); cf. Gauß (1809) [30]. Examples for the usually dimensionful continuous metrical quantity $y_i$ that can be described as arising from a Gauß process are

- the price of a 1 kg loaf of bread in a medium-sized town of your home country,
- the average monthly waiting time in minutes spent by car users in traffic jams during the morning rush hour near an industrial centre,
- the IQ of an adult female or male individual, or
- the wavelength in nanometres of the red line in the visible hydrogen emission spectrum.
Often one finds the natural logarithm of a strictly positive metrical statistical variable \( Y \), after properly normalising the latter via division by a convenient reference quantity of the same physical dimension, to be describable as approximately originating from a Gauß process. Note that departures of Gauß-distributed data from their common mean by more than three standard deviations are very rare, and by more than six standard deviations are practically impossible.

Gauß distributions have the properties (see, e.g., Rinne (2008) [86, Subsec. 3.10.1]):

Spectrum of values:
\[ y_i \in \mathbb{R} \; . \tag{2.20} \]

Probability density function (pdf):
\[
f(y_i|\theta_1, \theta_2, I) = \frac{1}{\sqrt{2\pi} \theta_2} \exp \left[ -\frac{1}{2} \left( \frac{y_i - \theta_1}{\theta_2} \right)^2 \right] , \quad \text{with} \quad \theta_1 \in \mathbb{R} \; , \; \theta_2 \in \mathbb{R}_{>0} \; ; \tag{2.21} \]

\( \theta_1 \) constitutes a location parameter and \( \theta_2 \) a scale parameter, both of which share the physical dimension of \( y_i \) itself. The reciprocal of the squared scale parameter, \( 1/\theta_2^2 \), is conventionally referred to as the precision. Note that the Gauß probability density function is normalised with respect to the continuous variable \( y_i \) but not with respect to the continuous parameters \( \theta_1 \) and \( \theta_2 \).

Its graph is shown in Fig. 2.4 for four different combinations of values of \( \theta_1 \) and \( \theta_2 \).

Expectation value and variance:
\[
\begin{align*}
\mathbb{E}(y_i) &= \theta_1 \; , \tag{2.22} \\
\text{Var}(y_i) &= \theta_2^2 \; . \tag{2.23} 
\end{align*}
\]

\( \text{R: dnorm}(y_i, \theta_1, \theta_2), \text{pnorm}(y_i, \theta_1, \theta_2), \text{qnorm}(p, \theta_1, \theta_2), \text{rnorm}(n_{\text{simulations}}, \theta_1, \theta_2) \)

\( \text{JAGS: dnorm}(\theta_1, 1/\theta_2^2) \) (sampling)

\( \text{Stan: normal}(\theta_1, \theta_2) \) (sampling)

\subsection{2.2.2 Non-central \( t \)--distributions}

The three-parameter family of non-central \( t \)--distributions,
\[
y_i|\theta_1, \theta_2, \nu, I \sim \text{t}(\theta_1, \theta_2, \nu) \; , \tag{2.24} \]

constitutes a generalisation of a well-known family of continuous probability distributions discovered by the English statistician William Sealy Gosset (1876–1937). Profoundly confusing for the scientific community, he published his findings under the pseudonym of “Student;” cf. Student (1908) [97]. While being qualitatively similar to Gauß distributions, their main characteristic is the larger probability weight contained in the “tails” of the distributions. Therefore, non-central \( t \)--distributions are being employed to model data-generating processes for usually dimensionful continuous metrical quantities \( y_i \) which regularly produce outliers. Specific features of non-central \( t \)--distributions are (see, e.g., Rinne (2008) [86, Subsec. 3.10.6]):
**2.2. UNIVARIATE CONTINUOUS DATA**

![Gauss distributions](image)

Figure 2.4: Some examples of Gauss sampling distributions for an uncertain continuous quantity $y$.

Spectrum of values:

$$y_i \in \mathbb{R} \quad (2.25)$$

Probability density function (pdf):

$$f(y_i | \theta_1, \theta_2, \nu, I) = \frac{\Gamma((\nu + 1)/2)}{\Gamma(\nu/2) \sqrt{\pi \nu \theta_2}} \left[ 1 + \frac{1}{\nu} \left( \frac{y_i - \theta_1}{\theta_2} \right)^2 \right]^{-(\nu+1)/2}, \quad \text{with } \nu \in \mathbb{R}_{\geq 1}; \quad (2.26)$$

$\theta_1 \in \mathbb{R}$ represents a location parameter and $\theta_2 \in \mathbb{R}_{>0}$ a scale parameter, both of which share the physical dimension of $y_i$, and $\nu \geq 1$ is the dimensionless positive degrees of freedom parameter. All three parameters are continuous. The Gamma function used above is defined via an Euler integral of the second kind by (see, e.g., Rinne (2008) [86, p 168])

$$\Gamma(x) := \int_0^\infty t^{x-1} \exp(-t) \, dt, \quad \text{with } \, x \in \mathbb{R}_{\geq 0}. \quad (2.27)$$

For later application it is important to note that for positive integer values of $x$, i.e., $x = n \in \mathbb{N}$, it holds true that

$$\Gamma(n + 1) = n! \quad (2.28)$$

The graph of the non-central $t$–probability density function is shown in Fig. 2.5 for four different combinations of values of $\theta_1$, $\theta_2$ and $\nu$. Gosset’s one-parameter family of standard $t$–distributions is contained in Eq. (2.26) for the special parameter choices $\theta_1 = 0$ and $\theta_2 = 1$. 
CHAPTER 2. LIKELIHOOD FUNCTIONS AND SAMPLING DISTRIBUTIONS

Expectation value and variance (cf. Greenberg (2013) [41, p 230]):

\[ E(y_i) = \theta_1, \quad \text{if} \quad \nu > 1 \]  
\[ \text{Var}(y_i) = \frac{\nu}{\nu - 2} \theta_2^2, \quad \text{if} \quad \nu > 2. \]  

(2.29)  
(2.30)

Figure 2.5: Some examples of non-central \( t \)-sampling distributions for an uncertain continuous quantity \( y \).

\[ R: (1/\theta_2) \ast \text{dt}((y_i + \theta_1)/\theta_2, \nu), (1/\theta_2) \ast \text{pt}((y_i + \theta_1)/\theta_2, \nu) \]  
\[ \text{JAGS:} \ \text{dt}(\theta_1, 1/\theta_2^2, \nu) \ \text{(sampling)} \]  
\[ \text{Stan:} \ \text{student}t(\nu, \theta_1, \theta_2) \ \text{(sampling)} \]

In the limit \( \nu \to +\infty \), non-central \( t \)-distributions asymptote towards Gaussian distributions. In actual practical situations, differences between the two kinds of distributions become effectively irrelevant when \( \nu \geq 50 \), in which case Gaussian distributions may be used to simplify computations.

2.2.3 Exponential distributions

The one-parameter family of exponential distributions,

\[ y_i | \theta, I \sim \text{Exp}(\theta), \]  

(2.31)
2.2. **UNIVARIATE CONTINUOUS DATA**

is regularly employed in modelling distributions for waiting times or spatial distances. For example, the generically dimensionful continuous metrical quantity $y_i$ may represent

- the lifetime in months of a fashion hype,
- the distance in kilometres a commuter travels from their home to their workplace near an industrial centre,
- the time in minutes until the next incoming telephone call in a call centre, or
- the lifetime in seconds of a rainbow.

Main properties of **exponential distributions** are (see, e.g., Rinne (2008) [86, Subsec. 3.9.3]):

Spectrum of values:

$$y_i \in \mathbb{R}_{\geq 0}. \quad (2.32)$$

Probability density function (pdf):

$$f(y_i|\theta, I) = \theta \exp (-\theta y_i), \quad \text{with} \quad \theta \in \mathbb{R}_{>0}, \quad (2.33)$$

and $\theta$ represents a **rate parameter** of physical dimension inverse to $y_i$. Note that the exponential probability density function is normalised with respect to the continuous variable $y_i$ but not with respect to the continuous parameter $\theta$. Its graph is shown in Fig. 2.6 for four different values of $\theta$.

Expectation value and variance:

$$E(y_i) = \frac{1}{\theta} \quad (2.34)$$
$$\text{Var}(y_i) = \frac{1}{\theta^2}. \quad (2.35)$$

**R:** `dexp(y_i, \theta)`, `pexp(y_i, \theta)`, `qexp(p, \theta)`, `rexp(n_{\text{simulations}}, \theta)`

**JAGS:** `dexp(\theta)` (sampling)

**Stan:** `exponential(\theta)` (sampling)

Exponential distributions constitute a special case of the two-parameter family of **Gamma distributions** (cf. Greenberg (2013) [41, p 225]), which will be introduced in Subsec. 3.4.2 below. We remark in passing that, in hierarchical models (see Ch. 8), exponential distributions, which represent a certain type of maximum entropy distribution, may also serve as (weakly or strongly regularising) prior distributions for scale parameters $\theta_2$ of Gauß likelihood functions, or of degree-of-freedom parameters $\nu$ of $t$–likelihood functions; cf. McElreath (2016) [68, p 364], and Kruschke (2015) [58, p 462].
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Figure 2.6: Some examples of exponential sampling distributions for an uncertain continuous quantity \( y \).

### 2.2.4 Pareto distributions

The two-parameter family of univariate **Pareto distributions**, 
\[
y_i \mid \theta, y_{\text{min}}, I \sim \text{Par}(\theta, y_{\text{min}}),
\]
was introduced, to Economics in the first place, by the Italian engineer, sociologist, economist, political scientist and philosopher **Vilfredo Federico Damaso Pareto** (1848–1923); cf. Pareto (1896) [79]. The usually dimensionful continuous positive quantity \( y_i \) could represent, for example,

- the annual revenue of a company listed at the New York Stock Exchange,
- the number of clicks attracted by a video on YouTube that was watched at least once,
- the number of books sold by a writer in a given year, or
- the mass of a galaxy cluster.

**Pareto distributions** possess the features (see, e.g., Rinne (2008) [86, Subsec. 3.11.7]):

Spectrum of values:
\[
y_{\text{min}} \leq y_i \in \mathbb{R}^{>0}.
\]
2.2. UNIVARIATE CONTINUOUS DATA

Probability density function (pdf):

\[
f(y_i | \theta, y_{\text{min}}, I) = \frac{\theta}{y_{\text{min}}} \left(\frac{y_{\text{min}}}{y_i}\right)^{\theta + 1}, \quad \text{with} \quad \theta \in \mathbb{R}_{>0};
\]  

(2.38)

\(\theta\) constitutes a dimensionless scale parameter and \(y_{\text{min}}\) a location parameter of the same physical dimension as \(y_i\). Note that the Pareto probability density function is normalised with respect to the continuous variable \(y_i\), but not with respect to the continuous parameters \(\theta\) and \(y_{\text{min}}\). Its graph is shown in Fig. 2.7 for four different combinations of values of \(\theta\) and \(y_{\text{min}}\).

Expectation value and variance:

\[
E(y_i) = \frac{\theta}{\theta - 1} y_{\text{min}} \quad \text{for} \quad \theta > 1
\]

(2.39)

\[
\text{Var}(y_i) = \frac{\theta}{(\theta - 1)^2(\theta - 2)} y_{\text{min}}^2 \quad \text{for} \quad \theta > 2.
\]

(2.40)

Figure 2.7: Some examples of Pareto sampling distributions for an uncertain continuous quantity \(y\).

\textbf{R}: \texttt{dpareto}(y_i, \theta, y_{\text{min}}), \texttt{ppareto}(y_i, \theta, y_{\text{min}}), \texttt{qpareto}(p, \theta, y_{\text{min}}), \texttt{rpareto}(n_{\text{simulations}}, \theta, y_{\text{min}}) \quad \text{(extraDistr package)}

\textbf{JAGS}: \texttt{dpar}(\theta, y_{\text{min}}) \quad \text{(sampling)}

\textbf{Stan}: \texttt{pareto}(y_{\text{min}}, \theta) \quad \text{(sampling)}
2.3 Multivariate data

The single-datum likelihood functions introduced in this section apply to multivariate data \( y \) from a continuous vector-valued, \( m \)-dimensional \textit{statistical variable} \( Y \). They depend on unobservable and therefore unknown continuously varying scalar-, vector- and matrix-valued parameters. We will here briefly review only the two most frequently used multivariate single-datum likelihood functions for vector-valued continuously varying data.

2.3.1 Multivariate Gauss distributions

Multivariate Gauss processes are described by a single-datum likelihood function for a vector-valued \( y \in \mathbb{R}^{m \times 1} \) given by (see, e.g., Rinne (2008) [86, Subsec. 3.10.4], Gelman et al (2014) [35, Sec. 3.5], or Gill (2015) [39, Sec. 3.5])

\[
    f(y|\mu, \Sigma, I) = \frac{1}{\sqrt{(2\pi)^m \det(\Sigma)}} \exp \left[ -\frac{1}{2} (y - \mu)^T \Sigma^{-1} (y - \mu) \right],
\]

wherein \( \mu \in \mathbb{R}^{m \times 1} \) represents a \textit{mean vector}, and \( \Sigma \in \mathbb{R}^{m \times m} \) a regular \textit{covariance matrix} which is always symmetric and positive semi-definite.

\( \text{R:} \ \text{dmvnorm}(y, \mu, \Sigma), \ \text{rmvnorm}(n_{\text{simulations}}, \mu, \Sigma) \) (\text{mvtnorm} package)

\( \text{JAGS:} \ \text{dnorm}(\mu[1 : m], \Omega[1 : m, 1 : m]) \) (precision matrix: \( \Omega \)) (sampling)

\( \text{Stan:} \ \text{multi_normal}(\mu, \Sigma) \) (sampling)

2.3.2 Multivariate non-central \( t \)--distributions

The generalisation of the three-parameter non-central \( t \)--distribution discussed in Subsec. [2.2.2] to the multivariate case is given by the single-datum likelihood function for a vector-valued \( y \in \mathbb{R}^{m \times 1} \) (see, e.g., Gelman et al (2014) [35, Tab. A.1])

\[
    f(y|\mu, \Sigma, \nu, I) = \frac{\Gamma \left[ \left( \nu + m \right)/2 \right]}{\Gamma \left( \nu/2 \right) (\pi \nu)^{m/2} \sqrt{\det(\Sigma)}} \left[ 1 + \frac{1}{\nu} (y - \mu)^T \Sigma^{-1} (y - \mu) \right]^{-(\nu+m)/2},
\]

where \( \mu \in \mathbb{R}^{m \times 1} \) is a \textit{mean vector}, \( \Sigma \in \mathbb{R}^{m \times m} \) is a regular symmetric and positive semi-definite \textit{covariance matrix}, and \( \nu \geq 1 \) is the positive dimensionless \textit{degrees of freedom parameter}.

\( \text{R:} \ \text{dmvt}((\text{data vector}), (\text{ncp vector}), (\text{scale matrix}), \nu), \ \text{rmvt}(n_{\text{simulations}}, (\text{ncp vector}), (\text{scale matrix}), \nu) \) (\text{mvtnorm} package)

\( \text{JAGS:} \ \text{dmt}(\mu[1 : m], \Omega[1 : m, 1 : m], \nu) \) (precision matrix: \( \Omega \)) (sampling)

\( \text{Stan:} \ \text{multi_student_t}(nu, mu, Sigma) \) (sampling)

2.4 Exponential family

It is of some practical interest to realise that each of the binomial, Poisson, Gauss and exponential distributions belong to a larger class of probability distributions referred to as the \textit{exponential}
family, first discussed by Fisher (1935) \[28\]. These are particularly important as they can be used to quantitatively model data-generating processes for a wide spectrum of observable natural phenomena in a comprehensive fashion. It can be shown that each member of this family constitutes a maximum entropy probability distribution, given specific constraints corresponding to available information in the different contexts where they appear; cf. McElreath (2016) \[68\] p 7, and Sec. 3.3 below.

In a statistical model which aims to capture the distributional features of a statistical variable \(Y\) by employing a set of \(k + 1\) parameters \(\{\theta_0, \ldots, \theta_k\}\), the total-data likelihood function for members of the exponential family exhibits the general structure (cf. Lee (2012) \[63\] Sec. 2.11, Gelman et al (2014) \[35\] Sec. 2.4, Gill (2015) \[39\] Subsec. 4.3.2, or McElreath (2016) \[68\] Sec. 9.2.)

\[
P(\{y_i\}_{i=1}^{n} | \theta_0, \ldots, \theta_k, I) = \left[ \prod_{i=1}^{n} r(y_i) \right] s^n(\theta_0, \ldots, \theta_k) \times \exp \left[ u^T(\theta_0, \ldots, \theta_k) \cdot \sum_{i=1}^{n} t(y_i) \right], \tag{2.43}
\]

with, in general, vector-valued factors \(u \in \mathbb{R}^{(k+1)\times 1}\) and \(t \in \mathbb{R}^{(k+1)\times 1}\). In the special one-parameter case, \(k = 0\), both of these reduce to scalars. The vector-valued quantity \(\sum_{i=1}^{n} t(y_i) \in \mathbb{R}^{(k+1)\times 1}\) is referred to as a sufficient statistic for the set of parameters \(\{\theta_0, \ldots, \theta_k\}\), as in the total-data likelihood function the latter interact with the data \(\{y_i\}_{i=1}^{n}\) only via the former. If a prior probability distribution possesses the same structure as the total-data likelihood function given in Eq. (2.43), then it will be of the conjugate type; cf. Sec. 3.4 below.

We now turn to discuss in the next chapter prior probability distributions, which serve to model initial states of knowledge of a researcher concerning the range of plausible values of a single parameter in specific empirical situations of enquiry.
CHAPTER 2. LIKELIHOOD FUNCTIONS AND SAMPLING DISTRIBUTIONS
Chapter 3

Prior probability distributions

It lies at the very heart of the methodological philosophy of the Bayes–Laplace approach to data analysis and statistical inference that unknown quantities such as parameters in statistical models are treated probabilistically by assigning to them probability distributions that represent a state of knowledge on the part of the researcher. Therefore, there is an immediate necessity in statistical modelling to specify a prior joint probability distribution for all unknown model parameters. This mode of action is to be viewed as a mathematical formalisation of including all available background information I on a matter of interest, such as obtained from related past data analyses, scientific discourse, or even from personal prejudices; cf. Coles (2006) [12, p 61]. The latter option provides the psychological basis for many people to associate with the Bayes–Laplace approach the notion of “subjective probabilities,” although such a view neglects some deep epistemological issues.

Prior probability distributions represent a researcher’s state of knowledge before gaining access to relevant observational data on the problem under investigation. They can be broadly classified into one of three qualitative categories, ranked according to information content:

- uninformative prior probability distributions,
- weakly informative prior probability distributions, and
- sceptical prior probability distributions, resp. regularising prior probability distributions.

For practical reasons, and as an expression of ignorance of a researcher of parameter correlations prior to data analysis, it is often assumed that a prior joint probability distribution for multiple model parameters factorises into a product of single-parameter prior probability distributions ¹ cf. the remarks made in Sec. 1.4.

In the following we will review the cases of single-parameter prior probability distributions that are most important for actual practical model-building, and how some of them can be motivated conceptually. The different options that will be outlined offer a sufficient amount of flexibility in that they let a researcher express a diverse range of prior states of knowledge, from

¹Single-parameter prior probability distributions treat a single parameter in a model-building process probabilistically prior to data analysis. These distributions themselves depend generically on further parameters, which may be specified as fixed, or as adaptive to additional information input.
uninformed to sceptical, by tuning accordingly the free parameters in the various probability distributions employed. We will begin by addressing formal ways of specifying a state of complete ignorance as a reference point for prior probability distributions.

3.1 Principle of indifference

Suppose given a set of $k \in \mathbb{N}$ mutually exclusive and exhaustive propositions $\{A_1, \ldots, A_k\}$, conditioned on background information $I$, so that $P(A_i | A_j | I) = 0$ for $i \neq j$. If $I$ provides no reason to assign a higher plausibility to any one proposition in the set than to any other, thus expressing a state of complete ignorance, then Keynes (1921) [55, p 41] suggested the only consequential probability assignment to be

$$P(A_i | I) = \frac{1}{k}, \quad i = 1, \ldots, k.$$  \hspace{1cm} (3.1)

Originally, this approach was introduced by the Swiss mathematician Jakob Bernoulli (1654–1705), who referred to it as the “principle of non-sufficient reason;” Keynes (1921) [55, p 41] himself preferred to call it the principle of indifference, which is the term that spread in the literature.

The assignment (3.1) yields univariate discrete uniform distributions for sets of propositions $\{A_1, \ldots, A_k\}$ that are properly normalised, in line with Eq. (1.16). The graph of the probability function is shown in Fig. 3.1 below for four different values of $k$.

![Discrete uniform distributions](image)

Figure 3.1: Some examples of discrete uniform distributions for an uncertain integer quantity $x$. 
3.2 Transformation invariance

A different method for establishing in mathematical terms a state of complete ignorance has been elucidated by Jaynes (2003) [48, Subsec. 12.4.1], and by Sivia and Skilling (2006) [92, Subsec. 5.1.2]. Here the requirement imposed on probability distributions for model parameters is that they remain invariant under transformations of the parameters. We will now address the two simplest examples of transformation-invariant single-parameter distributions:

(i) Let \( \rho \in \mathbb{R} \) be a continuous location parameter. When invariance is demanded under a shift of the parameter’s origin, i.e., a translation \( \rho \mapsto \rho + a \), for a constant \( a \in \mathbb{R} \), then the condition

\[
P(\rho|I) \, d\rho = P(\rho + a|I) \, d(\rho + a) \quad \Rightarrow \quad P(\rho|I) \, d\rho = P(\rho + a|I) \, d\rho
\]

needs to be solved to determine an adequate form for \( P(\rho|I) \). The general solution is given by

\[
P(\rho|I) = \text{constant}
\]

which expresses uniformity of \( P(\rho|I) \), irrespective of the value of \( \rho \). To obtain a properly normalised continuous uniform distribution satisfying Eq. (3.16) below, additional information as to the range of \( \rho \in [a, b] \subset \mathbb{R} \) needs to be injected, provided it is available. In that case one obtains

\[
\rho|a,b,I \sim U(a,b) , \quad P(\rho|a,b,I) = \frac{1}{b - a} .
\]

The graph of this probability density function is shown in Fig. 3.2 for four different combinations of values of \( a \) and \( b \).

(ii) Let \( \ell \in \mathbb{R}_{>0} \) be a continuous positive scale parameter. When invariance is demanded under a change of the parameter’s size, i.e., a re-scaling \( \ell \mapsto \beta \ell \), for a positive constant \( \beta \in \mathbb{R}_{>0} \), then the condition

\[
P(\ell|I) \, d\ell = P(\beta \ell|I) \, d(\beta \ell) \quad \Rightarrow \quad P(\ell|I) \, d\ell = \frac{1}{\beta} P(\beta \ell|I) \, d\ell
\]

needs to be solved to determine an adequate form for \( P(\ell|I) \). The general solution is given by

\[
P(\ell|I) = \frac{\text{constant}}{\ell}
\]

which is generally referred to as a Jeffreys prior; cf. Jeffreys (1939) [50], Sivia and Skilling (2006 [92, p 109], or Gill (2015) [39, Subsec. 4.4.2]. To obtain a properly normalised probability distribution satisfying Eq. (3.16) below, additional information as to the range of \( \ell \in [a, b] \subset \mathbb{R}_{>0} \) needs to be injected, provided it is available. In that case one obtains a truncated Jeffreys distribution given by

\[
\ell|a,b,I \sim \text{Jeff}(a,b) , \quad P(\ell|a,b,I) = \frac{1}{\ln(b/a)} \left( \frac{1}{\ell} \right) .
\]

The graph of this probability density function is shown in Fig. 3.3 for four different combinations of values of \( a \) and \( b \).
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Figure 3.2: Some examples of uniform distributions for a continuous location parameter $\rho$.

Figure 3.3: Some examples of truncated Jeffreys distributions for a continuous positive scale parameter $\ell$. 
3.3 Principle of maximum entropy

The most sophisticated technical procedure for systematically converting relevant background information $I$ into usable specific prior probability distributions, while still striving to maintain a practical and profoundly modest state of ignorance, has been proposed by Jaynes (1957) through his principle of maximum entropy; see also Jaynes (2003) Ch. 11.

In this procedure he employs the notion of an information entropy associated with a specific probability distribution for a set of $k \in \mathbb{N}$ mutually exclusive and exhaustive propositions $\{A_1, \ldots, A_k\}$, conditioned on background information $I$, that was developed by the US-American mathematician, electrical engineer, and cryptographer Claude Elwood Shannon (1916–2001); see Shannon (1948) . This is defined by

$$S := - \sum_{i=1}^{k} P(A_i|I) \ln \left( \frac{P(A_i|I)}{m_i} \right). \quad (3.8)$$

As Jaynes (2003) suggests, it may be interpreted as a measure of the “amount of uncertainty” represented by a probability distribution. His modification of the information entropy formula (3.8) by a normalised Lebesgue measure, keeps this non-negative quantity invariant under re-parametrisations of the set of propositions $\{A_1, \ldots, A_k\}$; cf. Jaynes (2003) Sec. 12.3 and Sivia and Skilling (2006) p 116.

To maximise the information entropy of the probability assignment for a given set of propositions $\{A_1, \ldots, A_k\}$ and pertinent background information $I$, Jaynes devises a variational principle for a scalar-valued Lagrange function that is a linear combination of the information entropy (3.8) itself, the normalisation condition (1.16), and a set of $l \in \mathbb{N}$ further constraints $0 = C_i, i = 1, \ldots, l$, each of which represents testable pertinent information $I$. These constraints usually depend on the unknown probabilities $P(A_i|I)$. Setting $p_i := P(A_i|I)$ to simplify notation, the Lagrange function is given by

$$L = - \sum_{i=1}^{k} p_i \ln \left( \frac{p_i}{m_i} \right) - \lambda_0 \left( \sum_{i=1}^{k} p_i - 1 \right) - \sum_{i=1}^{l} \lambda_i C_i; \quad (3.9)$$

the unknown coefficients $\lambda_0$ and $\lambda_i$ are referred to as Lagrange multipliers.

To attain a maximum for the information entropy (3.8), the unknowns $p_i$, $\lambda_0$ and $\lambda_i$ must neces-

---

2 The minus sign preceding the expression on the right-hand side of Eq. (3.8) ensures for the information entropy $S$ a spectrum of non-negative values.

3 Named after the French mathematician Henri Léon Lebesgue (1875–1941).

4 Named after the an Italian mathematician and astronomer Joseph-Louis Lagrange (1736–1813).

5 Here the signs of the second and third terms are motivated by computational convenience.
sarily satisfy the system of \( k + l + 1 \) non-linear algebraic equations given by

\[
0 = \frac{\partial L}{\partial p_j} = -1 - \ln \left( \frac{p_j}{m_j} \right) - \lambda_0 - \sum_{i=1}^{l} \lambda_i \frac{\partial C_i}{\partial p_j}, \quad j = 1, \ldots, k, \quad (3.10)
\]

\[
0 = \frac{\partial L}{\partial \lambda} = \sum_{i=1}^{k} p_i - 1 \quad (3.11)
\]

\[
0 = \frac{\partial L}{\partial \lambda_j} = C_j, \quad j = 1, \ldots, l. \quad (3.12)
\]

The general solution to condition (3.10) is given by

\[
p_j = m_j e^{-(1+\lambda_0)} \exp \left[ - \sum_{i=1}^{l} \lambda_i \frac{\partial C_i}{\partial p_j} \right], \quad j = 1, \ldots, k, \quad (3.13)
\]

while Eqs. (3.11) and (3.12) serve to enforce the normalisation condition and the \( l \) constraints on the \( p_i \). Viewed from a qualitative perspective, it turns out that, amongst all competitors, those probability distributions attain maximum information entropy which spread out probability as evenly as possible between the given propositions, while fully incorporating the available background information by respecting all the given constraints. The extremisation procedure outlined aims at rendering a probability distribution as uniform as possible, in the sense of the principle of indifference. However, the more testable information is available, the more non-uniform the resultant probability distribution will become.

We point the interested reader to Sivia and Skilling (2006) [92, Sec. 5.3] for specific applications of the principle of maximum entropy. Representing for a discrete resp. continuous statistical variable \( Y \) its expectation value and variance as constraints by

\[
0 = C_1 = \sum_{i=1}^{k} y_i p_i - \mu, \quad \text{resp.} \quad 0 = C_1 = \int_{-\infty}^{+\infty} y f(y) \, dy - \mu, \quad (3.14)
\]

\[
0 = C_2 = \sum_{i=1}^{k} (y_i - \mu)^2 p_i - \sigma^2, \quad \text{resp.} \quad 0 = C_2 = \int_{-\infty}^{+\infty} (y - \mu)^2 f(y) \, dy - \sigma^2, \quad (3.15)
\]

and giving the normalisation condition and the information entropy for the continuous case as

\[
0 = \int_{-\infty}^{+\infty} f(y) \, dy - 1 \quad (3.16)
\]

\[
S = \int_{-\infty}^{+\infty} f(y) \ln \left( \frac{f(y)}{m(y)} \right) \, dy, \quad (3.17)
\]

these authors demonstrate how some standard probability distributions for discrete and continuous \( Y \) arise as maximum entropy distributions. In particular, combining the information entropy (3.8) or (3.17) with

(i) the normalisation conditions (1.16) or (3.16) and a uniform Lebesgue measure, the discrete or continuous uniform distributions discussed in Subsecs. 3.1 and 3.2 can be derived;
3.4 Conjugate prior probability distributions

In the first place, conjugate prior probability distributions for single unknown model parameters constitute a welcome computational convenience. But the choice of a conjugate prior in actual data analysis is by no means compulsory. The ultimate selection depends on the quality of the information \( I \) available to a researcher prior to gaining access to relevant empirical data.

Conjugate prior probability distributions are characterised by their property that, in combination with total-data likelihood functions, they generate posterior probability distributions that belong to the very same family of distributions as the priors one started from. In particular, for total-data likelihood functions from the exponential family, discussed in Sec. 2.4 before, it is straightforward to specify related conjugate prior probability distributions; see, e.g., Gelman et al (2014) [35, Sec. 2.4], or Gill (2015) [39, Sec. 4.3] and Tab. 4.1 therein.

In the following, we will discuss the most frequently encountered conjugate prior probability distributions used to describe single unknown model parameters probabilistically.

3.4.1 Beta distributions

The two-parameter family of univariate Beta distributions,

\[
x | \alpha, \beta, I \sim \text{Be}(\alpha, \beta),
\]

is signified by the properties (see, e.g., Greenberg (2013) [41, p 226]):

Spectrum of values:

\[
x \in [0, 1].
\]

Probability density function (pdf):

\[
f(x | \alpha, \beta, I) = \frac{1}{B(\alpha, \beta)} x^{\alpha - 1} (1 - x)^{\beta - 1}, \quad \text{with } \alpha, \beta \in \mathbb{R}_{> 0},
\]

where \( \alpha \) and \( \beta \) are dimensionless shape parameters. The pdf-normalising Beta function is defined via an Euler integral of the first kind by (see, e.g., Rinne (2008) [86, p 340))

\[
B(\alpha, \beta) := \int_0^1 x^{\alpha - 1} (1 - x)^{\beta - 1} \, dx = \frac{\Gamma(\alpha) \Gamma(\beta)}{\Gamma(\alpha + \beta)};
\]
the definition of the Gamma function was given in Eq. (2.27). The graph of the probability density function is shown in Fig. 3.4 for four different combinations of values of $\alpha$ and $\beta$. Note that the continuous uniform distribution on $[0, 1]$ is contained as the special case $\text{Be}(1, 1) = U(0, 1)$.

Expectation value and variance:

$$\begin{align*}
E(x) &= \frac{\alpha}{\alpha + \beta} \\
\text{Var}(x) &= \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}.
\end{align*}$$

Figure 3.4: Some examples of pdfs of Beta distributions for an uncertain quantity $x$.

**R:** dbeta$(x, \alpha, \beta)$, pbeta$(x, \alpha, \beta)$, qbeta$(p, \alpha, \beta)$, rbeta$(n_{\text{simulations}}, \alpha, \beta)$

**JAGS:** dbeta$(\alpha, \beta)$ (sampling)

**Stan:** beta$(\alpha, \beta)$ (sampling)

Prior Beta distributions for a probability for “success” parameter lead to posterior Beta distributions for a probability for “success” when they are combined with the binomial likelihood functions introduced in Subsec. 2.1.2.
3.4. CONJUGATE PRIOR PROBABILITY DISTRIBUTIONS

3.4.2 Gamma distributions

The two-parameter family of univariate Gamma distributions,
\[ x \mid \alpha, \beta, I \sim \text{Ga}(\alpha, \beta) , \]  
(3.24)
has characteristic features (see, e.g., Greenberg (2013) [41, p 225]):

Spectrum of values:
\[ x \in \mathbb{R}_{\geq 0} . \]  
(3.25)

Probability density function (pdf):
\[ f(x\mid \alpha, \beta, I) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} \exp(-\beta x) , \quad \text{with} \quad \alpha, \beta \in \mathbb{R}_{>0} ; \]  
(3.26)
\(\alpha\) constitutes a dimensionless shape parameter, while \(\beta\) is a rate parameter of physical dimension inverse to \(x\). The Gamma function was defined in Eq. (2.27). The graph of the probability density function is shown in Fig. 3.5 for four different combinations of values of \(\alpha\) and \(\beta\).

Expectation value and variance:
\[ \mathbb{E}(x) = \frac{\alpha}{\beta} \]  
(3.27)
\[ \text{Var}(x) = \frac{\alpha}{\beta^2} . \]  
(3.28)

R: \texttt{dgamma}(x, \alpha, \beta), \texttt{pgamma}(x, \alpha, \beta), \texttt{qgamma}(p, \alpha, \beta), \texttt{rgamma}(n_{\text{simulations}}, \alpha, \beta)
JAGS: \texttt{dgamma}(\alpha, \beta) (sampling)
Stan: \texttt{gamma}(\alpha, \beta) (sampling)

Notice that for the particular choice of parameters \(\alpha = \nu/2, \beta = 1/2\), Gamma distributions contain the one-parameter family of \(\chi^2\)-distributions with \(\nu\) degrees of freedom as a special case. Similarly, for \(\alpha = 1, \beta = \beta\), one obtains the one-parameter family of exponential distributions considered in Subsec. 2.2.3; cf. Greenberg (2013) [41, p 225].

Prior Gamma distributions for a precision parameter lead to posterior Gamma distributions for a precision parameter when they are combined with the Gaussian likelihood functions introduced in Subsec. 2.2.1. Also, prior Gamma distributions for a rate parameter lead to posterior Gamma distributions for a rate parameter when, for discrete count data, they are combined with the Poisson likelihood functions introduced in Subsec. 2.1.3 or, for continuous interval data, when they are combined with the exponential likelihood functions discussed in Subsec. 2.2.3.

3.4.3 Inverse Gamma distributions

The two-parameter family of univariate inverse Gamma distributions,
\[ x \mid \alpha, \beta, I \sim \text{IG}(\alpha, \beta) , \]  
(3.29)
Figure 3.5: Some examples of pdfs of Gamma distributions for an uncertain quantity $x$. 

is related to Gamma distribution by a simple inversion transformation of the independent variable, namely $x \rightarrow 1/x$; see, e.g., Greenberg (2013) [41] p 225f. They have the properties:

Spectrum of values:

$$x \in \mathbb{R}_{>0}.$$  

(3.30)

Probability density function (pdf):

$$f(x|\alpha, \beta, I) = \frac{\beta^\alpha}{\Gamma(\alpha)} \frac{1}{x^{\alpha+1}} \exp\left(-\frac{\beta}{x}\right), \quad \text{with} \quad \alpha, \beta \in \mathbb{R}_{>0},$$

(3.31)

where $\alpha$ is a dimensionless shape parameter and $\beta$ a rate parameter of the same physical dimension as $X$. The graph of the probability density function is shown in Fig. 3.6 for four different combinations of values of $\alpha$ and $\beta$.

Expectation value and variance:

$$E(x) = \frac{\beta}{\alpha - 1}, \quad \text{if} \quad \alpha > 1.$$  

(3.32)

$$\text{Var}(x) = \frac{\beta^2}{(\alpha - 1)^2(\alpha - 2)}, \quad \text{if} \quad \alpha > 2.$$  

(3.33)

R: dinvgamma($x, \alpha, \beta$), pinvgamma($x, \alpha, \beta$), qinvgamma($p, \alpha, \beta$), rinvgamma($n_{\text{simulations}}, \alpha, \beta$) (invgamma package)

Stan: inv.gamma($\alpha, \beta$) (sampling)
3.5. **OTHER PRIOR PROBABILITY DISTRIBUTIONS**

3.4.4 **Gauß distributions**

For the two-parameter family of Gauß distributions,

\[
f(x|m_0, \tau_0, I) = \frac{1}{\sqrt{2\pi} \tau_0} \exp \left[ -\frac{1}{2} \left( \frac{x - m_0}{\tau_0} \right)^2 \right], \quad \text{with} \quad m_0 \in \mathbb{R}, \; \tau_0 \in \mathbb{R}_{>0}, \tag{3.34}
\]

the location parameter \( m_0 \) and the scale parameter \( \tau_0 \) both have the physical dimension of \( x \). Prior Gauß distributions for a location parameter lead to posterior Gauß distributions for a location parameter when they are combined with the Gauß likelihood functions introduced in Subsec. [2.2.1](#).

Lastly, we introduce two more families of probability distributions that are also often used as prior probability distributions for certain kinds of single unknown model parameters.
3.5.1 Cauchy distributions

The two-parameter family of univariate Cauchy distributions,

\[ x \mid x_0, \gamma, I \sim \text{Ca}(x_0, \gamma) , \]  

(3.35)

put forward by the French mathematician, engineer and physicist Augustin–Louis Cauchy (1789–1857) is given by (see, e.g., Rinne (2008) [86, Subsec. 3.11.2]):

Spectrum of values:

\[ x \in \mathbb{R} . \]

(3.36)

Probability density function (pdf):

\[
f(x \mid x_0, \gamma, I) = \frac{1}{\pi \gamma} \frac{1}{1 + \left(\frac{x - x_0}{\gamma}\right)^2}, \quad \text{with} \quad x_0 \in \mathbb{R}, \quad \gamma \in \mathbb{R}_{>0},
\]

(3.37)

the location parameter \( x_0 \) and the scale parameter \( \gamma \) both carry the physical dimension of \( x \).

The graph of the probability density function is shown in Fig. 3.7 for four different combinations of values of \( x_0 \) and \( \gamma \). Formally, as follows from Eq. (2.26), Cauchy distributions correspond to non-central \( t \)-distributions with one degree of freedom, \( \nu = 1 \).

Expectation value and variance:

\[
E(x) = \text{does NOT exist due to a diverging integral} \quad \quad \text{(3.38)}
\]

\[
\text{Var}(x) = \text{does NOT exist due to a diverging integral} \quad \quad \text{(3.39)}
\]

The R:

\[
dcauchy(x, x_0, \gamma), \quad \text{pcauchy}(x, x_0, \gamma), \quad \text{qcauchy}(p, x_0, \gamma), \quad \text{rcauchy}(n_{\text{simulations}}, x_0, \gamma)
\]

JAGS:

\[
dt(x_0, 1/\gamma^2, 1) \text{ (sampling)}
\]

Stan:

\[
\text{cauchy}(x_0, \gamma) \text{ (sampling)}
\]

Half-Cauchy distributions (meaning the half to the right of the mode) have become a standard in modern data analysis as weakly regularising prior probability distributions for unknown scale parameters such as standard deviations: in fixed-prior models and, in particular, in adaptive-prior, hierarchical models, in which they control the degree of shrinkage of model parameters for data obtained from different but related groups; cf. Gelman (2006) [33], Gill (2015) [39, p 178], Kruschke (2015) [58, p 558], and McElreath (2016) [68, pp 260, 363].

3.5.2 Laplace distributions

The two-parameter family of univariate Laplace distributions,

\[ x \mid \mu, b, I \sim \text{Laplace}(\mu, b) , \]  

(3.40)

has the properties (see, e.g., Rinne (2008) [86, Subsec. 3.11.5]):
Figure 3.7: Some examples of PDFs of Cauchy distributions for an uncertain quantity $x$.

Spectrum of values:

$$x \in D \subseteq \mathbb{R}.$$  

(3.41)

Probability density function (PDF):

$$f(x|\mu, b, I) = \frac{1}{2b} \exp\left[-\frac{|x - \mu|}{b}\right], \quad \text{with} \quad \mu \in \mathbb{R}, \ b \in \mathbb{R}_{>0};$$  

(3.42)

$\mu$ constitutes a location parameter, $b$ a scale parameter, and both carry the physical dimension of $x$. The graph of the probability density function is shown in Fig. 3.8 for four different combinations of values of $\mu$ and $b$.

Expectation value and variance:

$$\mathbf{E}(x) = \mu$$  

(3.43)

$$\text{Var}(x) = 2b^2.$$  

(3.44)

**R:** dlaplace($x, \mu, b$), plaplace($x, \gamma, b$), qlaplace($p, \gamma, b$), rlaplace($n_{\text{simulations}}, \mu, b$) (extrabistr package)

**JAGS:** ddexp($\mu, 1/b$) (sampling)

**Stan:** double_exponential($\mu, b$) (sampling)

We will now turn to highlight in the next two chapters a few of those prominent rare cases of single- and two-parameter estimations which can be solved analytically.
Figure 3.8: Some examples of pdfs of Laplace distributions for an uncertain quantity $x$. 
Chapter 4

Single-parameter estimation

In the special case of single-parameter estimation in inductive statistical inference, a few analytical solutions for the posterior probability distribution for the unknown parameter in question are available, and well-known. Typically this is possible in those cases where either uniform or conjugate prior probability distributions are employed to express a researcher’s state of knowledge as to the range of values of the unobservable model parameter of interest, before seeing relevant empirical data.

In the single-parameter instance, Bayes’ theorem, in its model-building variant of Eq. (1.24), reduces to

\[
P(\theta | \{y_i\}_{i=1,...,n}, I) = \frac{P(\{y_i\}_{i=1,...,n} | \theta, I) P(\theta | I)}{P(\{y_i\}_{i=1,...,n} | I)}.
\]  

(4.1)

This is the relationship, for which some exact solutions can be derived.

The known analytical solutions for single-parameter posterior probability distributions possess a certain pedagogical merit. Therefore, some prominent examples will be reviewed in the next few sections.

4.1 Binomial-distributed univariate discrete data

Suppose given \( n \) exchangeable and logically independent repetitions of a Bernoulli experiment, with unknown but constant probability for “success,” \( 0 \leq \theta \leq 1 \). Let the observed total number of “successes” in this experiment be

\[
y := \sum_{i=1}^{n} y_i,
\]  

(4.2)

with \( 0 \leq y \leq n \). Then, as discussed in Subsec. (2.1.2), the full data-generating process is described by

\[
y | \theta, n, I \sim \text{Bin}(n, y),
\]  

(4.3)

with total-data likelihood function

\[
P(y | n, \theta, I) = \binom{n}{y} \theta^y (1 - \theta)^{n-y}.
\]  

(4.4)
This is to be viewed as a function of \( \theta \), for fixed data \( n \) and \( y \). Note that, by Eq. (2.43), \( y = n \bar{y} \), where the sample mean of a univariate metrically scaled data set is defined by

\[
\bar{y} := \frac{1}{n} \sum_{i=1}^{n} y_i ,
\]

constitutes a sufficient statistic for \( \theta \).

### 4.1.1 Uniform prior

Adopting for \( \theta \) a uniform prior probability distribution [cf. Eq. (3.4)],

\[
\theta | n, I \sim U(0, 1) ,
\]

and forming the product with (4.4), then, after some algebra that involves the definition of the binomial coefficient in Eq. (2.10) and the Gamma function identity of Eq. (2.28), one is led to the normalised posterior probability distribution for \( \theta \) given by

\[
P(\theta | y, n, I) = \frac{\Gamma(n+2)}{\Gamma(y+1) \Gamma(n-y+1)} \theta^y (1-\theta)^{n-y} ,
\]

i.e., a Beta distribution

\[
\theta | y, n, I \sim \text{Be}(y+1, n-y+1) .
\]

In the present case, it is also easy to obtain the prior predictive probability distribution for \( y \), when no observations have yet been made. With Eq. (1.27) one finds that

\[
P(y|n, I) = \int_0^1 P(y|n, \theta, I) P(\theta|n, I) \, d\theta = \int_0^1 \left( \frac{n}{y} \right)^\theta (1-\theta)^{n-y} \times 1_{\text{prior}} \, d\theta
\]

\[
= \frac{1}{n+1} \times \int_0^1 \frac{(n+1)!}{y!(n-y)!} \theta^y (1-\theta)^{n-y} \, d\theta
\]

\[
= \frac{1}{n+1} \times \int_0^1 \frac{\Gamma(n+2)}{\Gamma(y+1) \Gamma(n-y+1)} \theta^y (1-\theta)^{n-y} \, d\theta
\]

\[
= \frac{1}{n+1} ,
\]

where, in the final step, the normalisation condition for Beta distributions according to Eq. (3.21) was used. Clearly, this result represents an initial discrete uniform probability distribution over the set of possible outcomes, \( y \in \{0, \ldots, n\} \).
Similarly, starting from Eq. (1.28) to calculate the posterior predictive probability distribution for a new observation $y_{\text{new}}$ to be a “success,” given the information that $y$ “successes” were observed in $n$ previous iid-repetitions of the Bernoulli experiment, one arrives at

\[
P(y_{\text{new}} = 1|y, n, I) = \int_0^1 P(y_{\text{new}} = 1|y, n, \theta, I) P(\theta|y, n, I) \, d\theta
\]

\[
= \int_0^1 \theta \frac{\Gamma(n+2)}{\Gamma(y+1) \Gamma(n-y+1)} \theta^y (1-\theta)^{n-y} \, d\theta
\]

\[
= \frac{y+1}{n+2} \times \int_0^1 \frac{\Gamma(n+3)}{\Gamma(y+2) \Gamma(n-y+1)} \theta^y (1-\theta)^{n-y} \, d\theta
\]

\[
= \frac{y+1}{n+2};
\]

(4.10)

again, use was made of the normalisation condition for Beta distributions given in Eq. (3.21). This last result constitutes Laplace’s famous “rule of succession;” cf. Keynes (1921) [55, p 372], Cox (1946) [13, p 11], Jaynes (2003) [48, pp 155, 165], and Gelman et al (2014) [35, p 32]. In the present context, this may actually be interpreted as the posterior expectation value for $\theta$, viz.

\[
\frac{y+1}{n+2} = \frac{2}{n+2} \times \frac{1}{2} + \frac{n}{n+2} \times \frac{y}{n} = E(\theta|y, n, I).
\]

(4.11)

It exemplifies the notion of the posterior probability distribution being a “compromise” between the prior probability distribution and the likelihood function; see, e.g., Gill (2015) [39, p 42] or Kruschke (2015) [58, p 112]. In particular, in this representation it becomes apparent that with increasing sample size $n$ the weight is being pushed away from prior information towards data information, which is a very compelling and elegant feature.

From Eq. (3.23), the posterior variance for $\theta$ amounts to

\[
\text{Var}(\theta|y, n, I) = \frac{(y+1)(n-y+1)}{(n+2)^2(n+3)}.
\]

(4.12)

Further summary statistics can be easily computed with pre-programmed R-functions.

### 4.1.2 Conjugate prior

Alternatively, selecting for $\theta$ instead a conjugate Beta prior probability distribution [cf. Eq. (3.20)],

\[
\theta|\alpha, \beta, n, I \sim \text{Be}(\alpha, \beta)
\]

(4.13)

and forming the product with (4.4), then, again, algebra involving Eqs. (2.10) and (2.28) yields a normalised posterior probability distribution for $\theta$ given by

\[
P(\theta|y, \alpha, \beta, n, I) = \frac{\Gamma(\alpha + \beta + n)}{\Gamma(\alpha + y) \Gamma(\beta + n-y)} \theta^{\alpha+y-1} (1-\theta)^{\beta+n-y-1},
\]

(4.14)
i.e., a Beta distribution

\[ \theta \mid y, \alpha, \beta, n, I \sim \text{Be}(\alpha + y, \beta + n - y) \]  

(4.15)

see, e.g., Lee (2012) [63, Subsec. 3.1.1], Gelman et al. (2014) [35, Sec. 2.4], Gill (2015) [39, Subsec. 2.3.4], or Kruschke (2015) [58, Sec. 6.3]. By means of re-arranging, one finds from Eq. (3.22) that the posterior expectation value for \( \theta \) is given by

\[ E(\theta \mid y, \alpha, \beta, n, I) = \frac{\alpha + y}{\alpha + y + \beta + n - y} = \frac{\alpha + \beta}{\alpha + \beta + n} \times \frac{\alpha}{\alpha + \beta} + \frac{n}{\alpha + \beta + n} \times \frac{y}{n} \]  

(4.16)

it thus can be interpreted as weighted average of the prior mean and the sample mean, where the numerators of the respective weighting factors represent a prior effective sample size \((\alpha + \beta)\) and the actual data sample size \((n)\), respectively. Note that for \( n \gg \alpha + \beta \) the sample mean will dominate.

From Eq. (3.23), the posterior variance for \( \theta \) amounts to

\[ \text{Var}(\theta \mid y, \alpha, \beta, n, I) = \frac{(\alpha + y)(\beta + n - y)}{(\alpha + \beta + n)^2(\alpha + \beta + n + 1)} \]  

(4.17)

Sampling from the single-parameter posterior distribution (4.15) and calculating further summary statistics can be easily accomplished by use of pre-programmed R-functions.

### 4.2 Poisson-distributed univariate discrete data

Suppose given from a Poisson process measurements of \( n \) exchangeable and logically independent counts \( y_i \),

\[ \{y_i\}_{i=1,...,n} \mid \theta, I \overset{iid}{\sim} \text{Pois}(\theta) \]  

(4.18)

so that the total-data likelihood function is

\[ P(\{y_i\}_{i=1,...,n} \mid \theta, I) = \theta^{\sum_{i=1}^{n} y_i} \frac{\prod_{i=1}^{n} y_i! \exp(-n\theta)}{n!} \]  

(4.19)

with unknown rate parameter \( \theta \in \mathbb{R}_{>0} \). By Eq. (2.43), \( \sum_{i=1}^{n} y_i = n\bar{y} \) is a sufficient statistic for \( \theta \).

Assuming for \( \theta \) a conjugate Gamma prior probability distribution [cf. Eq. (3.26)],

\[ \theta \mid \alpha, \beta, I \sim \text{Ga}(\alpha, \beta) \]  

(4.20)

and forming the product with (4.19), then a few simple algebraic manipulations yield a posterior probability distribution for \( \theta \) proportional to

\[ P(\theta \mid \{y_i\}_{i=1,...,n}, \alpha, \beta, I) \propto \theta^{(\alpha + \sum_{i=1}^{n} y_i) - 1} \exp\left[-(\beta + n)\theta \right] \]  

(4.21)

i.e., upon normalisation, a Gamma distribution

\[ \theta \mid \{y_i\}_{i=1,...,n}, \alpha, \beta, I \sim \text{Ga}(\alpha + \sum_{i=1}^{n} y_i, \beta + n) \]  

(4.22)
4.3. GAUSS-DISTRIBUTED UNIVARIATE CONTINUOUS DATA

cf. Lee (2012) [63, Subsec. 3.4.1], or Gelman et al (2014) [35, Sec. 2.6]. From Eq. (3.27), the decomposed posterior expectation value for $\theta$ is

$$E(\theta|\{y_i\}_{i=1,\ldots,n}, \alpha, \beta, I) = \frac{\alpha + \sum_{i=1}^{n} y_i}{\beta + n} \times \frac{\alpha}{\beta} + \frac{n}{\beta + n} \times \frac{\sum_{i=1}^{n} y_i}{n}; \quad (4.23)$$

the prior effective sample size thus amounts to $\beta$. For $n \gg \beta$ the sample mean will dominate.

From Eq. (3.28), the posterior variance for $\theta$ amounts to

$$\text{Var}(\theta|\{y_i\}_{i=1,\ldots,n}, \alpha, \beta, I) = \frac{\alpha + \sum_{i=1}^{n} y_i}{(\beta + n)^2}. \quad (4.24)$$

Sampling from the single-parameter posterior distribution (4.22) and calculating further summary statistics can be easily accomplished by use of pre-programmed R-functions.

4.3 Gauß-distributed univariate continuous data

In this section we will suppose given $n$ exchangeable and logically independent measurements $y_i$ from a Gauß process,

$$\{y_i\}_{i=1,\ldots,n} | \theta_1, \theta_2, I \overset{\text{iid}}{\sim} \mathcal{N}(\theta_1, \theta_2^2). \quad (4.25)$$

To simplify entailing algebra for demonstrational purposes, an assumption that is usually unrealistic in practice will be imposed, viz. that one of the two parameters in the Gauß total-data likelihood (2.21) is known and, therefore, fixed.

4.3.1 Known variance

When the scale parameter $\theta_2 = \sigma_0$ is fixed, the total-data likelihood function is given by

$$P(\{y_i\}_{i=1,\ldots,n} | \theta_1, \sigma_0, I) = \left(\frac{1}{\sqrt{2\pi} \sigma_0}\right)^n \exp \left[-\frac{1}{2\sigma_0^2} \sum_{i=1}^{n} (y_i - \theta_1)^2\right], \quad (4.26)$$

which is to be viewed as a function of an unknown location parameter $\theta_1$. Upon evaluating the $(y_i - \theta_1)^2$-term in the exponent, one finds that $\sum_{i=1}^{n} y_i = n\bar{y}$ is a sufficient statistic for $\theta_1$ according to Eq. (2.43).

Choosing for $\theta_1$ a conjugate Gauß prior probability distribution [cf. Eq. (3.34)],

$$\theta_1 | m_0, s_0, I \sim \mathcal{N}(m_0, s_0^2), \quad (4.27)$$

and forming the product with (4.26), then a few algebraic steps lead to a posterior probability distribution for $\theta_1$ proportional to

$$P(\theta_1|\{y_i\}_{i=1,\ldots,n}, m_0, s_0, \sigma_0, I) \propto \exp \left[-\frac{1}{2} \left(\frac{\theta_1 - \mu_1}{\sigma_1}\right)^2\right], \quad (4.28)$$
CHAPTER 4. SINGLE-PARAMETER ESTIMATION

with posterior expectation value and posterior variance for \( \theta_1 \) given by

\[
\mu_1 := \left( \frac{1}{s_0^2} + \frac{n}{\sigma_0^2} \right)^{-1} \times \left( \frac{1}{s_0^2} m_0 + \frac{n}{\sigma_0^2} \bar{y} \right), \quad \sigma_1^2 := \left( \frac{1}{s_0^2} + \frac{n}{\sigma_0^2} \right)^{-1}.
\]

Upon normalisation, this yields a Gauß distribution

\[
\theta_1 \mid \{y_i\}_{i=1,...,n}, m_0, s_0, \sigma_0, I \sim N(\mu_1, \sigma_1^2);
\]

see, e.g., Lee (2012) [63, Subsec. 2.3.1], Gelman et al (2014) [35, Sec. 2.5], or Gill (2015) [39, Sec. 3.2]. In a fashion identical to previous cases, the posterior expectation value may be decomposed so that

\[
E(\theta_1 \mid \{y_i\}_{i=1,...,n}, m_0, s_0, \sigma_0, I) = \mu_1 = \frac{1/s_0^2}{1/s_0^2 + n/\sigma_0^2} \times \text{prior mean} + \frac{n/\sigma_0^2}{1/s_0^2 + n/\sigma_0^2} \times \bar{y} \text{ sample mean};
\]

the prior effective sample size, 1, and the actual sample size, \( n \), are weighted by the precisions \( 1/s_0^2 \) and \( 1/\sigma_0^2 \), respectively. Depending on the values of these two precisions, the sample mean will usually dominate for \( n \gg 1 \). Sampling from the single-parameter posterior distribution (4.30) and calculating further summary statistics can be easily accomplished by use of pre-programmed \( \mathbb{R} \)-functions.

4.3.2 Known mean

When the location parameter \( \theta_1 = \mu_0 \) is fixed, the total-data likelihood function is given by

\[
P(\{y_i\}_{i=1,...,n} \mid \mu_0, \theta_2^2, I) = \frac{1}{(\sqrt{2\pi})^n} \frac{1}{(\theta_2^2)^{n/2}} \exp \left[ -\frac{1}{2\theta_2^2} \sum_{i=1}^n (y_i - \mu_0)^2 \right],
\]

which is to be viewed as a function of an unknown squared scale parameter \( \theta_2^2 \). By inspection, one finds that \( \sum_{i=1}^n (y_i - \mu_0)^2 =: n v \) is a sufficient statistic for \( \theta_2^2 \) according to Eq. (2.43).

Now choosing for \( \theta_2^2 \) a conjugate inverse Gamma prior probability distribution [cf. Eq. (3.31)],

\[
\theta_2^2 \mid \alpha_0, \beta_0, I \sim IG(\alpha_0, \beta_0),
\]

and forming the product with (4.32), then a little algebra yields a posterior probability distribution for \( \theta_2^2 \) proportional to

\[
P(\theta_2^2 \mid \{y_i\}_{i=1,...,n}, \mu_0, \alpha_0, \beta_0, I) \propto \frac{1}{(\theta_2^2)^{(n+\alpha_0)/2} + 1} \exp \left[ -\left( \frac{\beta_0 + n}{2} v \right) / \theta_2^2 \right],
\]

i.e., upon normalisation, an inverse Gamma distribution

\[
\theta_2^2 \mid \{y_i\}_{i=1,...,n}, \mu_0, \alpha_0, \beta_0, I \sim IG\left(\alpha_0 + \frac{n}{2}, \beta_0 + \frac{n}{2} v\right);
\]
4.4 Exponentially distributed univariate continuous data

Lastly, when there are given from an exponential process measurements of \( n \) exchangeable and logically independent interval lengths \( y_i \),

\[
\{ y_i \}_{i=1,...,n} \mid \theta, I \overset{\text{id}}{\sim} \text{Exp}(\theta),
\]

then the total-data likelihood function is

\[
P(\{ y_i \}_{i=1,...,n} \mid \theta, I) = \theta^n \exp \left( -\theta \sum_{i=1}^{n} y_i \right),
\]

with unknown rate parameter \( \theta \in \mathbb{R}_{>0} \). By Eq. (2.43), \( \sum_{i=1}^{n} y_i = n \bar{y} \) is a sufficient statistic for \( \theta \). Introducing for \( \theta \) a conjugate Gamma prior probability distribution [cf. Eq. (3.26)],

\[
\theta \mid \alpha, \beta, I \sim \text{Ga}(\alpha, \beta),
\]

and forming the product with (4.39), then a few re-arrangements lead to a posterior probability distribution for \( \theta \) proportional to

\[
P(\theta \mid \{ y_i \}_{i=1,...,n}, \alpha, \beta, I) \propto \theta^{(\alpha+n)-1} \exp \left[ -\left( \beta + \sum_{i=1}^{n} y_i \right) \theta \right],
\]

i.e., upon normalisation, a Gamma distribution

\[
\theta \mid \{ y_i \}_{i=1,...,n}, \alpha, \beta, I \sim \text{Ga}(\alpha + n, \beta + \sum_{i=1}^{n} y_i);
\]

cf. Gelman et al (2014) [35 Sec. 2.6]. From Eq. (3.27), the decomposed posterior expectation value for \( \theta \) is

\[
\mathbb{E}(\theta \mid \{ y_i \}_{i=1,...,n}, \alpha, \beta, I) = \frac{\alpha + n}{\beta + \sum_{i=1}^{n} y_i} = \frac{\beta}{\beta + \sum_{i=1}^{n} y_i} \times \bar{y} + \frac{\beta}{\beta + \sum_{i=1}^{n} y_i} \times \frac{n}{\sum_{i=1}^{n} y_i}.
\]
For $\sum_{i=1}^{n} y_i \gg \beta$, the sample mean for $\theta$, which is $n/\sum_{i=1}^{n} y_i = 1/\bar{y}$, will dominate over its prior mean, $\alpha/\beta$.

From Eq. (3.28), the posterior variance for $\theta$ amounts to

$$\text{Var}(\theta | \{y_i\}_{i=1,...,n}, \alpha, \beta, I) = \frac{\alpha + n}{(\beta + \sum_{i=1}^{n} y_i)^2}.$$  \hspace{1cm} (4.44)

Sampling from the single-parameter posterior distribution (4.42) and calculating further summary statistics can be easily accomplished by use of pre-programmed R-functions.

We now turn to discuss some exactly solvable two-parameter estimation problems in the next chapter.
Chapter 5

Joint two-parameter estimation for univariate Gauß processes

The principles remain the same, but the entailing computations become considerably more complex quite quickly, when the posterior joint probability distribution for two or more unknown parameters in a model-building project is to be estimated from background information and available empirical data. In fact, there are not many cases in which this goal can be achieved by means of closed-form analytical solutions after all. To provide a taste of the technical complexities involved in the model-building process in higher dimensions, we will outline in this chapter the derivation of the posterior joint probability distribution and its associated posterior marginal probability distributions in two dimensions for univariate continuous data originating from a Gauß process. In consequence, the discussion to follow proves a wee bit formula-(integration)-heavy, though this should not deter the favourably inclined reader from continuing the exciting journey through modern techniques of inductive statistical inference.

Suppose given a sample of size \( n \) of iid-measurements \( \{y_i\}_{i=1,...,n} \) gained from a univariate Gauß process. Then the total-data likelihood function is constructed as the product of \( n \) copies of the single-datum likelihood function given in Eq. (2.21). In the following we will employ standard notation for the model parameters in a Gauß process context and set \( \theta_1 = \mu \) for the location parameter and \( \theta_2^2 = \sigma^2 \) for the scale parameter. The starting point is thus given by

\[
P(\{y_i\}_{i=1,...,n} | \mu, \sigma^2, I) = \left( \frac{1}{\sqrt{2\pi} \sigma} \right)^n \exp \left[ -\frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \mu)^2 \right] .
\] (5.1)

Then, evaluating first the squared term in the exponent of the exponential function, re-ordering resultant terms, and compactifying again by completing two convenient squares upon adding in a
zero via the identity \( 0 = n\bar{y} - n\bar{y} \) that involves the sample mean, one arrives at

\[
P\left( \{y_i\}_{i=1}^{n} | \mu, \sigma^2, I \right) = \frac{1}{(\sqrt{2\pi})^n (\sigma^2)^{n/2}} \times \exp \left[ -\frac{1}{2\sigma^2} \left( \sum_{i=1}^{n} y_i^2 - 2\mu \sum_{i=1}^{n} y_i + \mu^2 \sum_{i=1}^{n} 1 \right) \right]
\]

\[
= \frac{1}{(\sqrt{2\pi})^n (\sigma^2)^{n/2}} \exp \left[ -\frac{1}{2\sigma^2} \left( \sum_{i=1}^{n} y_i^2 - 2n\bar{y}\mu + n\mu^2 \right) \right]
\]

\[
0 = n\bar{y} - n\bar{y} \equiv \frac{1}{(\sqrt{2\pi})^n (\sigma^2)^{1/2}} \exp \left[ -\frac{1}{2} \left( \frac{\mu - \bar{y}}{\sigma/\sqrt{n}} \right)^2 \right]
\]

\[
\times \frac{1}{(\sigma^2)^{(n-1)/2}} \exp \left[ -\frac{1}{2} \sum_{i=1}^{n} \left( y_i - \bar{y} \right)^2 / \sigma^2 \right]. \quad (5.2)
\]

Altogether, we recognise in this result the product between the kernels of a univariate Gauß distribution on the one-hand side, and of a univariate inverse Gamma distribution on the other, viz.,

\[
P\left( \{y_i\}_{i=1}^{n} | \mu, \sigma^2, I \right) = \frac{1}{(\sqrt{2\pi})^n (\sigma^2)^{1/2}} \exp \left[ -\frac{1}{2} \left( \frac{\mu - \bar{y}}{\sigma/\sqrt{n}} \right)^2 \right]
\]

\[
\times \frac{1}{(\sigma^2)^{(n-1)/2}} \exp \left[ -\frac{1}{2} \sum_{i=1}^{n} \left( y_i - \bar{y} \right)^2 / \sigma^2 \right]. \quad (5.3)
\]

In this last expression we defined a total sum of squared deviations of the univariate data from their common sample mean by

\[
\text{TSS} := \sum_{i=1}^{n} (y_i - \bar{y})^2. \quad (5.4)
\]

By inspection, it becomes apparent that, according to Eq. (2.43), the quantity \( \sum_{i=1}^{n} y_i = n\bar{y} \), which is proportional to the sample mean, constitutes a sufficient statistic for the location parameter \( \mu \). Likewise, the quantity TSS, in terms of which one defines the sample variance, is a sufficient statistic for the scale parameter \( \sigma^2 \).

Let us now supply the total-data likelihood function (5.3) with a bivariate prior joint probability distribution for the model parameters \( \mu \) and \( \sigma^2 \). We will factorise it by making use of the product rule (1.11), so that

\[
P(\mu, \sigma^2 | I) = P(\mu | \sigma^2, I) \times P(\sigma^2 | I) \quad (5.5)
\]

obtains. In the next two sections we will consider specific choices for \( P(\mu, \sigma^2 | I) \) that are motivated by computational convenience and the fact that they lead to closed form solutions for the bivariate posterior joint probability distribution. Of course, both examples possess high practical relevance, too.
5.1 Uniform joint prior

The simplest choice is that of an improper, non-normalised but transformation-invariant uniform prior joint probability distribution for $\mu$ and $\sigma^2$ according to Eqs. (3.3) and (3.6), which takes the form

$$P(\mu, \sigma^2 | I) = c_1 \propto P(\mu | \sigma^2, I) \times c_2 \propto P(\sigma^2 | I),$$

(5.6)

with $c_1 > 0$, $c_2 > 0$. This choice expresses the assumption of initial logical independence between $\mu$ and $\sigma^2$.

Presently the derivation of the posterior joint probability distribution for $\mu$ and $\sigma^2$, which is obtained from multiplying the total-data likelihood function by the prior joint probability distribution, does not require a lot of computational effort. The result exhibits the product structure (see, e.g., Lee (2012) [63, Sec. 2.12], or Gelman et al (2014) [35, Sec. 3.2])

$$P(\mu, \sigma^2 | \{y_i\}_{i=1, \ldots, n}, I) \propto \frac{1}{(\sigma^2)^{1/2}} \exp \left[ -\frac{1}{2} \left( \frac{\mu - \bar{y}}{\sigma/\sqrt{n}} \right)^2 \right] \propto N(\bar{y}, \sigma^2/n)$$

$$\times \frac{1}{(\sigma^2)^{(n-1)/2+1}} \exp \left( -\frac{1}{2} \frac{TSS}{\sigma^2} \right) \propto IG((n-1)/2, TSS/2).$$

(5.7)

Upon normalisation, this gives a bivariate Gauß–inverse Gamma model to describe the uncertainty inherent in the joint estimation of $\mu$ and $\sigma^2$, i.e.\[^1\]

$$\mu, \sigma^2 | \{y_i\}_{i=1, \ldots, n}, I \sim N(\bar{y}, \sigma^2/n) \times IG((n-1)/2, TSS/2).$$

(5.8)

In practice, one is often primarily interested in the posterior probability distribution for a single model parameter, which can be derived from the posterior joint probability distribution by way of marginalisation. That is, averaging the posterior joint probability distribution over the full range of the scale parameter $\sigma^2$, and applying the substitution method to compactify the exponent of the exponential function, one finds that the posterior marginal probability distribution for $\mu$

\[^1\]Sivia and Skilling (2006) [92, Sec. 3.3] discuss the case of estimating $\mu$ and $\sigma^2$ for a univariate Gauß process with improper prior probability distributions that are constants for both parameters.
CHAPTER 5. JOINT TWO-PARAMETER ESTIMATION

is proportional to

\[
P(\mu | \{y_i\}_{i=1,...,n}, I) = \int_0^\infty P(\mu, \sigma^2 | \{y_i\}_{i=1,...,n}, I) \, d\sigma^2
\]

\[
\propto \int_0^\infty \frac{1}{(\sigma^2)^{(n-1)/2+3/2}} \exp \left[ -\frac{1}{2\sigma^2} (TSS + n (\mu - \bar{y})^2) \right] \, d\sigma^2
\]

\[
\propto \left[ TSS + n (\mu - \bar{y})^2 \right]^{-n/2} \times \int_0^\infty t^{(n/2)-1} e^{-t} \, dt
\]

\[
\propto \left[ TSS + n (\mu - \bar{y})^2 \right]^{-n/2} \times \left[ 1 + \frac{1}{n-1} \left( \frac{\mu - \bar{y}}{\sqrt{TSS/(n-1)n}} \right)^2 \right]^{-n/2}
\]

so that, upon proper normalisation, this yields a univariate non-central \(t\)-distribution,

\[
\mu | \{y_i\}_{i=1,...,n}, I \sim t(\bar{y}, \sqrt{TSS/(n-1)n}, n-1) .
\]

(5.9)

Analogously, averaging the posterior joint probability distribution over the full range of the location parameter \(\mu\) leads to the posterior marginal probability distribution for \(\sigma^2\) being proportional to

\[
P(\sigma^2 | \{y_i\}_{i=1,...,n}, I) = \int_{-\infty}^{+\infty} P(\mu, \sigma^2 | \{y_i\}_{i=1,...,n}, I) \, d\mu
\]

\[
\propto \frac{1}{(\sigma^2)^{(n-1)/2+1}} \exp \left( -\frac{1}{2} \frac{TSS}{\sigma^2} \right) \times \int_{-\infty}^{+\infty} \frac{1}{(\sigma^2)^{1/2}} \exp \left[ -\frac{1}{2} \left( \frac{\mu - \bar{y}}{\sigma/\sqrt{n}} \right)^2 \right] \, d\mu
\]

\[
\propto \frac{1}{(\sigma^2)^{(n-1)/2+1}} \exp \left( -\frac{1}{2} \frac{TSS}{\sigma^2} \right) .
\]

(5.11)

Normalisation gives a univariate inverse Gamma distribution,

\[
\sigma^2 | \{y_i\}_{i=1,...,n}, I \sim IG((n-1)/2, TSS/2) .
\]

(5.12)

5.2 Conditionally conjugate joint prior

More flexibility for practical applications offers the choice of a conditionally conjugate prior joint probability distribution for \(\mu\) and \(\sigma^2\). This is expressed by

\[
P(\mu, \sigma^2 | I) \propto \frac{1}{(\sigma^2)^{1/2}} \exp \left[ -\frac{1}{2} \left( \frac{\mu - m_0}{\sigma} \right)^2 \right] \times \frac{1}{(\sigma^2)^{\alpha+1}} \exp \left( -\frac{\beta_0}{\sigma^2} \right) ;
\]

\[
\propto P(\mu | \sigma^2, I): \text{Gauß} \propto P(\sigma^2 | I): \text{inverse Gamma}
\]

(5.13)
the prior probability distribution for $\mu$ here is conditioned on the value of $\sigma^2$.

Next, a number of algebraic manipulations that involve the completion of squares in the exponents of the exponential functions yield the posterior joint probability distribution for $\mu$ and $\sigma^2$ in the product structure given by (see, e.g., Lee (2012) [63, Sec. 2.13], Greenberg (2013) [41, Sec. 4.3], Gelman et al (2014) [35, Sec. 3.3], or Gill (2015) [39, Sec. 3.4])

\[
P(\mu, \sigma^2 | \{y_i\}_{i=1,...,n}, I) \propto \frac{1}{(\sigma^2)^{1/2}} \exp \left[ -\frac{1}{2} \left( \frac{\mu - \mu_n}{\sigma/\sqrt{n + 1}} \right)^2 \right]
\]

\[
\propto N(\mu_n, \sigma^2/(n+1))
\]

\[
\times \frac{1}{(\sigma^2)^{\alpha_n+1}} \exp \left( -\beta_n/\sigma^2 \right),
\]

where we defined

\[
\mu_n := \frac{1}{n+1} m_0 + \frac{n}{n+1} \bar{y}
\]

\[
\alpha_n := \alpha_0 + \frac{n}{2}
\]

\[
\beta_n := \beta_0 + \frac{TSS}{2} + \frac{1}{2} \frac{n}{n+1} (m_0 - \bar{y})^2.
\]

Note that the parameter $\mu_n$ is a weighted average of the prior mean, $m_0$, and the sample mean, $\bar{y}$. Normalisation again obtains a bivariate Gauß–inverse Gamma model for the joint estimation of $\mu$ and $\sigma^2$, viz.,

\[
\mu, \sigma^2 | \{y_i\}_{i=1,...,n}, I \sim N(\mu_n, \sigma^2/(n+1)) \times IG(\alpha_n, \beta_n).
\]

Marginalisation to find the corresponding univariate posterior probability distributions for $\mu$ and $\sigma^2$ proceeds along the same lines as outlined in the previous section. Hence, averaging the posterior joint probability distribution over the full range of the scale parameter $\sigma^2$, and applying the substitution method to compactify the exponent of the exponential function, the posterior marginal probability distribution for $\mu$ is proportional to

\[
P(\mu | \{y_i\}_{i=1,...,n}, I) = \int_0^\infty P(\mu, \sigma^2 | \{y_i\}_{i=1,...,n}, I) \, d\sigma^2
\]

\[
\propto \int_0^\infty \frac{1}{(\sigma^2)^{\alpha_n+3/2}} \exp \left[ -\frac{1}{2\sigma^2} \left( 2\beta_n + (n+1) (\mu - \mu_n)^2 \right) \right] \, d\sigma^2
\]

\[
\propto \left[ 2\beta_n + (n+1) (\mu - \mu_n)^2 \right]^{-(\alpha_n+1/2)} \times \int_0^\infty \left\{ \frac{(\alpha_n+1/2)-1}{\Gamma((\alpha_n+1/2)-1)} e^{-t} \, dt \right\}
\]

\[
\propto \left[ 2\beta_n + (n+1) (\mu - \mu_n)^2 \right]^{-(\alpha_n+1/2)}
\]

\[
\propto \left[ 1 + \frac{1}{2\alpha_n} \left( \frac{\mu - \mu_n}{\sqrt{(\beta_n/\alpha_n)/(n+1)}} \right)^2 \right]^{-(2\alpha_n+1)/2},
\]

(5.19)
so that, after normalisation, a non-central $t$–distribution arises,
\[
\mu \mid \{y_i\}_{i=1,...,n}, I \sim t(\mu_n, \sqrt{\beta_n/\alpha_n}/(n+1), 2\alpha_n).
\] (5.20)

Lastly, averaging the posterior joint probability distribution over the full range of the location parameter $\mu$, the kernel of the posterior marginal probability distribution for $\sigma^2$ is given by
\[
P(\sigma^2 \mid \{y_i\}_{i=1,...,n}, I) = \int_{-\infty}^{+\infty} P(\mu, \sigma^2 \mid \{y_i\}_{i=1,...,n}, I) \, d\mu
\]
\[
\propto \frac{1}{(\sigma^2)^{\alpha_n+1}} \exp\left(-\frac{\beta_n}{\sigma^2}\right) \times \left[ \frac{1}{(\sigma^2)^{1/2}} \exp\left(-\frac{1}{2} \left(\frac{\mu - \mu_n}{\sigma/\sqrt{n+1}}\right)^2\right) \right] \, d\mu
\]
\[
\propto \frac{1}{(\sigma^2)^{\alpha_n+1}} \exp\left(-\frac{\beta_n}{\sigma^2}\right),
\] (5.21)
and normalisation converts this into a univariate inverse Gamma distribution,
\[
\sigma^2 \mid \{y_i\}_{i=1,...,n}, I \sim IG(\alpha_n, \beta_n).
\] (5.22)

Sampling from all four of the exact posterior marginal probability distributions given above, and calculating further summary statistics, can be easily accomplished by use of pre-programmed R-functions.

The extension of the parameter estimation procedure discussed in this section to cases of data from Gauß processes with more than two model parameters is conceptually (though not computationally) straightforward. In the next chapter we will describe in some detail how multivariate posterior joint probability distributions and their marginal accomplices over multi-dimensional parameter spaces can be simulated numerically by resorting to techniques that make use of Markov Chain Monte Carlo iteration codes, so they can be used in inductive statistical inference.
Chapter 6

Fitting and assessing generalised linear models

So how, in the context of a research problem of interest, does one pursue the building of a concrete statistical model from relevant background information and direct observational or experimental evidence, when the related model parameter space becomes high-dimensional due to problem-inherent complexity, and closed-form analytical solutions are no longer possible?

Regression analysis of quantitative–empirical data has long been the workhorse of inductive statistical inference. Its prime objective is the construction of an empirically validated statistical model which is to be viewed as a representation of a specific scientific theory in the realm of one’s research activities. In the Bayes–Laplace approach the construction of a statistical model means foremost determining a posterior joint probability distribution for a certain finite number of unknown model parameters from a suitable joint prior probability distribution for these model parameters and the sample measurements for the different statistical variables the researcher included in her/his portfolio on the grounds of intensive theoretical considerations. Making valuable progress in the task of finding the sought-after posterior joint probability distribution has, by now, been possible for a few decades via employing one of the many well-distributed powerful and efficient numerical algorithms for simulation that yield discrete approximations of an accuracy sufficient for reliable inference. For example, in this way hitherto unknown bivariate correlations between essential model parameters can be learned, and also the posterior marginal probability distributions for single model parameters that are of central interest can be captured. Any statistical model, whether obtained by analytical means or via simulation, needs to be checked for its sensitivity to the prior assumptions injected in the model-building process, and it also has to be assessed for its posterior predictive accuracy.

We will outline in the following the main steps of regression analysis within the Bayes–Laplace approach for different types of quantitative–empirical data in the context of generalised linear models (see Nelder and Wedderburn (1972) [74]). We will describe how the numerical approximation of high-dimensional posterior joint probability distributions can be activated within some of the many freely available software implementations in R of the most reliable and widespread simulation algorithms. To keep matters simple, we will be working in this chapter exclusively with fixed prior probability distributions for each of the unknown model parameters.
CHAPTER 6. FITTING AND ASSESSING GENERALISED LINEAR MODELS

6.1 Generalised linear models

Let us first introduce some compact notation that is to be used in the applications presented in subsequent sections. The empirical data, \( \{ x_{ij} \}_{i=1}^n \), for a set of \( k \in \mathbb{N} \) independent variables, is to be collected in a design matrix,

\[
X := \begin{pmatrix}
1 & x_{11} & x_{12} & \ldots & x_{1k} \\
1 & x_{21} & x_{22} & \ldots & x_{2k} \\
\vdots & \vdots & \ddots & \vdots \\
1 & x_{n1} & x_{n2} & \ldots & x_{nk}
\end{pmatrix} \in \mathbb{R}^{n \times (k+1)},
\]

(6.1)

and is conventionally augmented by a column of ones, \( x_{i0} = 1 \), for reasons that will soon become apparent. The data contained in the design matrix \( X \) can be either metrically scaled, or of a binary nature as arising from indicator variables that take values in the set \( \{0, 1\} \).

In the model-building process, the data for the independent variables will be employed as predictors, and, typically, no assumptions are made concerning their distributional origin, or as to the accuracy of their measurement. Potential problems are associated with the metrical data in the design matrix \( X \). When multicollinearity abounds, the posterior predictive accuracy of a statistical model is weakened from the outset; see, e.g., McElreath (2016) [68, Sec. 5.3.]. Multicollinearity amounts to redundant information in the \( X \)-data that is due to strong bivariate correlations between some of the metrically scaled "independent variables." It has the effect that posterior probability distributions for model parameters become unnecessarily spread out more strongly, and so uncertainty will increase. The inclusion of redundant information in the model-building process should thus be avoided. In the following we will assume that bivariate correlations in the metrical part of the \( X \)-data are negligibly small.

Next, a vector of \( k + 1 \) real-valued regression coefficients is introduced by

\[
\beta := \begin{pmatrix}
\beta_0 \\
\beta_1 \\
\vdots \\
\beta_k
\end{pmatrix} \in \mathbb{R}^{(k+1) \times 1},
\]

(6.2)

so that arbitrary linear combinations of the data for the independent variables can be represented by the matrix product

\[
X \beta.
\]

(6.3)

The \( n \) measured values \( \{ y_i \}_{i=1}^n \) for the single dependent variable are assembled in a vector

\[
y := \begin{pmatrix}
y_1 \\
y_2 \\
\vdots \\
y_n
\end{pmatrix} \in \mathbb{R}^{n \times 1}.
\]

(6.4)

The \( y \)-data may be discrete or continuous, it may be binary by nature, represent counts, or take any real value from a pre-specified range. The data for the dependent variable \( y \) is to be predicted
from the data for the independent variables contained in $X$ via the statistical model one seeks to construct. In describing the model-building process, we will limit considerations to the discussion of additive main effects of the independent variables, and point to the literature for the numerous possibilities of including non-additive interaction effects. The latter are to be seen as an option for devising statistical models of a higher degree of flexibility, though at the price of being more difficult to interpret.

In generalised linear models (GLM), the relationship between the dependent variable $y$ and the independent variables contained in $X$ need no longer be linear, nor does the dispersion of the data have to be of the Gaussian type; see Nelder and Wedderburn (1972) [74], Lee (2012) [63, Sec. 6.7], Gelman et al (2014) [35, Ch. 16], Kruschke (2015) [58, Sec. 15.4], Gill (2015) [39, App. A], or McElreath (2016) [68, Sec. 9.2.]. GLM exhibit a generic two-level structure, comprising both a deterministic and a probabilistic component. These are given by

$$E(y|X, \beta, \text{dispersion parameter(s)}, I) = f^{-1}(X\beta) =: \mu \quad \text{(6.5)}$$

$$y|X, \beta, \text{dispersion parameter(s)}, I \sim \text{pdf}(\mu, \text{dispersion parameter(s)}) \quad \text{(6.6)}$$

Eq. (6.5) relates the expectation value $\mu$ for $y$ to the deterministic linear form $X\beta$ via a continuously differentiable and invertible scalar-valued inverse link function, $f^{-1}$, while Eq. (6.6) represents a suitable total-data likelihood function for the $y$-data-generating process, which, besides $\mu$, may also depend on some dispersion parameter(s).

In preparation of the subsequent discussion on the application of iterative numerical simulations for advancing the building of a statistical model, we draw the reader’s attention to the empirical fact that standardisation of the metrically scaled components in the $y$- and $X$-data, and, consequently, of the related regression coefficients $\beta$, renders iterative numerical simulations more efficient by reducing autocorrelation in the sampling outcomes. This immediately improves the mixing properties of the sampling outcomes, and, ultimately, the overall numerical stability of the approximative solutions for posterior probability distributions; cf. Kruschke (2015) [58, Sec. 17.2] and McElreath (2016) [68, p 226]. Standardisation amounts to a homogenisation of scales. It proves to be a straightforward algebraical exercise to transform back variables and model parameters from standardised scales to original scales, once simulations have been completed.

### 6.2 Monte Carlo sampling algorithms

The Polish–US-American mathematician and nuclear physicist Stanislaw Marcin Ulam (1909–1984) and the Hungarian–US-American mathematician, physicist and computer scientist John von Neumann (1903–1957) pioneered the development of a family of algorithmic techniques that have come to be known across the empirical scientific disciplines as Monte Carlo simulations. For their numerical experiments these researchers employed the first generation of computers. The specific term “Monte Carlo” (MC) was coined as a code name for undisclosed activities in a joint paper by Metropolis and Ulam (1949) [70]. It is a historical fact that the first powerful simulation algorithms were a spin-off of intense conceptual research work at Los Alamos National Laboratory, NM, USA during the 1940ies and 1950ies which was invested with the aim of acquiring nuclear fission and fusion bombs.
The developments on the algorithmic front were followed from the 1990ies onwards by revolutionising technological advances in the hardware sector that triggered an incredible boost of computing power on standard household notebooks and similar computing devices. With boundary conditions so hospitable to transformation, the ensuing Markov chain Monte Carlo (MCMC) simulation techniques and their integration into the Bayes–Laplace approach to data analysis and statistical inference were offered a real chance to excel. The term “Markov Chain” refers to the property of the algorithms driving the simulations that an iteration step in a multi-dimensional parameter space to a new position depends only on the present position, and not on any earlier positions. The targeted high-dimensional, stationary posterior joint probability distribution used in inductive statistical inference is gradually built over typically thousands of iteration steps.

There are three types of MCMC sampling algorithms that find widespread use in statistical model-building:

1. The Metropolis–Hastings (MH) sampling algorithm was originally put forward in the paper by Metropolis et al. (1953) [71], and significantly upgraded by Hastings (1970) [43] nearly two decades later. The basic principles of MH sampling are nicely explained and motivated with simple simulations by Kruschke (2015) [58, Sec. 7.2] and by McElreath (2016) [68, Sec. 8.2]. Full details of the MH sampling algorithm are given by Greenberg (2013) [41, Sec. 7.2] and by Gill (2015) [39, Sec. 10.4].

Some MH routines are contained in the R package MCMCpack by Martin et al. (2011) [67]. Given how the core proposal distribution, the acceptance ratio and the decision rule are designed to operate, the MH sampling algorithm does not necessarily update simulated parameter values and their associated posterior joint probability distribution in every iteration step; it so proves computationally less efficient.

2. The Gibbs sampling algorithm, a special case of the MH sampling algorithm, was developed by Geman and Geman (1984) [36], and popularised through an influential review paper by Gelfand and Smith (1990) [41]. This method requires as input a complete set of analytically expressible full conditional probability distributions for all the model parameters involved. The simulated parameter values and their associated conditional probability distributions are being updated in cyclical order, one in every iteration step, while holding the remaining ones fixed. Consequently, the targeted posterior joint probability distribution is improved in every iteration step and no computing time is squandered. The Gibbs sampling algorithm is up to now the most frequently employed MCMC simulation method. Full details of its structure are given by Greenberg (2013) [41, Sec. 7.1] and by Gill (2015) [39, Sec. 10.3].

The MRC Biostatistics Unit at the University of Cambridge, UK spearheaded the dissemination of the Gibbs sampling algorithm with their BUGS (“Bayesian inference Using Gibbs Sampling”) project. The BUGS code is freely available from the website

\footnote{To put this into perspective: today, for example, every average mobile telephone outperforms by a few orders of magnitude the gigantic computing machines that were available to NASA when landing human beings on the Moon during the late 1960ies and early 1970ies. See URL (cited on August 7, 2018): www.zmescience.com/research/technology/smartphone-power-compared-to-apollo-432/}

\footnote{Named after the US-American scientist Josiah Willard Gibbs (1839–1903).}
6.3 MCMC SIMULATIONS WITH JAGS

www.mrc-bsu.cam.ac.uk/software/bugs/ and its use is described by Lunn et al (2000) [66]. A closely related product is the GNU-licensed software package JAGS (“Just Another Gibbs Sampler”) developed by Martyn Plummer that is available from the website mcmc-jags.sourceforge.net; see Plummer (2016, 2017) [83, 84]. JAGS can be operated in an \( R \) environment upon loading the packages rjags and coda; cf. Plummer (2016) [83] and Plummer et al (2006) [85]. The \( R \) package runjags by Denwood (2016) [17] offers the possibility for parallel MCMC generation with JAGS by activating more than one processor on the computing device one uses for the simulation.

3. The Hamiltonian Monte Carlo (HMC) sampling algorithm was devised by Duane et al (1987) [18] for simulating the quantum dynamic motion of nuclear particles that are subjected to the strong nuclear force. In broad terms, the method models a trapped massive quantum point particle that is moving under the influence of an external attractive potential. The acceleration experienced by such a particle is proportional to the local spatial gradient (“slope”) of the external potential. When adapted to the type of simulations needed in statistical modelling, one finds that the HMC sampling algorithm traverses a high-dimensional parameter space and scales a posterior joint probability distribution much more efficiently than either of the HM and Gibbs variants. This is of great advantage especially when simulating very complex, multi-level hierarchical models. Qualitative details of the HMC sampling algorithm are described by Kruschke (2015) [58, Sec. 14.1] and by McElreath (2016) [68, Sec. 8.2.].

The leading implementation of the HMC sampling algorithm is the Stan code distributed freely by the Stan Development Team (mc-stan.org); cf. Stan Development Team (2017) [94]. Its operation in an \( R \) environment requires installation of the package rstan, also programmed by the Stan Development Team (2018) [95].

On the technical side it is worthwhile pointing out that in order to maintain numerical stability and accuracy the implementations of all three types of MCMC sampling algorithms operate with the natural logarithms of likelihood functions and prior and posterior probability distributions. In this way it is possible to handle successfully extremely tiny probability values as they are commonplace when probability needs to be spread out across multiple directions in a high-dimensional parameter space.

The application of one of the MC sampling algorithms in this list, e.g., when operating their implementation in an \( R \) environment, yields a discretised approximation to the targeted posterior joint probability distribution for a usually large set of unknown model parameters. Conceptually these discretised approximations to a posterior joint probability distribution, determined by Eq. (1.24), constitute higher-dimensional generalisations of the very structure of the contingency table displayed in Tab. [1.1].

6.3 MCMC simulations with JAGS

In this section we will now describe how to construct some standard GLMs from empirical data and relevant background information by means of MCMC simulations in JAGS, when operated from \( R \). We give the corresponding commands for HMC simulations in Stan in App. [B].
The process of building a statistical model from MCMC simulations comprises four main steps:

1. model specification
2. model fitting
3. model assessing
4. model application

We will here focus on the first three.

Before looking into the details, we briefly comment on the way continuously varying quantities of interest can be numerically approximated using the output of MCMC simulations. Probability-weighted integrals of continuous functions \( f \) of a single model parameter \( \theta \) are approximated by (see Gill (2015) \[39, Eq. (9.3)\] or Kruschke (2015) \[58, Eq. (10.7)\])

\[
\int_{\theta_{\text{range}}} f(\theta) \, P(\theta|I) \, d\theta \approx \frac{1}{n} \sum_{\theta_i \sim P(\theta|I)} f(\theta_i),
\]  

(6.7)

where \( n \) denotes the total number of values \( \theta_i \) sampled from the numerically simulated distribution \( P(\theta|I) \). The principle of approximation underlying this relation can be transferred to obtaining from the output of MCMC simulations discretised versions of the higher-dimensional integrals over the multivariate posterior joint probability distribution that express the univariate posterior marginal probability distributions for each of the \( k + 1 \) model parameters \( \beta_i \in \{\beta_0, \ldots, \beta_k\} \).

This is given by

\[
P(\beta_0, \ldots, \beta_k|y, X, I) \approx \frac{1}{n} \sum_{\beta_0 \sim P(\beta_0|y, X, I)} \cdots \sum_{\beta_k \sim P(\beta_k|y, X, I)} P(\beta_0, \ldots, \beta_k|y, X, I),
\]

(6.9)

which, conceptually, corresponds to a direct application of the marginalisation rule that was illustrated in Tab.1.1 of Ch.1. \( P(\beta_0, \ldots, \beta_k|y, X, I) \) denotes the numerically simulated posterior joint probability distribution.

So now let us address the main elements of MCMC simulations of posterior probability distributions with JAGS, and how the output so obtained can be checked for reliability.\(^3\) Comment lines in JAGS code are to be preceded by a hashtag symbol “#,” in full analogy to comment lines in R code. Please refer to the JAGS user manual by Plummer (2017) \[84, Sec. 4\] for further information on running JAGS from R.

\(^3\)For HMC simulations with Stan from R, McElreath makes available an easy to use routine called map2stan, which is contained in his package rethinking; see McElreath (2016) \[69\].
6.3. MCMC SIMULATIONS WITH JAGS

6.3.1 Specification of empirical data

We begin by loading into R the empirical data to be analysed, assuming that it does not contain missing values and that it is available in a data file of the *.csv-format. If the data file is in a different format, the R Data Import/Export manual at the website cran.r-project.org/doc/manuals/r-release/R-data.html advises the reader on how to proceed. The empirical data typically comprises measurements for a single dependent variable $y$ and for $k \in \mathbb{N}$ independent variables which have been gathered in a matrix $X$ (here, for simplicity, without a first column worth of ones!). The sample size be $n \in \mathbb{N}$. For the performance of MCMC simulations with JAGS, we also have to load the R package rjags. All of this information is communicated to R via the code below, as well as specifying the number of independent groups from which data was obtain, should this option apply to the case at hand.

Listing 6.1: Gibbs sampling with JAGS in R: specification of empirical data.

```r
# Load R package rjags
library("rjags")

# Load a specific data set from a *.csv file, creating a R data.frame
dataSet = read.csv( "<filename.csv>" , header = TRUE )

# Identify dependent and independent variables, sample size, number of independent variables, number of groups
y = dataSet[,"yVarName"]
X = as.matrix( dataSet[,c("xVarName1", ..., "xVarNamek")], ncol = k )
nSample = length(y)
nIndVars = ncol(X)
gp = as.numeric( dataSet[,"groupVarName"] ) # if relevant
nGroups = length( unique(gp) ) # if relevant

# Specify data list for JAGS simulations
dataList = list(
  nSample = nSample ,
  nIndVars = nIndVars ,
  nGroups = nGroups , # if relevant
  y = y ,
  X = X , # capital X!
  gp = gp # if relevant
)
```

6.3.2 Standardisation and specification of single-datum likelihood function and of prior probability distributions

In the next block of JAGS code in R, the metrically scaled and binary indicator data in the $y$- and $X$-input is subjected to standardisation for reasons given in Sec. 6.1. Foremost, the next block specifies for a statistical model to be fitted to the empirical data the single-datum likelihood function and the prior probability distribution for every single model parameter. Note that the
prior probability distributions enter the MCMC simulations of the multivariate posterior joint probability distribution only once, while the empirical data as a whole enters via the single-datum likelihood function a total of \( n \) times. The data and model blocks together need to be enclosed in an R string command as shown below.

Listing 6.2: Gibbs sampling with JAGS in R: standardisation of metrically scaled empirical data and specification of single-datum likelihood function and of prior probability distributions for model parameters.

```r
# JAGS data transformation and model: use a string command in R
modelString = "<following specifications to be inserted here>"

data {
    # Standardisation of dependent variable data
    ...
    # Standardisation of independent variables data
    ...
}

model {
    for ( i in 1:nSample ) {
        # Specify single-datum likelihood function
        y[i] ~ likelihoodFunction( parameter 1 , ... ,
                                    parameter k+1 )

        # Specify inverse link function, when applicable
        mu[i] <- ...

        # Specify prior distributions for k+1 model parameters
        parameter 1 ~ priorDistribution 1
        ...
        parameter k+1 ~ priorDistribution k+1
    }
}
```

6.3.3 Initialisation of MCMC simulations

The user may specify for the MCMC simulations with JAGS initial values for all model parameters. This option is optional. It can be a useful corrective tool, e.g., when one finds that the MCMC simulations have difficulties in locating the maximum of a unimodal posterior joint probability distribution. Most importantly, however, in this block the user specifies the number of Markov chains to be simulated.

Listing 6.3: Gibbs sampling with JAGS in R: specifying initial values for model parameters and initialisation of MCMC simulations.

```r
# Set initial values for k+1 model parameters (optional)
```
6.3. MCMC SIMULATIONS WITH JAGS

initList = function() {
  list(
    "parameter_1" = <value> , # parameter names in quotation marks
    ...,
    "parameter_k+1" = <value>
  )
}

# Initialise random number generator so simulations can be
# reproduced (optional)
set.seed(<positiveInteger>)

# Initialisation of JAGS simulations
modelJAGS = jags.model(
  textConnection(modelString) ,
  data = dataList ,
  inits = initList , # (optional)
  n.chains = <number of Markov chains to be generated>
)

6.3.4 Gibbs MCMC sampling

Now the core of the MCMC simulations with JAGS follows. When the MCMC simulations have
successfully initialised in the previous step, first a burn-in period with on the order of one thou-
sand iterations or more is activated. This gives the Gibbs sampler in JAGS the chance to find the
stationary distribution that is to approximate the multivariate posterior joint probability distri-
bution of interest. The data generated in this run is being discarded. The actual simulated data
to be used for inference is then generated and stored in a subsequent step. In particular, the user
specifies explicitly by name those model parameters for which she/he wants to obtain a MCMC
sample representation of the associated univariate posterior marginal probability distribution.
They also specify the number of iterations per Markov chain to be generated. The thin option
provides a tool for reacting to simulations that show a high degree of autocorrelation in the gener-
ated Markov chains. Finally, it is of some practical use to merge the simulated data from multiple
Markov chains in a single output in a matrix-valued MCMC object.

Listing 6.4: Gibbs sampling with JAGS in R: performance of burn-in and MCMC sampling.
# Burn-in period
update( modelJAGS , n.iter = <number of burn-in iterations> )

# Execution of JAGS simulations: saving simulated posterior samples;
# names of sampled parameters to be enclosed in quotation marks
modSim = coda.samples(
  model = modelJAGS ,
  variable.names = c( "parameter_1" , ... , "parameter_k+1" ) ,
  n.iter = <number of iterations> ,
  thin = <step size for thinning> # default: 1
6.3.5 Analysis of convergence properties of Markov chains

Tools for the analysis of the convergence properties of the MCMC simulations with JAGS are contained in the \textit{R} package \texttt{coda} by Plummer \textit{et al} (2006) \cite{plummer2006}, which is automatically loaded when calling the package \texttt{rjags}. These tools comprise a visualisation of the convergence and mixing properties of the Markov chains for each model parameter by means of trace plots, the calculation of the value of the benchmark Gelman–Rubin convergence diagnostic (which should be as close to the value 1 as possible), the determination of the degree of autocorrelation in the Markov chains for each model parameter, and the related effective MC sample size.

\begin{verbatim}
# Trace plots of MC chains for each parameter simulation
plot(modSim, ask = TRUE)

# Gelman-Rubin diagnostic for each parameter simulation
# (should be very close to 1)
gelman.diag(modSim)

# Autocorrelation of MC chains for each parameter simulation
# (should decline rapidly)
autocorr.diag(modSim)
autocorr.plot(modSim)

# Effective MC sample size for each parameter simulation
# (the larger, the better)
effectiveSize(modSim)
\end{verbatim}

6.3.6 Description of posterior probability distributions

In the last block of JAGS code in \textit{R} to be described here, properties of the MCMC sample representation of the univariate \textit{posterior marginal probability distribution} for each model parameter, and of the bivariate correlations between the latter are made explicit. This comprises information on the values of the mean, standard deviation, and some selected quantiles, the plotting of the graph of the \textit{pdf}, and the determination of the limits of highest posterior density intervals, the default setting for the probability enclosed of which is 95\%. In addition, the bivariate correlation matrix for the simulated model parameters is calculated, and mutual dependencies visualised via a scatter plot matrix.
6.4. LINEAR REGRESSION

Listing 6.6: Gibbs sampling with JAGS in R: description of posterior marginal probability distributions and of bivariate correlations.

```r
# Summary of simulated posterior marginal for each parameter
densplot(modCsim[,"parameter_1"] )
...
densplot(modCsim[,"parameter_k+1"] )

# Highest posterior density interval for each parameter; default: 95%
HPDinterval(modCsim)

# Bivariate correlation matrix for parameter simulations
cor( as.matrix(modCsim) )

# Bivariate scatter plot matrix for parameter simulations
pairs( as.matrix(modCsim) )

We will leave the MCMC simulations with JAGS of posterior predictive distributions until later.

6.4 Linear regression

As a first specific application of MCMC simulations with JAGS in R, we turn to address linear regression. This serves to model a linear relationship between data \( y \) for a single metrically scaled dependent variable, and data for \( k \in \mathbb{N} \) independent variables contained in \( X \), which may either be metrically scaled, or binary indicators. Many examples with one or more independent variables can be found in the discussions given by Sivia and Skilling (2006) [92, Subsec. 3.5.1], Albert (2009) [2, Sec. 9.2], Kruschke et al. (2012) [59], Lee (2012) [63, Sec. 6.3], Greenberg [41, Sec. 8.1], Gelman et al. (2014) [35, Ch. 14], Andreon and Weaver (2015) [4, Ch. 8], Kruschke (2015) [58, Ch. 18], or McElreath (2016) [68, Sec. 4.4].

One of the most frequently encountered approaches to devising a linear regression model is to start from a maximum entropy perspective and choose a Gaussian single-datum likelihood function according to Eq. (2.21), with a homogeneous variance, and supplement it with a conditionally conjugate Gaussian-inverse Gamma prior joint probability distribution for the unknown model parameters \( \beta \) and \( \sigma^2 \), in analogy to the application discussed in Sec. 5.2. The assumption of homogeneous
variance is commonly known as **homoscedasticity**. We thus obtain

\[
\begin{align*}
\text{likelihood: } & \quad y \mid X, \beta, \sigma^2, I \overset{\text{ind}}{\sim} N(\mu, \sigma^2) \tag{6.10} \\
\text{inverse link function: } & \quad \mu = X\beta \tag{6.11} \\
\text{priors: } & \quad \beta_0 | \sigma^2 \sim N(\mu_0, \sigma_0^2) \quad \text{(for intercept)} \tag{6.12} \\
& \quad \beta | \sigma^2 \sim N(0, \tau_0^2) \tag{6.13} \\
& \quad \sigma^2 \sim IG(\alpha_0, \delta_0) \tag{6.14}
\end{align*}
\]

where \( \mu_0, \sigma_0^2, \tau_0^2, \alpha_0, \text{ and } \delta_0 \) denote fixed hyperparameters of the conditionally conjugate Gaussian–inverse Gamma prior joint probability distribution. Note that in Eq. (6.13) zero-centred Gaussian prior probability distributions were specified for the unknown regression coefficients \( \beta \), apart from \( \beta_0 \).

This choice is to represent scepticism as to the presence of any of these regression coefficients in a best-fit model.

Presently the **identity map**

\[
y = z \tag{6.15}
\]

is selected as inverse link function according to Eq. (6.5), i.e., \( f^{-1}(X\beta) = X\beta \). This map is depicted in Fig. 6.1.

In the following we give the code for the specification in JAGS of a **linear regression model**, employing standardised metrically scaled variables, and a homogeneous variance and fixed prior

\[
\text{(6.15)}
\]

\[
\text{Figure 6.1: Plot of the identity map (6.15).}
\]

Of course, the link function itself is likewise an identity map: \( X\beta = f(\mu) = \mu \).
probability distributions for the model parameters. Note that in JAGS Gauss distributions are parametrised in terms of the precision, which is the inverse of the variance. Hence, a Gamma prior probability distribution will be fixed for this parameter. We confine our consideration to the inclusion of additive main effects of the independent variables, but point to the numerous possibilities of rendering the model more flexible by including also multiplicative interaction terms for the independent variables.

Listing 6.7: Gibbs sampling with JAGS in R: model specification for linear regression.

```r
# JAGS model: all of the following code needs to be embedded in a
# modelString = "..." command in R

data {
  # Standardisation of dependent variable data
  yMean <- mean(y)
yStdev <- sd(y)
  for ( i in 1:nSample ) {
    zy[i] <- ( y[i] - yMean ) / yStdev
  }

  # Standardisation of independent variables data
  for ( j in 1:nIndVars ) {
    xMean[j] <- mean(X[,j]) # capital X!
xStdev[j] <- sd(X[,j])
    for ( i in 1:nSample ) {
      zX[i,j] <- ( X[i,j] - xMean[j] ) / xStdev[j]
    }
  }
}

model {
  # likelihood (w/ homoscedasticity assumption)
  for ( i in 1:nSample ) {
    zy[i] ~ dnorm( zmu[i] , zprec ) # precision parameter!
    # inverse link function
    zmu[i] <- zb0 + sum( zb[1:nIndVars] * zX[i,1:nIndVars] )
  }

  # priors
  zb0 ~ dnorm( 0 , 1/1^2 ) # regularising
  for ( j in 1:nIndVars ) {
    zb[j] ~ dnorm( 0 , 1/1^2 ) # regularising
  }
  zprec ~ dgamma( <alpha0> , <delta0> )
  zsigma <- sqrt( 1 / zprec )

  # De-standardisation of model parameters
  b[1:nIndVars] <- ( zb[1:nIndVars] / xStdev[1:nIndVars] )
}
```
The corresponding code for the specification of a linear regression model in Stan when intending to perform HMC sampling is given in App. B.1.

When there is a need to deal with outliers in the \( y \)-data, one might resort to a non-central \( t \)-single-datum likelihood function according to Eq. (2.26), and then specify an additional fixed prior probability distribution for the degrees of freedom parameter \( \nu \geq 1 \); e.g., an exponential distribution from the family defined by Eq. (2.33).

\[ \text{6.5 ANOVA-like regression} \]

Now we describe coding MCMC simulations with JAGS in R for **ANOVA-like regression**. This serves to model a linear relationship between data \( y \) for a single metrically scaled dependent variable, and data \( g \) for a qualitative variable which can take values in \( k \in \mathbb{N} \) non-ordered categories. This method is useful when the researcher’s objective is to compare distributional features of one and the same metrically scaled variable between several independent groups. Examples can be found in the discussions given, e.g., by Lee (2012) [63, Sec. 6.5], Gelman et al (2014) [35, Sec. 15.6], and Kruschke (2015) [58, Ch. 19].

Again, taking the maximum entropy perspective, one chooses a Gauß single-datum likelihood function according to Eq. (2.21), with a homogeneous variance, and specifies a conditionally conjugate Gauß–inverse Gamma prior joint probability distribution for the unknown location parameters \( \mu_g \) and the scale parameter \( \sigma^2 \). Adopting the cell means view of ANOVA-like regression, this gives

\[
\begin{align*}
\text{likelihood:} & \quad y | g, \mu_g, \sigma^2, I \overset{\text{ind}}{\sim} N (\mu_g, \sigma^2) \\
\text{priors:} & \quad \mu_g | g, \sigma^2, I \sim N (0, \sigma_0^2) \\
& \quad \sigma^2 | g, I \sim IG (\alpha_0, \beta_0) ,
\end{align*}
\]

where \( \sigma_0^2, \alpha_0 \) and \( \beta_0 \) denote fixed hyperparameters of the conditionally conjugate Gauß–inverse Gamma prior joint probability distribution. Note that in Eq. (6.17) zero-centred Gauß prior probability distributions were specified for the unknown regression coefficients \( \mu_g \).

In the code for the specification in JAGS of an **ANOVA-like regression model** in the cell means view, we employ the homoscedasticity assumption and fixed prior probability distributions for the model parameters. Note that in JAGS Gauß distributions are parametrised in terms of the precision. Hence, a Gamma prior probability distribution will be fixed for this parameter. Experience shows that for the present kind of statistical models the Markov chains generated by the Gibbs algorithm are usually not plagued with autocorrelation, so there is no need for standardising the metrically scaled \( y \)-data.
6.6. LOGISTIC REGRESSION

Listing 6.8: Gibbs sampling with JAGS in R: model specification for ANOVA-like regression in the cell means view.

```r
# JAGS model: the following code needs to be embedded in a
# modelString = "...") command in R

model {
    # likelihood (cell means model w/ homoscedasticity assumption)
    for ( i in 1:nSample ) {
        y[i] ~ dnorm( mu[gp[i]] , prec )
    }
    # priors
    for ( j in 1:nGroups ) {
        mu[j] ~ dnorm( 0 , 1/(sigma0)^2 )
    }
    prec ~ dgamma( <alpha0> , <beta0> )
    sigma <- sqrt( 1 / prec )
}
```

The corresponding code for the specification of an ANOVA-like regression model in Stan when intending to perform HMC sampling is given in App. B.2.

If the group-specific \( y \)-data contains outliers, the single-datum likelihood function may be replaced by a non-central \( t \)-distribution according to Eq. (2.26). Also, the available \( y \)-data may suggest that an assumption of heteroscedasticity is more realistic. In this case, one specifies an adaptive prior probability distribution for the scale parameter \( \sigma^2 \). This case will be addressed in Sec. 8.2.

As this fits the present discussion, we remark that the Bayes–Laplace analogue of the frequentist Student’s independent samples \( t \)-test has been developed by Gönen et al (2005) [40]. Further applications and implementations in R are given by Kruschke (2013) [57] and Kruschke (2015) [58, Sec. 16.3].

6.6 Logistic regression

When the research objective is to explain the dependency of count data with a known finite maximum of \( n \in \mathbb{N} \) on a set of \( k \in \mathbb{N} \) either metrically scaled or binary indicator independent variables, logistic regression is the standard tool for model-building. We will here sketch the way of integrating this technique into MCMC simulations with JAGS in R. Many interesting examples of applications can be found in Albert (2009) [2, Sec. 4.4], Lee (2012) [63, Subec. 9.8.1], Greenberg [41, Subsec. 8.2.3], Gelman et al (2014) [35, Sec.16.3], Kruschke (2015) [58, Ch. 21], or McElreath (2016) [68, Sec. 10.1].

The maximum entropy perspective suggests to capture the individual instant of whether a count was observed or not by a Bernoulli single-datum likelihood function according to Eq. (2.4), so that, overall, a binomial total-data likelihood function according to Eq. (2.9) abounds as describing the data-generating process for the total count. Contrary to linear regression and ANOVA-like
regression discussed in Secs. 6.4 and 6.5 above, these likelihood functions have no explicit dependence on a dispersion parameter. In addition, it is meaningful to assign zero-centred Gaussian prior probability distributions for the unknown regression coefficients $\beta$, a choice we will comment on shortly. The standard set-up for logistic regression is given by

\[
\text{likelihood: } \ y | \ X, \beta, I \sim \text{Bin} (\theta) \quad (6.19)
\]

\[
\text{inverse link function: } \ \theta = \text{logistic} (X \beta) \quad (6.20)
\]

\[
\text{priors: } \ \beta \sim N (0, \sigma_0^2) , \quad (6.21)
\]

where $\sigma_0^2$ denotes a fixed hyperparameter of the Gaussian prior probability distributions.

In logistic regression the standard logistic function

\[
y = \text{logistic}(z) = \frac{1}{1 + e^{-z}} \quad (6.22)
\]

serves as the inverse link function according to Eq. (6.5), i.e., $f^{-1} (X \beta) = \text{logistic} (X \beta)$. This map is depicted in Fig. 6.2. The standard logistic function maps the unbounded real-valued linear form $X \beta$ to the interval $[0, 1]$. With the ranges of possible values now coinciding, the transformed linear form, $\text{logistic} (X \beta)$, can be related directly to the (dimensionless) probability for “success”

---

5 The link function itself is given by the logit function: $X \beta = f(\theta) = \ln \left( \frac{\theta}{1 - \theta} \right)$. 

---

Figure 6.2: Plot of the standard logistic function (6.22).
parameter $\theta$. A particular feature of logistic regression is the general choice of a “zero log-odds” reference baseline,

$$0 \equiv \ln \left( \frac{\theta}{1 - \theta} \right) = X \beta \quad \Leftrightarrow \quad \theta = \frac{1}{2},$$

(6.23)

i.e., equal probabilities for the binary outcomes “failure” or “success” according to Bernoulli’s “principle of non-sufficient reason” of Sec. 3.1. For non-zero data, $X \neq 0$, the implication is $\beta = 0$, explaining the zero-centring of the Gauss prior probability distributions.

The code for the specification in JAGS of a logistic regression model with fixed prior probability distributions for the model parameters is given in the following.

Listing 6.9: Gibbs sampling with JAGS in R: model specification for logistic regression.

```r
# JAGS model: all of the following code needs to be embedded in a
# modelString = "..." command in R

data {
  # Standardisation of independent variables data
  for ( j in 1:nIndVars ) {
    xMean[j] <- mean(X[,j])  # capital X!
    xStdev[j] <- sd(X[,j])
    for ( i in 1:nSample ) {
      zX[i,j] <- ( X[i,j] - xMean[j] ) / xStdev[j]
    }
  }
}

model {
  # likelihood: Bernoulli single-datum
  for ( i in 1:nSample ) {
    y[i] ~ dbern( theta[i] )
    # inverse link function
    theta[i] <- ilogit( zb0 + sum( zb[1:nIndVars] * zX[i,1:nIndVars] ) )
    # take care of linebreak!
  }

  # priors: zero-centred
  zb0 ~ dnorm( 0 , 1/1^2 )  # regularising
  for ( j in 1:nIndVars ) {
    zb[j] ~ dnorm( 0 , 1/1^2 )  # regularising
  }

  # De-standardisation of model parameters
  b[1:nIndVars] <- zb[1:nIndVars] / xStdev[1:nIndVars]
  b0 <- zb0 - sum( zb[1:nIndVars] * xMean[1:nIndVars] / xStdev[1:nIndVars] )
  # take care of linebreak!
}
```
The corresponding code for the specification of a logistic regression model in Stan when intending to perform HMC sampling is given in App. B.3.

### 6.7 Poisson regression

Qualitatively different to the previous case is the situation when the empirical data to be explained is count data with an unknown maximum. To model the respective data-generating process in dependence of a set of \( k \in \mathbb{N} \) either metrically scaled or binary indicator independent variables, it is best practice to employ Poisson regression. The implementation of corresponding MCMC simulations with JAGS in R will be the topic of this section. Many practical applications of this technique to interesting research problems are outlined by Sivia and Skilling (2006) \[92, \text{Sec. 3.1}\], Albert (2009) \[2, \text{Sec. 11.4}\], Gelman et al (2014) \[35, \text{Sec. 16.4}\], Andreon and Weaver (2015) \[4, \text{Subsec. 6.1.2}\], or McElreath (2016) \[68, \text{Sec. 10.2}\]. Kruschke (2015) \[58, \text{Ch. 24}\] discusses a count data case with two nominally scaled independent variables, which amounts to the analysis of data from a contingency table. Methodologically, this case can be broadly likened to a frequentist \( \chi^2 \)–test of independence.

Like all the methods of regression analysis discussed in this chapter, Poisson regression takes a prime motivation from a maximum entropy perspective. Hence the choice of a Poisson single-datum likelihood function according to Eq. (2.15), which represents a particular state of ignorance. It has no explicit dependence on a dispersion parameter. Again, we select zero-centred Gauß prior probability distributions for the unknown regression coefficients \( \beta \) to express scepticism as to their presence in a best-fit model. A resultant common set-up for Poisson regression is given by

\[
\begin{align*}
\text{likelihood:} \\
\theta | X, \beta, I & \sim \text{Pois}(\theta) \\
\text{inverse link function:} \\
\theta & = \exp(X\beta) \\
\text{priors:} \\
\beta & \sim \text{N}(0, \sigma_0^2)
\end{align*}
\]  

(6.24) (6.25) (6.26)

where \( \sigma_0^2 \) is a fixed hyperparameter of the Gauß prior probability distributions.

In Poisson regression the natural exponential function

\[y = \exp(z) \]  

(6.27)

serves as the inverse link function according to Eq. (6.5), i.e., \( f^{-1}(X\beta) = \exp(X\beta) \). This map is depicted in Fig. 6.3. The natural exponential function maps the unbounded real-valued linear form \( X\beta \) to the interval \((0, \infty)\). The transformed linear form, \( \exp(X\beta) \), can thus be directly related to the non-negative dimensionless rate parameter \( \theta \). The choice of zero-centred Gauß prior probability distributions for the \( \beta \) implies via the link function:

\[
\beta = 0 \quad , \quad X \neq 0 \quad \iff \quad \ln(\theta) = 0 \quad \Rightarrow \quad \theta = 1 ;
\]  

(6.28)

\footnote{The link function itself is given by the natural logarithmic function: \( X\beta = f(\theta) = \ln(\theta) \).}
the order-of-magnitude of \( \theta \) is the information that is most relevant in Poisson data-generating processes.

Often in practical applications this parameter is given a product structure \( \theta = \tau \lambda \), with the understanding that the dimensionful exposure \( \tau \) amounts to available empirical data, while \( \lambda \) is the unknown dimensionful rate parameter. The inverse link function then becomes \( \lambda = \frac{1}{\tau} \exp \left( X \beta \right) \).

The code for the specification in JAGS of a \textit{Poisson regression model} with fixed prior probability distributions for the model parameters is to follow. Note that we have included (but currently commented out) the alternative model specification for operating with exposures \( \tau \) and a rate parameter \( \lambda \).

Listing 6.10: Gibbs sampling with JAGS in R: model specification for Poisson regression.

```r
# JAGS model: all of the following code needs to be embedded in a
# modelString = "..." command in R

data {
  # Standardisation of independent variables data
  for ( j in 1:nIndVars ) {
    xMean[j] <- mean(X[,j]) # capital X!
    xStdev[j] <- sd(X[,j])
    for ( i in 1:nSample ) {
      zX[i,j] <- ( X[i,j] - xMean[j] ) / xStdev[j]
    }
  }
}
```
model {
  # likelihood
  for ( i in 1:nSample ) {
    y[i] ~ dpois( theta[i] )
    # y[i] ~ dpois( lambda[i] )
    # inverse link function
    theta[i] <- exp( zb0 + sum( zb[1:nIndVars] * zX[i,1:nIndVars] ) )
  }
  # take care of linebreak!
  # lambda[i] <- (1/tau[i]) * exp( zb0
  # + sum( zb[1:nIndVars] * zX[i,1:nIndVars] ) )
  ## take care of linebreak!

  # priors
  zb0 ~ dnorm( 0 , 1/1^2 ) # regularising
  for ( j in 1:nIndVars ) {
    zb[j] ~ dnorm( 0 , 1/1^2 ) # regularising
  }

  # De-standardisation of model parameters
  b[1:nIndVars] <- zb[1:nIndVars] / xStdev[1:nIndVars]
  b0 <- zb0 - sum( zb[1:nIndVars] * xMean[1:nIndVars] / xStdev[1:nIndVars] )
  # take care of linebreak!
}

The corresponding code for the specification of a Poisson regression model in Stan when intending to perform HMC sampling is given in App. [B.4]

Should one find that the empirical count data that one analysed is over-dispersed, which manifests itself by the property $E(y|X, \beta, I) \ll Var(y|X, \beta, I)$ (when near equality was expected initially), then a Gamma–Poisson mixture model is suggested as a viable alternative; cf., e.g., Gelman et al (2014) [35, p 437f], or McElreath (2016) [68, p 350f]. The Gamma–Poisson probability distribution is also referred to as negative binomial distribution.

**R:** `dnbinom(y, n, theta), pbinom(y, n, theta), qnbinom(p, n, theta), rnbinom(n_simulations, n, theta)
**JAGS:** dnegbin(\theta, n) (sampling)
**Stan:** `neg_binomial(n, \theta/(1 - \theta))` (sampling)

### 6.8 Exponential regression

The last type of regression analysis we want to introduce in this chapter is exponential regression. This can be employed to explain data $y$ for the lengths of temporal or spatial intervals, i.e., waiting times or spatial distances, in terms of a set of $k \in \mathbb{N}$ either metrically scaled or binary indicator
independent variables contained in \( \mathbf{X} \). Exponential regression is a rather “exotic type of regression” for reasons to be explained shortly, and is thus much less frequently encountered in practical applications discussed in the literature. An example, nevertheless, can be found in Gill (2015) \[39\] Sec. 12.4.

As outlined before in Sec. 3.3, also the exponential single-datum likelihood function is of a certain maximum entropy kind, thus expressing a corresponding specific state of ignorance. It, too, features no explicit dependence on a dispersion parameter. What complicates matters in the present case is the choice of a reasonable inverse link function. The so-called canonical choice is guided by the formal appearance of sufficient statistics in the total-data likelihood function (2.43) of members of the exponential family; cf. Gelman et al (2014) \[35\] p 407. This procedure, supplemented by dimensional considerations for the positive rate parameter \( \theta \), leads to a negative inverse map, i.e.,

\[
y = -\frac{1}{z}, \quad \text{for} \quad z \in \mathbb{R} \setminus \{0\},
\]

as the appropriate inverse link function. Excluding the singular argument of zero, the negative inverse map sends the unbounded real-valued linear form \( \mathbf{X} \beta \) to the split interval \((-\infty, 0) \cup (0, +\infty)\). Upon confinement to the negative regime of \( \mathbf{X} \beta \), it is thus possible to relate the transformed linear form, \(-1/ (\mathbf{X} \beta)\), directly to the dimensionful positive rate parameter \( \theta \). However, as this imposes a very strong constraint on the range of values of \( \mathbf{X} \beta \), the number of applications for this type of regression is rather small. The canonical inverse link function confined to its positive branch is depicted in Fig. 6.4. It should be stated that the canonical choice of inverse link function is by no means mandatory.

Selecting truncated fixed Gauß prior probability distributions for the regression parameters \( \beta \), and assuming \( \beta \in \mathbb{R}_{<0} \) and \( \mathbf{X} \in \mathbb{R}_{>0} \) so that \( \mathbf{X} \beta \in \mathbb{R}_{<0} \), the present set-up for exponential regression is given by

\[
\begin{align*}
\text{likelihood:} & \quad \theta | \mathbf{X}, \beta, I \overset{\text{ind}}{\sim} \text{Exp} (\theta) \\
\text{inverse link function:} & \quad \theta = -\frac{1}{\mathbf{X} \beta}, \quad \text{with} \quad \mathbf{X} \beta \in \mathbb{R}_{<0} \\
\text{priors:} & \quad \beta_0 | \sigma^2 \sim \mathcal{N} (\mu_0, \sigma_0^2), \quad \text{with} \quad \mu_0 \in \mathbb{R}_{<0}, \quad \text{(for intercept)} \\
& \quad \beta | \sigma^2 \sim \mathcal{N} (0, \tau^2_0), \quad \text{with} \quad \beta \in \mathbb{R}_{<0},
\end{align*}
\]

where \( \mu_0, \sigma_0^2 \) and \( \tau^2_0 \) are fixed hyperparameters of the Gauß prior probability distributions.

We now give the code for the specification in JAGS of an exponential regression model with fixed prior probability distributions for the model parameters. A special feature here is the truncation of all Gauß prior probability distributions at their mode so that an upper limit for the range of allowed parameter values is imposed.

Listing 6.11: Gibbs sampling with JAGS in \( \mathbb{R} \): model specification for exponential regression.

```R
# JAGS model: the following code needs to be embedded in a
# modelString = "..." command in R
```

\[7\]The canonical link function itself is also given by a negative inverse map: \( \mathbf{X} \beta = f(\theta) = -\frac{1}{\theta} \).
6.9 Simulating posterior predictive probability distributions

The researcher’s actual inferential work begins only when the model fitting process described in the previous sections has been finalised and the outcome of this activity sufficiently validated. At the centre of attention at this stage of inductive statistical inference are the posterior predictive probability distributions for a dependent variable $Y$ according to Eq. (1.28). Their special status
arises out of the dual role a single-datum likelihood function takes from operating in two directions: from an empirical datum to unknown model parameter values, and from known (simulated) model parameter values back to a yet unobserved empirical datum; cf. McElreath (2016) [68, p 62]. In order to evaluate the multi-dimensional integral of the single-datum likelihood function of a specific data-generating process, weighted by the posterior joint probability distribution of the proposed statistical model, over a \((k + 1)\)-dimensional parameter space on the basis of approximative MCMC simulations, direct application of the discretised integration over a continuous parameter according to Eq. (6.7) is imminent. By taking this action one averages the single-datum likelihood function over the parameter space after relevant information from available empirical data has been accounted for. Posterior predictive probability distributions combine observation uncertainty with parameter uncertainty and so provide a fairly conservative representation of a researcher’s state of knowledge on the given problem they subjected to statistical data analysis.

The main steps to be taken to gain MCMC simulations of posterior predictive probability distributions are as follows:

1. Evaluate the linear form \(X\beta\) from a researcher-specified design matrix \(X_{\text{new}}\) for \(m\) cases on \(k\) independent variables and the MCMC simulated regression parameters \(\beta\).

2. Apply the inverse link function \(f^{-1}\) to the linear form \(X_{\text{new}}\beta\) to obtain the expectation value \(\mu_{\text{new}}\) according to Eq. (6.5).

3. Sample repeatedly new values \(y_{\text{new}}\) for \(Y\) from the single-datum likelihood function with the MCMC posterior settings for \(\mu_{\text{new}}\) and possible further dispersion parameters to obtain simulated dependent data according to Eq. (6.6).

4. Visualise and summarise specific features of the MCMC simulated posterior predictive probability distributions for \(Y\).

\(R\) code that can be employed for simulating and visualising in a histogram representation posterior predictive probability distributions from user-specified input for \(k\) independent variables and the MCMC data for \(k + 1\) model parameters is provided next. Here we assume that the MCMC data for the intercept parameter \(\beta_0\) is contained in the first column of the MCMC object “modCsim.” In practice this could be different. Note that, as an important posterior predictive check, the code also super-imposes the original \(y\)-data and their common sample mean on the histogram representation, so that potential inconsistencies of the model-fitting process such as problems related to under-fitting or over-fitting become directly apparent.
Listing 6.12: Gibbs sampling with JAGS in R: simulation of posterior predictive probability distributions.

```r
# Record number of iterations performed in Gibbs MCMC sampling
(nIter <- nrow(modCsim))

# Specify values for m new cases on k independent variables
x1 <- c(<value 11>, <value 12>, ..., <value 1k>)
x2 <- c(<value 21>, <value 22>, ..., <value 2k>)
...  
xm <- c(<value m1>, <value m2>, ..., <value mk>)

Xproxy <- cbind(x1, x2, ..., xm)

# Construct new design matrix
Xnew <- t(rbind(rep(1, nrow(Xproxy)), Xproxy))
(nCases <- nrow(Xnew))

# Evaluate linear form from new design matrix and MCMC samples
# (i) Example: linear regression
mu <- Xnew %*% t(modCsim) # intercept in modCsim[,1]
# (ii) Example: other GLM
linkmu <- Xnew %*% t(modCsim) # intercept in modCsim[,1]

# Apply inverse link function to obtain mu
# Example: Poisson regression
mu <- exp(linkmu)

# Initialise matrix for simulated data for m cases on k variables
yNew <- matrix(rep(0, nIter*nCases), nrow = nIter, ncol = nCases, byrow = TRUE)

# Sample from likelihood function
# (i) Example: linear regression
for ( j in 1:nCases ) {
  yNew[,j] <- rnorm(n = nIter, mean = mu[,j], sd = modCsim,"sig")
}
# (ii) Example: Poisson regression
for ( j in 1:nCases ) {
  yNew[,j] <- rpois(n = nIter, lambda = mu[,j])
}

# Scan, plot and summarise posterior predictive samples
head(yNew)

hist(yNew[,1], freq = FALSE)
points(y, rep(0, nSample), pch = 1)
```

6.9. SIMULATING POSTERIOR PREDICTIVE DISTRIBUTIONS

points( mean(y) , 0 , pch = 19 )

hist( yNew[,2] , freq = FALSE )
points( y , rep(0, nSample) , pch = 1 )
points( mean(y) , 0 , pch = 19 )

... hist( yNew[,m] , freq = FALSE )
points( y , rep(0, nSample) , pch = 1 )
points( mean(y) , 0 , pch = 19 )

summary( yNew[,1] , freq = FALSE )
summary( yNew[,2] , freq = FALSE )
... summary( yNew[,m] , freq = FALSE )

An example of a histogram representation of a posterior predictive probability distributions for the case of a main-effects linear regression model with fixed prior probability distributions for five model parameters is displayed in Fig. 6.5.

Figure 6.5: Example of the histogram representation of a simulated posterior predictive probability distribution for a single new datum $y_{new}$ in the case of a five-parameter, main-effects linear regression model. The underlying MCMC simulation of the posterior joint probability distribution for the model parameters comprised 15,000 iterations. The original $y$-data points from a sample of size $n = 27$, as well as their common sample mean, have been super-imposed on this histogram.
If the data set available to the researcher is sufficiently large in size, it might be an option for improving the quality of the model fit to follow the standard practice of supervised machine learning and split it into a training set (ca. 60%), a cross-validation set (ca. 20%), and a test set (ca. 20%). Here, parameter estimation is performed with the training set, while posterior predictive accuracy is gauged with the remaining two sets. We point the reader to Gill (2015) [39, Sec. 6.4], Kruschke (2015) [58, Sec. 17.5] and McElreath (2016) [68, Sec. 3.3] for further information on simulating and interpreting posterior predictive probability distributions.

In the next chapter we will look at ways of discriminating between competing statistical models as regards their performance in fitting empirical data and predicting yet unobserved new data.
The comparison of statistical models that compete for an optimal fit to the same given set of quantitative–empirical data is an essential issue of reliability assessment which needs to be addressed in inductive statistical inference. Concerning their main objectives, some parallels can be drawn between model comparison in the Bayes–Laplace approach on the one-hand side, and frequentist null hypothesis significance testing on the other, but the former operation is based on a conceptually sound and transparent methodology, as we intend to sketch in this chapter.

In the Bayes–Laplace approach there have been developed two different kinds of frameworks to capture the relative performance of two or more competing statistical models as regards quality of model-fit attained, and their ensuing posterior predictive accuracy. The aim is to reduce potential over- and under-fitting of the data as much as possible. As, for a given research problem, no statistical model that was built from relevant prior information and available empirical evidence will ever be “correct” in the ontological sense, it is worthwhile considering the option of ultimately drawing inferences from a model that was obtained from averaging over two or more of the competing statistical models, should the fit of any of the models involved in the averaging process not be entirely unacceptable. The weight factors necessary for model averaging are obtained from normalising the differences in the quantified relative posterior predictive accuracy of the models which were taken into account.

A widely accepted guiding principle in statistical model-building is parameter parsimony. This is motivated by a particular view that dates back to the Middle Ages and proved highly influential in the history of Science. It was voiced by the English Franciscan friar, scholastic philosopher and theologian [William of Ockham (1288–1348)] who asserted:

“Frustra fit per plura, quod potest fieri per pauciora.”

1

In the various scientific communities of these modern days, this heuristic principle is known as Ockham’s razor, and it is often used as a justification for preferring one specific model as representing a proposed theoretical framework in place of an available competing model of comparable performance properties which, however, contains a larger number of model parameters.

---

1English translation: “It is vain to do with more, what can be done with less.” See URL (cited on August 17, 2018): www-history.mcs.st-and.ac.uk/Quotations/Ockham.html and Sivia and Skilling (2006) [92] p 81.
CHAPTER 7. MODEL COMPARISON AND HYPOTHESIS TESTING

7.1 Bayes factors

The idea behind the concept of Bayes factors as a practical tool for model comparison is a simple one. Start from Bayes’ theorem in its variant of Eq. (1.23) given in Ch. 1, and apply it, for a given fixed set of empirical data, to both a “model(i)” and a “model(j).” Upon forming the posterior odds, i.e., the ratio of the posterior probability for “model(i)” and the posterior probability for “model(j),” one obtains:

\[
\frac{P(\text{model}(i) | \text{data}, I)}{P(\text{model}(j) | \text{data}, I)} = \frac{P(\text{data} | \text{model}(i), I)}{P(\text{data} | \text{model}(j), I)} \times \frac{P(\text{model}(i) | I)}{P(\text{model}(j) | I)},
\]

where a common divisor of \(P(\text{data} | I)\) cancelled out along the way. Conventionally one defines the ratio multiplying the prior odds on the right-hand side of Eq. (7.1), i.e.,

\[
B_{ij} := \frac{P(\text{data} | \text{model}(i), I)}{P(\text{data} | \text{model}(j), I)}
\]

(7.2)

as the Bayes factor. In this form it gives the ratio of the average likelihoods for “model(i)” and “model(j).” By re-arranging Eq. (7.1), one find that this is equal to

\[
B_{ij} = \frac{P(\text{model}(i) | \text{data}, I)}{P(\text{model}(j) | \text{data}, I)} \times \frac{P(\text{model}(i) | I)}{P(\text{model}(j) | I)},
\]

(7.3)

i.e., the ratio of posterior odds and prior odds for “model(i)” and “model(j).” The Bayes factor provides an immediate manifestation of the very fact that within the Bayes–Laplace approach only the values of relative measures contain tangible information. In this framework it is often not possible to define absolute values in any sensible way.

Suppose “model(i)” contains a set of \(k+1\) parameters, \(\{\theta_0^{(i)}, \ldots, \theta_k^{(i)}\}\). Then its associated average likelihood is calculated by averaging the total-data likelihood function in \((k+1)\)-dimensional parameter space with the prior joint probability distribution,

\[
P(\text{data} | \text{model}(i), I) = \int_{\theta^{(i)}} \ldots \int_{\theta^{(i)}} P(\text{data} | \theta_0^{(i)}, \ldots, \theta_k^{(i)}, \text{model}(i), I) \times P(\theta_0^{(i)}, \ldots, \theta_k^{(i)} | \text{model}(i), I) \, d\theta_0^{(i)} \ldots d\theta_k^{(i)}. \tag{7.4}
\]

This calculation is to be repeated in an analogous fashion for “model(j),” which, however, usually contains a number of parameters different from \(k+1\). The point is that statistical models with a higher number of parameters need to spread out prior joint probability density (which, of course,
7.1. BAYES FACTORS needs to integrate to 1) over a larger number of dimensions in parameter space than statistical models with a smaller number of parameters. A larger number of dimensions of parameter space amounts to a larger hyper-volume to be covered by the prior joint probability density. In this respect, statistical models with a higher number of parameters automatically get penalised by the present procedure. Only if there is a sufficient amount of supporting evidence in the empirical data for the presence of additional parameters (which will factor into the procedure via the total-data likelihood function) can the penalty for a dimension-inflated hyper-volume be compensated.

Bayes factors can be calculated analytically for all the single-parameter estimation examples with exact solutions for the parameter’s posterior probability distribution that were discussed in Ch. 4. The reason is that in those cases only the prior probability distribution can be varied between competing models, while their total-data likelihood functions are identical. Here we present the explicit Bayes factor solution for the Beta–binomial model of Subsec. 4.1.2. Suppose given empirical data \{y, n\}, and introduce a “model (1)” and a “model (2)” as competing to explain the underlying data-generating process. The binomial total-data likelihood function has the same structure for both cases; only the parameter values of the two Beta prior probability distributions, \{\alpha_1, \beta_1\} and \{\alpha_2, \beta_2\}, will be different. Then the ratio of posterior model odds and prior model odds amounts to

\[
B_{12} = \frac{\text{Be}(\alpha_1 + y, \beta_1 + n - y)}{\text{Be}(\alpha_2 + y, \beta_2 + n - y)} \cdot \frac{\text{Be}(\alpha_1, \beta_1)}{\text{Be}(\alpha_2, \beta_2)}. \tag{7.5}
\]

Jeffreys (1939) [50, App. B] devised a heuristic scale for interpreting the values of Bayes factors when only two competing statistical models are considered. According to this scale, one classifies the explanatory power of the two models under investigation as

**Jeffreys’ scale for comparison of two competing models:**

- \(B_{12} > 1\): model (1) supported
- \(1 > B_{12} > 10^{-1/2}\): weak evidence against model (1)
- \(10^{-1/2} > B_{12} > 10^{-1}\): substantial evidence against model (1)
- \(10^{-1} > B_{12} > 10^{-3/2}\): strong evidence against model (1)
- \(10^{-3/2} > B_{12} > 10^{-2}\): very strong evidence against model (1)
- \(10^{-2} > B_{12}\): decisive evidence against model (1);

see also Gill (2015) [39, p 217]. Kass and Raftery (1995) [54, p 777], and Jaynes (2003) [48, p 91], transform Jeffreys’ scale to an orders-of-magnitude emphasising, base-10 logarithmic scale, which appears closer to intuition. In this case it holds that

\[
\log_{10}(B_{12}) = \log_{10} \left( \frac{P(\text{model}(1)|\text{data}, I)}{P(\text{model}(2)|\text{data}, I)} \right) - \log_{10} \left( \frac{P(\text{model}(1)|I)}{P(\text{model}(2)|I)} \right), \tag{7.6}
\]

which gives the difference between the posterior decadic log-odds and the prior decadic log-odds; see also Greenberg (2013) [41, p 36].

---

3For once, they have no X-data for independent variables blended in via an inverse link function like GLMs.
We draw the reader’s attention to the lively review by Jefferys and Berger (1992) [49] on the concept of **Bayes factors**. For illustrative purposes they relate their discussion to the prominent historical example from the early 20th Century of the two competing theories of gravitational interactions that were trying to explain the phenomenon of the advance of the perihelion of planet Mercury on its orbit around the Sun. This observation had been puzzling astronomers ever since the French astronomer and mathematician Urbain Jean Joseph Le Verrier (1811–1877) had reported on this problem for gravitational theory to the French Academy of Sciences on September 12, 1859.

The present exposition of **model comparison** elucidates that for **hypothesis testing** in the **Bayes–Laplace approach** one requires at least one proper, testable alternative hypothesis to a given “hypothesis(1),” where the former, too, can be assigned a well-defined **total-data likelihood function** so that decision-making as to the data-favoured hypothesis becomes possible. Simply making the choice

\[ \text{hypothesis(2)} := \text{hypothesis(1)} \]

will lead into a non-constructive dead end. There is no way to devise a meaningful **total-data likelihood function** \( P(\text{data}|\text{hypothesis(1),} I) \); see Sivia and Skilling (2006) [92, p 84], and Trotta (2008) [102, Sec. 4.1].

A computational challenge that had long plagued researchers was the evaluation of the **average likelihood** for multi-parameter models, when domain integrations have to be performed in high-dimensional parameter spaces. Some of the first algorithms that obtain this information by means of numerical simulation were given by Chib (1995) [11] and by Carlin and Chib (1995) [10]; see also Greenberg (2013) [41, Subsec. 7.1.2]. Specific routines for facilitating the practical task of computing **Bayes factors** have been made available within \( \mathbb{R} \) in the MCMCpack package by Martin et al (2011) [67].

\[ \mathbb{R}: \text{BayesFactor (MCMCpack output)} \] (MCMCpack package),

and in the **BayesFactor** package by Morey and Rouder (2018) [73]. Further information on conceptual aspects of model comparison with **Bayes factors** is given in the helpful practical tutorial by Lodewyckx *et al* (2011) [65], and in Gelman *et al* (2014) [35, Sec. 7.4], Gill (2015) [39, Ch. 7], or in Kruschke (2015) [58, Ch. 10].

For astrophysical and cosmological problems with only a small amount of available observational information, Trotta (2008) [102, Sec. 4.7] advocates the **Bayes factor** method for **model comparisons**. Gelman and Rubin (1995) [34] and Gelman *et al* (2014) [35, Sec. 7.4], on the other hand, generally advise against the use of **Bayes factors** as a selection criterion for **statistical models** due to their inherent **sensitivity** to the choice of **prior probability distributions**.

### 7.2 Information criteria and posterior predictive accuracy

Shannon’s **information entropy**, as defined in Eq. (3.8) for discrete cases and in Eq. (3.17) for continuous cases, is the universally approved unique measure of the amount of **uncertainty** rep-

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4 Presumably because the DIC-measure of Subsec. 7.2.1 that he also takes into consideration requires a relation of sample size to number of parameters of \( n \gg k + 1 \).
represented by a given probability distribution. Qualitatively speaking, information entropy is growing, the more probability (which sums to 1) is spread out across viable possibilities. In this respect, the number of dimensions of the space in which probability is distributed plays a particularly important role. Information entropy is also the central pillar of the currently most widely applied techniques for model comparison, for which relative posterior predictive accuracy is the criterion for evaluating the performance of competing statistical models. We will describe the details in this section.

The non-symmetric, directed Kullback–Leibler divergence, defined in terms of the information entropy in the discrete case of Eq. (3.8) by

$$D_{KL}(P, Q) := S(P, Q) - S(P) = \sum_{i=1}^{k} p_i \ln \left( \frac{p_i}{q_i} \right), \quad (7.7)$$

measures the additional information entropy generated when approximating one discrete probability distribution, $P = \{p_i\}_{i=1,...,k}$, by a second discrete probability distribution, $Q = \{q_i\}_{i=1,...,k}$; see Kullback and Leibler (1951) [61]. Note that, by construction, it holds that $D_{KL}(P, P) \equiv 0$.

Suppose given two candidate probability distributions, $Q^{(1)}$ and $Q^{(2)}$, that are competing to approximate an unknown target probability distribution, $P$. Then, when measured with the Kullback–Leibler divergence, the relative distance of $Q^{(1)}$ and $Q^{(2)}$ from the unknown target $P$ amounts to

$$D_{KL}(P, Q^{(1)}) - D_{KL}(P, Q^{(2)}) = \left[ S(P, Q^{(1)}) - S(P) \right] - \left[ S(P, Q^{(2)}) - S(P) \right] = S(P, Q^{(1)}) - S(P, Q^{(2)}) = -\sum_{i=1}^{k} p_i \ln \left( \frac{q_i^{(1)}}{q_i^{(2)}} \right) = -\sum_{i=1}^{k} p_i \left[ \ln \left( q_i^{(1)} \right) - \ln \left( q_i^{(2)} \right) \right]; \quad (7.8)$$

this is just the $P$-average of the difference in log-probability between $Q^{(1)}$ and $Q^{(2)}$. When this difference come out negative, $Q^{(1)}$ is closer to the unknown target $P$ than $Q^{(2)}$, and vice versa when the difference comes out positive. The snag is that the $P$-measure used for the averaging is not known, and so, to continue the comparison of $Q^{(1)}$ and $Q^{(2)}$, one needs to resort to a reliable estimation procedure. A tried and tested estimation procedure that has become commonplace employs the deviance of a probability distribution $Q$, defined by

$$D(Q) := -2 \sum_{i=1}^{n} \ln(q_i) \quad (7.9)$$

In terms of the deviance, the difference of Kullback–Leibler divergences in Eq. (7.8) can now
be estimated by
\[
D_{KL}(P, Q^{(1)}) - D_{KL}(P, Q^{(2)}) \approx D(Q^{(1)}) - D(Q^{(2)})
\]
\[
= -2 \sum_{i=1}^{k} \left[ \ln \left( q_i^{(1)} \right) - \ln \left( q_i^{(2)} \right) \right].
\] (7.10)

All of these considerations provide the foundation for a strategy that seeks to guard against over-fitting when approximating unknown posterior joint probability distributions by means of MCMC simulations. The objective of the model-building process is to compare competing statistical models on the basis of an estimation of their anticipated posterior predictive accuracy, or, in more technical terms, their expected out-of-sample deviance. We will now introduce the two most widely accepted estimators of a model’s expected out-of-sample deviance, so-called information criteria that take different aspects of the posterior average (or posterior expectation) of the natural logarithm of a model’s likelihood function as major building-blocks for valuing posterior predictive accuracy.

### 7.2.1 Deviance information criterion

Spiegelhalter et al (2002) \[93\] proposed the deviance information criterion (DIC) as a quantitative tool for estimating expected out-of-sample deviance. Its applicability is restricted in that it assumes a multivariate Gauss posterior joint probability distribution for the model parameters, and that the number of available observations is much larger than number of model parameters, i.e., \(n \gg k + 1\).

Spiegelhalter et al (2002) \[93, Eq. (10)\] start by defining a Bayesian deviance as capturing model performance in the fitting process by
\[
D_{\text{Bayes}}(\theta) := -2 \ln \left[ P(y|\theta, I) \right] + 2 \ln \left[ f(y|I) \right];
\] (7.11)

the first term amounts to minus two times the natural logarithm of the total-data-likelihood function, and \(f(y|I)\) is a standardising term that depends on the data only and so can be considered constant. Spiegelhalter et al (2002) \[93, Eq. (36)\] then continue to construct the DIC-measure as an additive combination of the posterior average of the Bayesian deviance as a measure of model fit, and an effective number of parameters \(p_{DIC}\) that acts as a penalty term to account for model complexity. This yields
\[
\text{DIC} := E_{\text{post}} \left( D_{\text{Bayes}}(\theta) \right) + p_{DIC},
\] (7.12)
\[
p_{DIC} := E_{\text{post}} \left( D_{\text{Bayes}}(\theta) \right) - D_{\text{Bayes}} \left( E_{\text{post}}(\theta) \right);
\] (7.13)

see also Trotta (2008) \[102, Sec. 4.7\], Gelman et al (2014) \[35, Sec. 7.2\], Gill (2015) \[39, Sec. 7.5\], and McElreath (2016) \[68, Sec. 6.4\]. Models with smaller DIC values are generally preferred, as,

---

\[6\]Here we have \(\theta \in \mathbb{R}^{(k+1) \times 1}\) and \(y \in \mathbb{R}^{n \times 1}\). Moreover, throughout we suppress conditioning on the data for potential independent variables, to keep notation reasonably simple.
by definition, they are closer to the unknown target. However, less well performing models should not be completely discarded from the outset, as they often contain valuable information.

The calculation in R of a model’s DIC score from MCMC simulations with JAGS has been made easy through Plummer’s (2016) \[83\] rjags package. This contains the taylor-made function R::dic.samples(modelJAGS, n.iter = number of iterations) (rjags package).

7.2.2 Watanabe–Akaike information criterion

The Watanabe–Akaike information criterion (WAIC), suggested by Watanabe (2010) \[107\] Eq. (6), offers a more refined, cumulative pointwise estimate of a model’s expected out-of-sample deviance, with much less restrictive prerequisites than the DIC-measure. Specifically it can be applied for assessing posterior predictive performance of highly skewed posterior joint probability distributions for model parameters, i.e., it does not assume that they be multivariate Gauss distributions. It also allows for arbitrary prior probability distributions.

Like the DIC-measure, WAIC is built from two additive components. This is on the one-hand side the sum of the natural logarithms of the posterior-averaged single-datum likelihood functions for every observation, \(y_i\), — this is referred to as the log-pointwise posterior predictive density (lppd) and is given by

\[
lppd := \sum_{i=1}^{n} \ln \left( \frac{1}{E_{\text{post}}[P(y_i|\theta, I)]} \right);
\]

on the other hand there is again a term representing an effective number of parameters that penalises model complexity, viz.,

\[
p_{\text{WAIC}} := -2 \sum_{i=1}^{n} E_{\text{post}} \left( \ln P(y_i|\theta, I) \right) + 2 \sum_{i=1}^{n} \ln \left( \frac{1}{E_{\text{post}}[P(y_i|\theta, I)]} \right).
\]

Altogether, the cumulative pointwise WAIC-estimate for a model’s expected out-of-sample deviance is thus given by

\[
\text{WAIC} := -2lppd + 2p_{\text{WAIC}},
\]

where the particular re-scaling proposed by Gelman et al (2014) \[35\] p 174] in order to comply with the usual deviance-based structure of other information criteria is employed; see also McElreath (2016) \[68\] Sec. 6.4. Again, models with smaller WAIC values are generally preferred, but it is advisable to retain weaker-performing competing models for further consideration. In recent years, the WAIC-measure has acquired in the pertinent research literature the status of the prime tool for comparing competing statistical models with respect to properties of over-fitting and posterior predictive accuracy.

The calculation in R of a model’s WAIC score from MCMC simulation output has been made possible via the \texttt{loo} package by Vehtari et al (2017) \[105\]. This contains the function R::waic(model) (\texttt{loo} package).
We refer to reader to the corresponding user manual for further practical coding instructions.

Now we turn to put into perspective in the next chapter various possibilities of increasing the flexibility of a statistical model by adapting it to a researcher’s state of knowledge when this exhibits a more complex structure than what was assumed in the examples of Ch. 6.
Chapter 8

Hierarchical modelling

The simple types of techniques of regression analysis we discussed in Ch. 6 in the context of generalised linear models confined their methodological considerations to constructing fixed-effects models. That is to say, the different families of statistical models that were presented are built on the implicit assumption that supposes effects to be the same for all sample units in the target population of the researcher's investigation. In practice, however, one often possesses information on some kind of existing substructure within the target population, such as sample units being members of exclusive groups or clusters, with the possibility of sample units belonging to the same group appearing more similar to one another on the characteristic features of the researcher's interest than across groups. If this kind of information is available, one might as well make use of it in the model-building process by integrating it into the calculation resp. simulation of posterior joint probability distributions for model parameters. Hierarchical models, as they are known within the Bayes–Laplace approach to data analysis and statistical inference, constitute the present state-of-the-art in Applied Statistics for devising flexible frameworks that can handle empirical data obtained from performing measurements on complex systems or/and dynamical processes. Some authors refer to hierarchical models as multi-level models, or as varying-effects models.

Technically speaking, varying-effects models are obtained by introducing for some model parameters adaptive prior probability distributions as opposed to the fixed ones that were employed in Ch. 6. The rationale behind this procedure is the view that the specific properties of some model parameters are captured more effectively when one describes them as arising from an entire distribution of possibilities across groups which have fixed prior probability distributions within groups. Such an approach has the consequence that information on the values of these parameters obtained from analysing empirical data is partially shared between groups — known as partial pooling of information — which leads via adaptive regularisation to more robust statistical models that are less vulnerable to the threat of over-fitting. This in turn will generally improve a model's overall posterior predictive accuracy: while within-group model-fits and predictions will get worse due to partial pooling, out-of-sample predictions will become more reliable; see, e.g., Gelman et al (2014) [35, Ch. 5], Gill (2015) [39, Ch. 12], Kruschke (2015) [58, Ch. 9], or McElreath (2016) [68, Ch. 12]. With partial pooling of information is associated the regularising phenomenon of shrinkage of estimates, these becoming less susceptible to the influence of outliers in the data. Because of learning from the exchanged information, parameter estimates on the
level of the individual group samples will “shrink” towards the total sample mean. The size of the shrinking effect is influenced by the amount of data within the groups and the amount of variation between the groups. In the empirical sciences this statistical phenomenon has long been known as regression towards the mean. It was made popular through the work of the English empiricist Sir Francis Galton FRS (1822–1911), who discovered it following years of intense research during the late 19th Century; see Galton (1886) [29], and also Kahneman (2011) [51, Ch. 17].

There are basically two kinds of varying-effects extensions of the fixed-effects generalised linear models specified in Ch. 6 one may consider: the reasonably straightforward varying-intercept models that suppose variation across groups of the \( \beta_0 \)-regression coefficient, which we will introduce in this chapter, and the technically more demanding varying-slopes models that require in particular the modelling of prior correlations amongst the full \( \beta \)-regression coefficients. The second option leads naturally to a significant increase in a model’s complexity, though not in the overall logic of making inferences in the Bayes–Laplace approach. This option is beyond the present scope of these lecture notes.

We now turn to take a look at fitting to adequate empirical data specific MCMC simulated varying-intercept extensions of the four classes of generalised linear models we presented in Secs. 6.4 to 6.7 using JAGS in R for their implementation. Again, the models so obtained need to be subjected to dedicated sensitivity analyses as to meaningful choices of prior probability distributions, and to critical posterior predictive checks.

### 8.1 Hierarchical linear regression

For the varying-intercept linear regression model, we here select a non-central \( t \)-distribution according to Eq. (2.26) as the single-datum likelihood function, to provide the flexibility needed for adapting to potential outliers in the data for the dependent metrically scaled variable \( Y \). We choose an exponential prior probability distribution according to Eq. (2.33) for the \( t \)-distribution’s degrees-of-freedom parameter \( \nu \). We take \( \nu > 2 \), so that by Eqs. (2.29) and (2.30) its expectation value and variance will be well-defined. A Gauß adaptive prior probability distribution is introduced for the group-level intercept parameter. We maintain the assumption of homogeneous variances. The resultant model is then described by

\[
\begin{align*}
\text{likelihood:} & \\ y | X, \beta, \sigma^2, \nu, [gp], I & \sim t \left( \mu, \sigma^2, \nu \right) \\
\text{inverse link function:} & \\ \mu & = \beta_0[gp] + \beta_1X_1 + \ldots + \beta_kX_k \\
\text{adaptive prior:} & \\ \beta_0[gp] & \sim N \left( \zeta, \omega^2 \right) \\
\text{fixed priors:} & \\ \zeta & \sim N \left( 0, s_0^2 \right) \\
\omega^2 & \sim IG \left( \psi_0, \chi_0 \right) \\
\beta_1, \ldots, \beta_k & \sim N \left( 0, \tau^2 \right) \\
\sigma^2 & \sim IG \left( \alpha_0, \delta_0 \right) \\
\nu - 2 & \sim \exp \left( \theta_0 \right) ,
\end{align*}
\]

where \( s_0^2, \psi_0, \chi_0, \tau^2, \alpha_0, \delta_0 \) and \( \theta_0 \) denote fixed hyperparameters of the various prior probability distributions. Examples of applications, in part with a Gauß single-datum likelihood function,
8.1. HIERARCHICAL LINEAR REGRESSION

can be found in Gill (2015) [39, Sec. 12.7] and in Kruschke (2015) [58, Sec. 17.3]. Andreon and Weaver (2015) [4, Secs. 8.4] employ logarithmic variables for modelling a simple linear regression relationship between galaxies’ velocity dispersions on the one hand, and the masses of their central black holes on the other, wherein the variables are subject to measurement error and object-specific intrinsic scatter.

We now give the code for the specification in JAGS of a varying-intercept linear regression model. Herein we suppressed the standardisation of the dependent and independent data, and the de-standardisation of the model parameters, both given already in Sec 6.4. No changes arise in this respect.

Listing 8.1: Gibbs sampling with JAGS in R: model specification for varying-intercept linear regression with non-central $t$–single-datum likelihood function.

```r
# JAGS model: all of the following code needs to be embedded in a
# modelString = "..." command in R

model {
    # likelihood: t-distribution w/ homoscedasticity assumption
    for ( i in 1:nSample ) {
        zy[i] ~ dt( zmu[i] , zprec , nu )
        # inverse link function
        zmu[i] <- zb0[gp[i]] + sum( zb[1:nIndVars] * zX[i,1:nIndVars] )
    }

    # adaptive prior
    # (i) varying intercept
    for ( j in 1:nGroups ) {
        zb0[j] ~ dnorm( zeta , precIntc )
    }

    # fixed priors
    zeta ~ dnorm( 0 , 1/<s0>^2 )
    precIntc ~ dgamma( <psi0> , <chi0> )
    omega <- sqrt( 1 / precIntc )

    # (ii) slopes
    for ( j in 1:nIndVars ) {
        zb[j] ~ dnorm( 0 , 1/1^2 ) # regularising
    }

    # (iii) precision for t-likelihood
    zprec ~ dgamma( <alpha0> , <delta0> )
    zsigma <- sqrt( 1 / zprec * nu / (nu-2) ) # stdev

    # (iv) degrees of freedom for t-likelihood
    nu <- 2 + nuTilde # nu > 2: existence of mean and variance
    nuTilde ~ dexp( <theta0> )
}
```

The corresponding code for the specification of a varying-intercept linear regression model in Stan when intending to perform HMC sampling is given in App. B.1.

## 8.2 Hierarchical ANOVA-like regression

We also choose a non-central \( t \)-distribution according to Eq. (2.26) as the single-datum likelihood function in hierarchical ANOVA-like regression. In the present case the specific multi-level feature follows from abandoning the assumption of homogeneous variances. We express this position by choosing an inverse Gamma adaptive prior probability distribution for the group-level scale parameter. For the degrees-of-freedom parameter, again an exponential prior probability distribution according to Eq. (2.33) is picked, imposing the condition \( \nu > 2 \) so that its expectation value and variance will be well-defined. The resultant model is then given by

likelihood: \[
y | g, \mu_0, \mu_g, \sigma_g^2, \nu, I \sim t \left( \mu_0 + \mu_g, \sigma_g^2, \nu \right)
\] (8.9)

adaptive priors:
- \( \mu_g \sim N \left( 0, \tau^2 \right) \) (8.10)
- \( \sigma_g^2 \sim IG \left( \alpha, \beta \right) \) (8.11)

fixed priors:
- \( \mu_0 \sim N \left( \bar{y}, s^2 \right) \) (8.12)
- \( \tau^2 \sim IG \left( \alpha_0, \beta_0 \right) \) (8.13)
- \( \alpha, \beta \sim Ga \left( \gamma_0, \delta_0 \right) \) (8.14)
- \( \nu - 2 \sim \text{exp} \left( \theta_0 \right) \) (8.15)

where \( \bar{y} \) and \( s^2 \) are the sample mean resp. sample variance of the \( y \)-data, and \( \alpha_0, \beta_0, \gamma_0, \delta_0 \) and \( \theta_0 \) denote fixed hyperparameters of the prior probability distributions. Examples of applications are presented in Gelman et al (2014) [35, Sec. 5.3] and in Kruschke (2015) [58, Sec. 19.5].

The code for the specification in JAGS of a hierarchical ANOVA-like regression model reads:

Listing 8.2: Gibbs sampling with JAGS in R: model specification for ANOVA-like regression with non-central \( t \)-single-datum likelihood function and heterogeneous variances.

```r
# JAGS model: the following code needs to be embedded in a
# modelString = "..." command in R

model {

  # likelihood (t-likelihood w/ heteroscedasticity assumption)
  for ( i in 1:nSample ) {
    y[i] ~ dt( mu0 + mu[gp[i]] , prec[gp[i]] , nu )
  }

  # adaptive priors
  for ( j in 1:nGroups ) {
    mu[j] ~ dnorm( 0 , 1/tau^2 ) # vage!
    prec[j] ~ dgamma( alpha , beta )
  }
}
```
8.3 Hierarchical logistic regression

The extension to the varying-intercept level of the next two classes of generalised linear models entails no further complication. The varying-intercept logistic regression model has at its core a binomial total-data likelihood function according to Eq. (2.9). A Gaussian adaptive prior probability distribution is selected for the group-level intercept parameter. The model is described by

\[
\begin{align*}
\text{likelihood:} & \quad y | X, \beta, [gp], I \sim \text{Bin} (\theta) \\
\text{inverse link function:} & \quad \theta = \text{logistic} (\beta_0 [gp] + \beta_1 X_1 + \ldots + \beta_k X_k) \\
\text{adaptive prior:} & \quad \beta_0 [gp] \sim N (\zeta, \omega^2) \\
\text{fixed priors:} & \quad \zeta \sim N (0, \sigma_0^2) \\
& \quad \omega^2 \sim \text{IG} (\alpha_0, \beta_0) \\
& \quad \beta_1, \ldots, \beta_k \sim N (0, \tau_0^2) 
\end{align*}
\]

where \( \sigma_0^2, \alpha_0, \beta_0 \) and \( \tau_0^2 \) denote fixed hyperparameters of the different prior probability distributions. Illustrative examples are discussed in Gelman et al (2014) [35, Sec. 5.3], Gill (2015) [39, Sec. 12.8], Kruschke (2015) [58, Sec. 21.4], and McElreath (2016) [68, Sec. 12.1].

We now give the code for the specification in JAGS of a varying-intercept logistic regression model. We suppressed the standardisation of the independent data, and the de-standardisation of the model parameters, which were both given in Sec. 6.6. No modifications are required in this part.

Listing 8.3: Gibbs sampling with JAGS in R: model specification for varying-intercept logistic regression with a binomial total-datum likelihood function.

# JAGS model: all of the following code needs to be embedded in a
# modelString = "..." command in R

model {
    # likelihood: binomial total-datum
    for ( i in 1:nSample ) {
        y[i] ~ dbin( theta[i] , nTrials[i] )
        # inverse link function
        theta[i] <- ilogit( zb0[gp[i]] + sum( zb[1:nIndVars] * zX[i,1:nIndVars] ) )
        # take care of linebreak!
    }

    # adaptive prior
    # (i) varying intercept
    for ( j in 1:nGroups ) {
        zb0[j] ~ dnorm( zeta , precIntc )
    }

    # fixed priors
    zeta ~ dnorm( 0 , 1/(<sigma0>)^2 )
    precIntc ~ dgamma( <alpha0> , <beta0> )
    omega <- sqrt( 1 / precIntc )

    # (ii) slopes
    for ( j in 1:nIndVars ) {
        zb[j] ~ dnorm( 0 , 1/l^2 ) # regularising
    }
}

The corresponding code for the specification of a varying-intercept logistic regression model in Stan when intending to perform HMC sampling is given in App. B.3.

## 8.4 Hierarchical Poisson regression

Lastly, we delineate the structure of a **varying-intercept Poisson regression model.** As before, the single-datum likelihood function is given by a Poisson distribution according to Eq. (2.15). A Gauß adaptive prior probability distribution is selected for the group-level intercept parameter. The model is given by

\[
\begin{align*}
\text{likelihood:} & \quad \theta | X, \beta, [gp], I \sim \text{Pois}(\theta) \\
\text{inverse link function:} & \quad \theta = \exp(\beta_c + \beta_0[gp] + \beta_1X_1 + \ldots + \beta_kX_k) \\
\text{adaptive prior:} & \quad \beta_0[gp] \sim N(0, \omega^2) \\
\text{fixed priors:} & \quad \beta_c \sim N(0, \sigma_0^2) \quad \omega^2 \sim IG(\alpha_0, \beta_0) \quad \beta_1, \ldots, \beta_k \sim N(0, \tau_0^2)
\end{align*}
\] (8.22-8.27)
where $\sigma_0^2$, $\alpha_0$, $\beta_0$ and $\tau_0^2$ denote fixed hyperparameters of the different prior probability distributions. Interesting applications of these models are outlined in Gelman et al (2014) [35, Sec. 16.4], Gill (2015) [39, Sec. 12.5], Kruschke (2015) [58, Sec. 21.4], and McElreath (2016) [68, Sec. 12.4]. Examples at an advanced level of hierarchical modelling with Poisson or binomial single-datum likelihood functions, or mixtures thereof, in an astrophysical context, can be found in Andreon and Weaver (2015) [4, Secs. 8.5 and 8.12].

The code for the specification in JAGS of a **varying-intercept Poisson regression model** follows. Therein we suppressed the standardisation of the independent data, as well as the destandardisation of the model parameters. Both can be obtained from the respective code for the fixed priors case given in Sec 6.7.

**Listing 8.4: Gibbs sampling with JAGS in R: model specification for varying-intercept Poisson regression.**

```r
# JAGS model: all of the following code needs to be embedded in a
# modelString = "..." command in R

model {
  # likelihood: Poisson
  for (i in 1:nSample) {
    y[i] ~ dpois( theta[i] )
  # inverse link function
  theta[i] <- exp( zbconst + zb0[gp[i]]
+ sum( zb[1:nIndVars] * zX[i,1:nIndVars] ) ) # linebreak!
  }
  
  # adaptive prior
  # (i) varying intercept
  for (j in 1:nGroups) {
    zb0[j] ~ dnorm( 0 , precIntc )
  }
  
  # fixed priors
  zbconst ~ dnorm( 0 , 1/(<sigma0>)^2 )
  precIntc ~ dgamma( <alpha0> , <beta0> )
  omega <- sqrt( 1 / precIntc )
  
  # (ii) slope
  for (j in 1:nIndVars) {
    zb[j] ~ dnorm( 0 , 1/1^2 ) # regularising
  }
}
```

The corresponding code for the specification of a varying-intercept Poisson regression model in Stan when intending to perform HMC sampling is given in App. B.4.

This concludes the present chapter. As indicated above, the next step towards enlargement of the technical capabilities of the **hierarchical models** depicted here would be to take varying-slopes...
effects due to **prior correlations** amongst the regression coefficients into consideration. Of direct practical interest is also the systematic handling of **multi-collinearity** and of **measurement error** within the data for the independent variables.

In the final chapter, we want to sketch elementary principles of an important field of application of probability theory, viz. the theory of decision under conditions of uncertainty, which forms a conceptual cornerstone of the frameworks of Economics, Political Science and the Organisational Sciences.
Chapter 9

Decision-making in the state space picture

Decision-making is a recurrent activity everyone is confronted with virtually on a daily basis. Economic theory in particular has long had a vested interest in a systematic formalisation of the principles underlying basic decision processes. A set-theoretical state space framework of descriptive character, developed in the middle of the 20th Century, has laid the foundation for a theory of decision under conditions of uncertainty. It continues to be upgraded by integrating insights gained from experimentation, and by adapting to pertinent new conceptual ideas. In this chapter, we want to review the standard model of decision theory for the case of static one-shot choice problems for a single decision-maker in the behavioural subjective expected utility (SEU) representation due to Savage (1954) [89] and Anscombe and Aumann (1963) [5], and outline its link to the Bayes–Laplace approach to inductive statistical inference. We will also briefly relate to a specific area of ongoing research. Full discussions of the principles of decision theory are given in the textbooks by Gilboa (2009) [37] and Peterson (2017) [82] at an introductory level, and in the monographs by Wald (1950) [106], Savage (1954) [89] and Berger (1985) [7] at a highly advanced technical level. Some pedagogical examples are provided in Gelman (1998) [32].

The simplest decision-theoretical models are built on the premiss of the rational-agent paradigm of Economics. Amongst other items, this entails the assumption of the existence of some form of reasoning ability on the part of the decision-maker, so that she/he can give justifications for the choices they made. The general set-up is as follows. A rational decision-maker faces a specific choice problem. She/he finds herself/himself in a certain individual prior state of knowledge on the matter to be decided. In particular, she/he takes into consideration which external states of Nature (or boundary conditions) could potentially take an influence on the consequences of the specific act the decision-maker eventually opts for, and what outcomes the decision could possibly lead to. At the end of the decision process, all uncertainty as to the actually realised momentary state of Nature and the consequences of the act preferred by the decision-maker will be resolved. Given this new empirical information, a basis for learning has opened on which the decision-maker attains a posterior state of knowledge. It is a central objective of decision theory to cast the scenario just depicted into formal language. This aims at capturing within an axiomatic framework a rational decision-maker’s state of knowledge concerning decision-relevant external states of Nature, the decision-makers choice behaviour under conditions of uncertainty, and resultant prospects for herself/himself. We will now turn to describe the main elements of this formal language, and the choice-specific operations defined therein.
CHAPTER 9. DECISION-MAKING IN THE STATE SPACE PICTURE

9.1 Primitives

The description of static one-shot choice problems for a single decision-maker in the set-theoretical state space formulation of Anscombe and Aumann (1963) \[5\] takes the following set of primitives as building blocks. There exist:

- a finite set of $n \in \mathbb{N}$ mutually exclusive and exhaustive consequence-relevant external states of Nature $\Omega$ that are unobservable; different kinds of decision-relevant events can be represented by arbitrary subsets $A \subseteq \Omega$,

- a finite set of outcomes $X$ that are observable,

- consequences given in the form of a set of “lotteries” (viz., discrete probability distributions), $\Delta(X|I)$, over the set of outcomes $X$; on this set of “lotteries” there is defined a mixing operation such that for every two distributions $p, q \in \Delta(X|I)$, every weight factor $\alpha \in (0, 1)$, and every outcome $x \in X$ it holds that $[\alpha p + (1-\alpha) q](x) = \alpha p(x) + (1-\alpha) q(x)$,

- the decision-makers objects of choice are elements from a finite set of $k \in \mathbb{N}$ alternative acts

$$F := \{ f | f : \Omega \rightarrow \Delta(X|I) \} ;$$  \hspace{1cm} (9.1)

acts are formally understood as maps of consequence-relevant states of Nature in $\Omega$ into the space of “lotteries” over outcomes, $\Delta(X|I)$,

- an ordinal binary preference relation $\succeq$ on $F$ and, by extension, on $\Delta(X|I)$, that is observable\footnote{The ordinal binary preference relation $\succeq$ is to be read as “preferred at least as.”}.

In some formulations of choice problems, the space of consequence-relevant external states of Nature is given a logic-based fine-structure; see, e.g., Gilboa (2009) \[37\]:

- canonical states of Nature arise as truth assignments $\{ 0 : \text{false}, 1 : \text{true} \}$ to a set of $l \in \mathbb{N}$ elementary propositions,

- the size of the resultant canonical state space is given by $\text{card}(\Omega) = 2^l$,

- in this picture, the number of distinguishable events amounts to $2^{2l}$; this number can easily grow very large as the number of elementary propositions taken into account increases.

9.2 Decision matrix

The primitives of static one-shot choice problems for a single decision-maker may be visualised by means of a decision matrix, a formal concept effectively anticipated by the French mathematician, physicist, inventor, writer and Catholic philosopher Blaise Pascal (1623–1662) in his famous reasoning that has come to be known as Pascal’s wager; see, e.g., Gilboa (2009) \[37\] Sec. 5.2. Figure 9.1 outlines the structure of the decision matrix in the behavioural subjective expected utility...
9.3. Axiomatisation

The next step in the formal construction of the behavioural subjective expected utility representation according to Savage (1954) [89] and Anscombe and Aumann (1963) [5], with earlier contributions by von Neumann and Morgenstern (1944) [75], is the axiomatisation of a rational decision-maker’s choice behaviour. This leads to the (cf. Gilboa (2009) [37, p 143])

**Representation theorem:** There exist a unique discrete prior probability distribution $P \in \Delta(\Omega|I)$ (synonymous with a decision-makers “beliefs”) and an interval-scaled von Neumann–Morgenstern utility function $U : X \rightarrow \mathbb{R}$ for outcomes in $X$ (the “moral value” of outcomes according to Bernoulli (1738) [8]) provided that the ordinal binary preference relation $\succeq$ on the set of alternative acts $F$ satisfies a minimal set of five axioms of rational choice:

2This is the same von Neumann we already encountered in Sec. [5.2] in the context of Monte Carlo simulations.

3In place of a utility function, many authors, in a decision-theoretical context, employ an equivalent loss function instead; see, e.g., Jaynes (2003) [48, Sec. 14.3], Lee (2012) [63, Sec. 7.5], or Gill (2015) [39, Sec. 8.1]. Kahneman and Tversky operate with a psychological value function; see Kahneman and Tversky (1979) [53] and Kahneman (2011) [51, p 282].

| prior distribution $P \in \Delta(\Omega|I)$ | $P(\omega_1|I)$ | $P(\omega_2|I)$ | $\ldots$ | $P(\omega_n|I)$ | $\sum_{i=1}^{n} P(\omega_i|I) = 1$ |
| acts $f_j \in F \setminus \text{states } \omega_i \in \Omega$ | $\omega_1$ | $\omega_2$ | $\ldots$ | $\omega_n$ | $k, n \in \mathbb{N}$ |
| $f_1$ | $p_{11}$ | $p_{12}$ | $\ldots$ | $p_{1n}$ | consequences: |
| $f_2$ | $p_{21}$ | $p_{22}$ | $\ldots$ | $p_{2n}$ | “lotteries” |
| $\vdots$ | $\vdots$ | $\vdots$ | $\ddots$ | $\vdots$ | $p_{ij} \in \Delta(X|I)$ |
| $f_k$ | $p_{k1}$ | $p_{k2}$ | $\ldots$ | $p_{kn}$ | over outcomes $x \in X$ |
| $f : \Omega \rightarrow \Delta(X|I)$ | $\sum_{x \in X} p_{ij} = 1$ |

Figure 9.1: Static one-shot decision matrix of subjective expected utility theory for a single decision-maker.

By learning from observation of the consequences of decisions made, and of the actual realisations of specific states of Nature, the decision-maker forms a personal discrete posterior probability distribution for states of Nature that can be an informative starting point for subsequent decision problems.
1. **weak order**: the ordinal binary preference relation $\succeq$ on the set of alternative acts $F$ is complete and transitive,

2. **continuity**: for every three acts $f, g, h \in F$, if the strong preference order $f \succ g \succ h$ applies, there exist weight factors $\alpha, \beta \in (0, 1)$ such that the strong preference order $\alpha f + (1 - \alpha)h \succ g \succ \beta f + (1 - \beta)h$ follows,

3. **independence**: for every three acts $f, g, h \in F$ and weight factor $\alpha \in (0, 1)$, the weak preference order $f \succeq g$ obtains iff the weak preference order $\alpha f + (1 - \alpha)h \succeq \alpha g + (1 - \alpha)h$ obtains,

4. **monotonicity**: for every two acts $f, g \in F$, the weak preference order $f \succeq g$ for all states $\omega \in \Omega$ implies the general weak preference order $f \succeq g$,

5. **non-triviality**: there exist at least two acts $f, g \in F$ such that the strong preference order $f \succ g$ is true.

### 9.4 Subjective expected utility model

Lastly, the subjective expected utility model for describing a rational decision-maker’s choice behaviour in the context of static one-shot choice problems is embodied by the (Anscombe and Aumann (1963) [5], Gilboa (2009) [37, p 144])

**Anscombe–Aumann theorem:** The ordinal binary preference relation $\succeq$ on the set of alternative acts $F$ satisfies the set of five axioms of rational choice if and only if there exists a unique discrete prior probability distribution $P \in \Delta(\Omega|I)$ for the state space $\Omega$ and a non-constant interval-scaled von Neumann–Morgenstern utility function $U : X \to \mathbb{R}$ for outcomes in $X$ such that, for every two acts $f, g \in F$, the weak preference order

$$f \succeq g$$

is true iff for the expected utility of these two acts the condition

$$\sum_{\omega \in \Omega} \left( \sum_{x \in X} U(x)f(\omega)(x) \right) P(\omega|I) \geq \sum_{\omega \in \Omega} \left( \sum_{x \in X} U(x)g(\omega)(x) \right) P(\omega|I)$$

is satisfied.

This states that a rational decision-maker’s choice behaviour can be interpreted as if they apply a personal prior probability distribution to express their uncertainty as to ensuing consequence-relevant states of Nature, and as if they always maximise subjective expected utility. The concept of an expected utility of an outcome was introduced into economic theory by the Swiss mathematician and physicist Daniel Bernoulli FRS (1700–1782); cf. Bernoulli (1738) [8].

Savage (1954) [89] posits the possibility of reconstructing, via the axiomatic formulation, both a decision-maker’s prior probability distribution and their utility function when a sufficient amount of empirical data on her/his choice behaviour, and the preferences so revealed, becomes available.
9.5  Caveats of the SEU model

A number of conceptual inconsistencies have been spotted over the years by various authors within the **subjective expected utility model** for a **rational decision-maker’s choice behaviour**, when confronted with experimental data. Particularly well-known in this respect are the following caveats:

- **Allais (1953)** [3] paradox: the violation of some axioms of rational choice by decision-makers in empirical tests of the SEU model, providing strong indication for a so-called **certainty effect**; see also Kahneman (2011) [51]* pp 312–314*,

- **Ellsbergs (1961)** [21] paradox: his experiments revealed that in simple specific choice situations decision-makers often prefer known probability distributions over unknown ones, even when the latter promise the possibility of larger ensuing pay-offs; this effect has been termed **uncertainty aversion**,

- **Kahneman and Tversky (1979)** [53] emphatically criticised the lack in the SEU framework of a **reference point** for a decision-maker’s individual utility function for outcomes; in their own work they had gathered compelling empirical evidence that vividly suggested that outcomes acquire a **different psychological value** for a decision-maker, depending on whether she/he perceives the outcome as a gain or as a loss; they referred to this (in their view) omission as “Bernoulli’s error,”

- **Dekel, Lipman and Rustichini’s (1998)** [16] impossibility results: in theoretical work these authors demonstrated that the standard state space formulation precludes **non-trivial forms of unawareness** of a decision-maker within an SEU model; a standard state space model is incapable of consistently incorporating the dimension of a decision-makers unawareness of future contingencies. In this respect, SEU model cannot adequately capture the concept of **surprises**.

All in all, the works listed, as well as other less prominent publications, hinted at the possibility that decision-makers do **not** necessarily act as though they were following the premiss of maximising their subjective expected utility on all occasions. In contrast, decision-makers do regularly exhibit **bounded rationality**. One particular line of investigation started undertaking a revision of the **rational-agent paradigm** in theories of human decision-making by integrating in a comprehensible fashion the complex dimension of a decision-maker’s psychological variability. This lead to the initiation of the field of **Behavioural Economics**, which is strongly associated with the names of the IsraeliUS-American experimental psychologists **Daniel Kahneman (born 1934)** and Amos Tversky (19371996), and the US-American economist **Richard H Thaler (born 1945)**; see Kahneman (2011) [51]* p 282f*, Thaler and Sunstein (2008) [101]*, and also Taleb (2007) [100]. For their ground-breaking work, both Kahneman in 2002 and Thaler in 2017 were awarded the **Sveriges Riksbank Prize in Economic Sciences in Memory of Alfred Nobel**.
9.6 Representations of non-knowledge

During the last 20 years or so, researchers in economic theory have become strongly interested again in finding coherent ways of including in a consistent formalisation of a decision-maker’s choice behaviour in the light of uncertainty the decision-maker’s non-knowledge of consequence-relevant states of Nature, and of unknown outcomes to acts she/he is going to pursue. Presumably unintended, this topic was brought spectacularly to the attention of an international public audience by Donald Rumsfeld, the former U.S. Secretary of Defense, on Feb 12, 2002, when responding to a journalist’s question at a U.S. Department of Defense news briefing [87] with the following explanation:

“Reports that say that something hasn’t happened are always interesting to me, because as we know, there are known knowns; there are things we know we know. We also know there are known unknowns; that is to say we know there are some things we do not know. But there are also unknown unknowns – the ones we don’t know we don’t know. And if one looks throughout the history of our country and other free countries, it is the latter category that tend to be the difficult ones.”

The inclusion of representations of different forms of a decision-maker’s non-knowledge in a comprehensive conceptual framework proves to be a challenging theoretical task. Starting from the decision matrix of static one-shot choice problems for a single decision-maker displayed in Fig. 9.1, the immediate points for potential modification and extension are (i) the decision-maker’s individual prior probability distribution for expressing degrees-of-belief for the plausibility of different states of Nature, and (ii) the issue of the completeness of the space of states of Nature itself. Some approaches that follow one or the other of these two lines of investigation have been reviewed by Svetlova and van Elst (2012, 2014) [98, 99]. Further interesting discussions on potential ways of advancing this intriguing topic have been collected in the “Handbook of Ignorance Studies” edited by Gross and McGoey (2015) [42].

Our introductory journey through the foundations of inductive statistical inference as practised within the Bayes-Laplace approach to data analysis and statistical inference has now come to an end. We hope the reader could sense a glimpse of the fascination induced by the simplicity and elegance of this framework, but, even more so, picked up some very useful and efficient practical tools for building scientifically sound statistical models, and for providing adequate interpretations and predictions.
Concluding remarks

Undoubtedly, an era of incomprehensibly huge big-data reservoirs has become a reality in present-day human societies as an immediate consequence of the changes and innovations brought about by the all-pervasive digital transformation. The question is what meaningful social purpose can all the information thereby generated and collected be delivered to?

I think this provides us with a great opportunity for making sustainable progress on practical as well as intellectual issues, though these two areas do not necessarily constitute orthogonal dimensions. There exists a multitude of intriguing and awe-inspiring phenomena, based, located, and rooted in both the natural and the social domains of human experience, that are accessible to observation and measurement. Equipped with naturally inherited curiosity that gets passed on from one generation to the next, and sticking to the guidelines of the scientific method, when given access to relevant empirical data, we can use analytical skills to try to read the plot behind the different kinds of natural and social interactions and interconnections that continue to pose complex and confusing puzzles to our everyday-life situations. The prospect of success for creating new common values should experience a boost when humility, courage, independent and unconstrained thinking, a diversity of ideas, taking care of one another, and an attitude of openness towards surprises are to be found in the portfolio of tools for investigation. Plausible reasoning leaves no room for “alternative facts.” Pseudo-argumentations based on the latter have a rather poor track record concerning their yield of tangible communal benefits. The US-American theoretical physicist Richard Phillips Feynman (1918–1988) has long been an outspoken critical voice against populist approaches towards tackling real problems in any kind of field of societal interest; cf. his thought-stimulating essay “Cargo Cult Science” published in Ref. [25] [pp 308–317]. And there certainly are some really pressing issues these days that need to be addressed by the human community; see, e.g., Helbing (2013) [46].

The human community anticipates in about 4 to 5 billion years a transition of the Sun from its present nuclear hydrogen-burning state to a then nuclear helium-buring state, in the process of which it will drastically inflate its volume to become a red giant, so the fate of the three innermost planets of the Solar System is practically known already today; see, e.g., Lesch and Müller (2003) [64] p 405]. Nevertheless, we have potentially much more time ahead of us for realising our potentials for creativity and sharing knowledge and understanding when compared to the period that is factually on record as regards the past history of the human species. Up to now, quite an impressive legacy of common goals, cultural values and outstanding intellectual triumphs has accumulated: in music, the visual and the performing arts, in drama, poetry and novel-writing, in sports, the different languages, and, of course, in view of the great scientific achievements of a very diverse spectrum of human minds. There are many prominent examples of seminal advances.
in the human understanding of different kinds of dynamical processes that have a direct bearing on human existence, among them

- the natural evolution of organic creatures according to the English naturalist, geologist and biologist Charles Robert Darwin, FRS FRGS FLS FZS (1809–1882) (see Darwin (1859) [15]),

- the nature of gravitational interactions as explained by Albert Einstein (1871–1955) (see Einstein (1915) [20], Hawking and Ellis (1973) [45], Misner et al (1973) [72], Abbott et al (2016) [1]; and also Ref. [24]), or

- the genetic coding mechanism underlying the reproduction of any living organism as deciphered by the British molecular biologist, biophysicist, and neuroscientist Francis Harry Compton Crick OM FRS (1916–2004), the US-American molecular biologist, geneticist and zoologist James Dewey Watson (born 1928), and the New Zealand physicist and molecular biologist Maurice Hugh Frederick Wilkins CBE FRS (1916–2004) (see Watson and Crick (1953) [108] and Wilkins et al (1953) [109]).

The face of planet Earth has been radically changed by the influence on Nature taken by humans over a period of only a few hundred, possibly a few thousand years — a far cry compared to the minimum 10 billion years it took to forge all the different kinds of natural resources, now available to the human community, in various kinds of astrophysical furnaces. This leaves at best a large two-digit figure of generations that have since been involved in exploiting these resources for generating and sharing material as well as immaterial goods, in the large majority for very sensible and helpful, but regrettably also for less sensible courses. If we manage to keep an eye on the upper limits presented to these resources, develop a common sense for the principle of reciprocity binding wo/man-kind to Nature, foster a related emotional connectivity, and ultimately safeguard the habitability of planet Earth for many generations to come, we might stand a real chance of being perceived by fellow beings in the vast stretches of the spacetime continuum as respectable citizens of the Universe.

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Appendix A

Essential commands in R

An official R reference card can be obtained from the URL (cited on July 10, 2018): https://cran.r-project.org/doc/contrib/Short-refcard.pdf

A
anova(model): outputing an ANOVA table for a linear model
autocorr.diag(model): autocorrelation diagnostic for a Markov chain Monte Carlo simu-
lution (coda package)
autocorr.plot(model): autocorrelation plot for a Markov chain Monte Carlo simulation
(coda package)

B
boxplot(variable ~ group variable, data = data frame): compiling a box plot for comparing metrically scaled univariate data between groups

cbind(object 1, object 2): combining matching objects (vectors, matrices, data frames) by columns
colMeans(data frame): computing means of column entries of data frame or matrix
colnames(data frame): listing column names of data frame or matrix
cor(data frame): obtains bivariate correlation matrix for for metrically scaled data from a data frame

D
data("data set"): loading a data set
data.frame(y=variable 1, X1=variable 2, ..., Xk+1=variable k+1): creating a data frame from the data of the specified variables
density(data): computes density estimates for given data; combination with plot(..) yields density plots
densplot(modCsim[,column specifications], xlim = c(lower limit, upper limit)): plotting the posterior densities for variables estimated in a Markov chain Monte Carlo simulation (coda package)
dic.samples(model, n.iter=number): computing the value of the deviance information criterion (DIC) for a Markov chain Monte Carlo simulation (rjags package)
dim(data frame): dimension of a data frame
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E
effectiveSize(model): effective sample size of a Markov chain Monte Carlo simulation

G
gelman.diag(model): Gelman–Rubin diagnostic for a Markov chain Monte Carlo simulation (coda package)
gelman.plot(model): plotting the development of Gelman–Rubin diagnostic with number of MCMC iterations (coda package)

H
head(data frame): scanning the first few rows of a data frame
HPDinterval(model): computing intervals of highest posterior density for model parameters (coda package)
hist(data frame$variable, freq = FALSE): plotting a histogram of relative frequencies for metrically scaled univariate data

I
install.packages("package"): installing a specific package
is.na(data frame): checking for missing values ("NA") in a data frame

L
length(variable): sample size of data for a specific variable
library("package"): loading a specific package
lm(variable1 ~ variable2, data = data frame): compiling a linear model for bivariate data

M
mean(variable): computing the sample mean for metrically scaled univariate data
median(variable): computing the sample median for metrically scaled univariate data

N
na.omit(data frame): removing cases with missing values ("NA") from a data frame
ncol(data frame): number of columns of a data frame
nrow(data frame): number of rows of a data frame
numeric(m): initialising an m-component (zero) vector

P
pairs(data frame): generating a matrix of pairwise scatter plots for metrically scaled data from a data frame
plot(variable1 ~ variable2, data = data frame): compiling a scatter plot for metrically scaled bivariate data

Q
quantile(variable, α): computing the α–quantile for metrically scaled univariate data

R
raftery.diag(model): Raftery–Lewis autocorrelation diagnostic for a Markov chain Monte Carlo simulation (coda package)
rbind(object 1, object 2): combining matching objects (vectors, matrices, data frames) by rows
rowMeans(data frame): computing means of row entries of data frame or matrix
rep(x, times): replicate “x” as often as indicated by “times”
rownames(data frame): listing row names of data frame or matrix

S
sample(elements, prob = posterior, size = <number of samples>,
replace = TRUE): sampling elements with repetition from a simulated posterior distribution
scale(variable, center = TRUE, scale = TRUE): standardisation of metrically scaled univariate data
sd(variable): computing the sample standard deviation for metrically scaled univariate data
[(n−1)-convention]
set.seed(integer): initialising the random number generator to a specific integer
str(data frame): scanning the structure of a data set
summary(model): outputing values of key statistical measures of a model

T
t(matrix): transposition of a matrix
table(variable): generating a table of absolute frequencies for univariate data
tail(data frame): scanning the last few rows of a data frame
traceplot(as.mcmc(data set$variable)): trace plot for a Markov chain Monte Carlo simulation for a specific variable (coda package)

V
var(variable): computing the sample variance for metrically scaled univariate data [(n−1)-
convention]

W
waic(model) (loo package)
APPENDIX A. ESSENTIAL COMMANDS IN R
Appendix B

Stan codes for HMC simulations

In this appendix we give the main elements of HMC simulations of posterior probability distributions with Stan, assuming a complete data set with no missing values is available. Some remarks on reading data sets in a file format other than *.csv into R were made in Subsec. 6.3.1. Comment lines in Stan code are to be preceded by a double slash “//”. Please refer to the Stan user manual [94, Sec. 8] and the publication [95] by the Stan Development Team for further information on running Stan from R.

To maintain generality, the data input formulation below is given for non-standardised metrically scaled data in the design matrix $X$.

Listing B.1: HMC sampling with Stan in R: general structure of code.

```r
# Load R package rstan
library("rstan")

# Load a specific data set from a *.csv file, creating a R data.frame
dataSet = read.csv("<filename.csv>", header = TRUE)

# Identify dependent and independent variables, sample size,
# number of independent variables, number of groups
y = dataSet[,"yVarName"]
xIn = as.matrix(dataSet[,c("xVarName1", ..., "xVarNamek")], ncol = k)
X = cbind(c(rep(1, nrow(xIn))), xIn) # design matrix: capital X!
nSample = length(y)
nIndVars = ncol(xIn)
gp = as.numeric(dataSet[,"groupVarName"])) # if relevant
nGroups = length(unique(gp)) # if relevant

# Specify data list for Stan simulation
dataList = list(
  nSample = nSample,
  nIndVars = nIndVars,
  nGroups = nGroups, # if relevant
  y = y,
  X = X, # design matrix
)
```

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`gp = gp # if relevant
```

# Stan model, specified via a string command in R
modelString = "<model specification, etc. to be inserted here>"

# Generate dynamic shared object (DSO) in C++
stanDSO = stan_model(model_code = modelString)

# Execution of Stan simulation: saving simulated posterior samples
modSimStan = sampling(
    object = stanDSO, data = dataList, chains = <number of HMC chains to be generated>,
    cores = <number of cores used for parallel computing (max: 3)>,
    iter = <total number of iterations>,
    warmup = <number of warmup iterations>,
    thin = 1, init = 'random'
)

# Trace plots of HMC chains
plot(modSimStan)

# Summary of simulated posterior marginal for each parameter
summary(modSimStan)

B.1 Linear regression

B.1.1 Fixed priors

We specify a linear regression model with a Gaussian single-datum likelihood function according to Eq. (2.21), with homogeneous variance. Contrary to Sec. 6.4 we here employ a half-Cauchy prior probability distribution for the scale parameter \( \sigma^2 \) as described in Subsec. 3.5.1. The regression coefficients \( \beta \) are given regularising Gaussian prior probability distributions. The following code assumes standardised data for the dependent and independent variables. It activates the calculation of the WAIC-estimate for a model’s out-of-sample deviance.

Listing B.2: HMC sampling with Stan in R: model specification for linear regression.

`# Stan model: all of the following code needs to be embedded in a
# modelString = "..." command in R

data {
    int<lower=1> N;
`
### B.1. LINEAR REGRESSION

```plaintext
real zy[N]; // standardised variables!
real zX0[N];
real zX1[N];
...
real zXk[N];
}

parameters{
  real<lower=0> zsigma; // standardised parameters!
  real zb0;
  real zbl;
  ...
  real zbk;
}

model{
  vector[N] zmu;
  zsigma ~ cauchy( 0 , 2 ); // half-Cauchy prior
  zbk ~ normal( 0 , 1 ); // regularising zero-centred Gauss priors
  ...
  zbl ~ normal( 0 , 1 );
  zb0 ~ normal( 0 , 1 );
  for ( i in 1:N ) {
    zmu[i] = zb0 * zX0[i] + zbl * zX1[i] + ... + zbk * zXk[i];
  }
  zy ~ normal( zmu , zsigma );
}

generated quantities{
  vector[N] zmu;
  real dev;
  dev = 0;
  for ( i in 1:N ) {
    zmu[i] = zb0 * zX0[i] + zbl * zX1[i] + ... + zbk * zXk[i];
  }
  dev = dev + (-2)*normal_lpdf( zy | zmu , zsigma );
}
```

#### B.1.2 Adaptive priors

We give the code for a varying-intercepts linear regression model with a non-central \( t \)-single-datum likelihood function according to eq. (2.26), and a Gauß adaptive prior for the group-level intercept parameter. Half-Cauchy priors are chosen for the scale parameters. The code assumes standardised data for the dependent and independent variables. It activates the calculation of the WAIC-estimate for a model’s out-of-sample deviance.
Listing B.3: HMC sampling with Stan in R: model specification for varying-intercept linear regression with non-central $t$–single-datum likelihood function.

```stan
# Stan model: all of the following code needs to be embedded in a
# modelString = "..." command in R

data{
  int<lower=1> N;
  int<lower=1> N_gp; // number of groups
  real zy[N]; // standardised variables!
  real zX0[N];
  real zX1[N];
  ...
  real zXk[N];
  int gp[N]; // group variable
}

parameters{
  real<lower=2> nu // nu > 2: existence of mean and variance
  real<lower=0> zsigmaIntc; // standardised parameters!
  real<lower=0> zsigma;
  vector[N_gp] zb0;
  real zeta;
  real zbl;
  ...
  real zbk;
}

model{
  vector[N] zmu;
  nu ~ exponential( <theta0> ); // exponential prior
  zsigma ~ cauchy( 0 , 2 ); // half-Cauchy prior
  zbk ~ normal( 0 , 1 ); // regularising zero-centred Gauss priors
  ...
  zbl ~ normal( 0 , 1 );
  zsigmaIntc ~ cauchy( 0 , 2 ); // half-Cauchy prior
  zeta ~ normal( 0 , <s0> ); // zero-centred Gauss prior
  zb0 ~ normal( zeta , zsigmaIntc ); // Gauss adaptive prior
  for ( i in 1:N )
    zmu[i] = zb0[gp[i]] * zX0[i] + zbl * zX1[i] + ... + zbk * zXk[i];
  zy ~ student_t( nu , zmu , zsigma ); // t-likelihood
}

generated quantities{
  vector[N] zmu;
}
B.2 ANOVA-LIKE REGRESSION

B.2.1 Fixed priors

We give an ANOVA-like regression model with a Gaussian single-datum likelihood function according to Eq. (2.21), with homogeneous variance. Contrary to Sec. 6.5, we employ a half-Cauchy prior probability distribution for the scale parameter $\sigma^2$ as described in Subsec. 3.5.1. The location parameters $\mu_g$ are given Gaussian prior probability distributions. It activates the calculation of the WAIC-estimate for a model’s out-of-sample deviance.

Listing B.4: HMC sampling with Stan in R: model specification for homoscedastic ANOVA-like regression.

```stan
# Stan model: all of the following code needs to be embedded in a # modelString = "..." command in R
data{
  int<lower=1> N;
  int<lower=1> N_gp; // number of groups
  real y[N];
  int gp[N]; // group variable
}
parameters{
  real<lower=0> sigma;
  real a;
  vector[N_gp] a_gp;
}
model{
  vector[N] mu;
  sigma ~ cauchy( 0 , 2 ); // half-Cauchy prior
  a_gp ~ normal( 0 , 1 );
  a ~ normal( <mean y> , <stdev y> );
  for ( i in 1:N ) {
    mu[i] = a + a_gp[gp[i]];
  }
}
APPENDIX B. STAN CODES FOR HMC SIMULATIONS

y ~ normal( mu , sigma );
}
generated quantities{
    vector[N] mu;
The real dev;
    dev = 0;
    for ( i in 1:N ) {
        mu[i] = a + a_gp[gp[i]];
    }
    dev = dev + (-2)*normal_lpdf( y | mu , sigma );
}

B.2.2 Adaptive priors

We give the code for a hierarchical ANOVA-like regression model with a non-central \( t \)-single-datum likelihood function according to Eq. (2.26). A half-Cauchy adaptive prior is chosen for the group-level scale parameter. The code activates the calculation of the WAIC-estimate for a model’s out-of-sample deviance.

Listing B.5: HMC sampling with Stan in R: model specification for heteroscedastic ANOVA-like regression with non-central \( t \)-single-datum likelihood function.

# Stan model: all of the following code needs to be embedded in a
# modelString = "..." command in R

data{
    int<lower=1> N;
    int<lower=1> N_gp; // number of groups
    real y[N];
    int gp[N]; // group variable
}

parameters{
    real<lower=2> nu // nu > 2: existence of mean and variance
    real<lower=0> tau;
    vector<lower=0>[N_gp] sigma_gp;
    real<lower=0> gamma;
    vector[N_gp] a_gp;
    real a;
}

model{
    vector[N] sigma;
    vector[N] mu;
    nu ~ exponential( <theta0> ); // exponential prior
B.3 Logistic regression

B.3.1 Fixed priors

We specify a logistic regression model with a Bernoulli single-datum likelihood function according to Eq. (2.4), and regularising zero-centred Gauß prior probability distributions for the unknown regression coefficients $\beta$. The following code assumes standardised data for the independent variables. It activates the calculation of the WAIC-estimate for a model’s out-of-sample deviance.

Listing B.6: HMC sampling with Stan in R: model specification for logistic regression.

```stan
data{
    int<lower=1> N;
}
parameters{
    real<lower=0> lambda0;
    real<lower=0> alpha0;
    real<lower=0> mean_y;
    real<lower=0> std_y;
    vector[N] gp;
    real<lower=0> sigma_gp[N];
    real<lower=0> sigma; // half-Cauchy adaptive prior
    real<lower=0> mu[N]; // zero-centred Gauss adaptive prior
}
model{
    gamma ~ exponential( lambda0 );
    tau ~ cauchy( 0, alpha0 );
    a ~ normal( mean_y, std_y );
    for ( j in 1:N )
        sigma_gp[j] ~ cauchy( 0, gamma ); // half-Cauchy adaptive prior
    for ( i in 1:N )
        sigma[i] = sigma_gp[gp[i]]; // zero-centred Gauss adaptive prior
    for ( i in 1:N )
        mu[i] = a + a_gp[gp[i]];
    y ~ student_t( nu, mu, sigma ); // t-likelihood
}
generated quantities{
    vector[N] sigma; // half-Cauchy adaptive prior
    vector[N] mu; // zero-centred Gauss adaptive prior
    real dev;
    dev = 0;
    for ( i in 1:N )
        sigma[i] = sigma_gp[gp[i]]; // half-Cauchy adaptive prior
    for ( i in 1:N )
        mu[i] = a + a_gp[gp[i]]; // zero-centred Gauss adaptive prior
    dev = dev + (-2)*student_t_lpdf( y | nu, mu, sigma );
}
```

B.3 Logistic regression
int y[N];
real zX0[N];
real zX1[N]; // standardised independent variables!
...;
real zXk[N];
}

parameters{
  real zb0; // standardised parameters!
  real zb1;
  ...;
  real zbk;
}

model{
  vector[N] theta;
  zbk ~ normal( 0 , 1 ); // regularising zero-centred Gauss priors
  ...;
  zbl ~ normal( 0 , 1 );
  zbo ~ normal( 0 , 1 );
  for ( i in 1:N ) {
    theta[i] = zb0 * zX0[i] + zbl * zX1[i] + ... + zbk * zXk[i];
  }
  y ~ binomial_logit( 1 , theta ); // logit link function
}

generated quantities{
  vector[N] theta;
  real dev;
  dev = 0;
  for ( i in 1:N ) {
    theta[i] = zb0 * zX0[i] + zbl * zX1[i] + ... + zbk * zXk[i];
  }
  dev = dev + (-2)*binomial_logit_lpmf( y | 1 , theta );
}

B.3.2 Adaptive priors

We specify a varying-intercept logistic regression model with a binomial total-data likelihood function according to Eq. (2.9). A Gauss adaptive prior probability distribution is introduced for the group-level intercept parameter. The following code assumes standardised data for the independent variables. It activates the calculation of the WAIC-estimate for a model’s out-of-sample deviance.

Listing B.7: HMC sampling with Stan in R: model specification for varying-intercept logistic regression with binomial total-data likelihood function.
# Stan model: all of the following code needs to be embedded in a # modelString = "..." command in R

data{
  int<lower=1> N;
  int<lower=1> N_gp; // number of groups
  int y[N]; // number of successes
  int n[N]; // number of trials
  int gp[N]; // group variable
  real zX0[N];
  real zX1[N]; // standardised independent variables!
  ...;
  real zXk[N];
}

parameters{
  vector[N_gp] zb0;
  real gpMu;
  real zb1; // standardised parameters!
  ...;
  real zbk;
  real<lower=0> gpSigma;
}

model{
  vector[N] theta;
  gpSigma ~ cauchy( 0 , 2 ); // half-Cauchy prior
  zbk ~ normal( 0 , 1 ); // regularising zero-centred Gauss priors
  ...;
  zbl ~ normal( 0 , 1 );
  gpMu ~ normal( 0 , 10 );
  zb0 ~ normal( gpMu , gpSigma ); // Gauss adaptive prior
  for ( i in 1:N ) {
    theta[i] = zb0[gp[i]] * zX0[i] + zb1 * zX1[i] + ... + zbk * zXk[i];
  }
  y ~ binomial_logit( n , theta ); // logit link function
}

generated quantities{
  vector[N] theta;
  real dev;
  dev = 0;
  for ( i in 1:N ) {
    theta[i] = zb0[gp[i]] * zX0[i] + zb1 * zX1[i] + ... + zbk * zXk[i];
  }
  dev = dev + (-2)*binomial_logit_lpmf( y | n , theta );
}

B.3. LOGISTIC REGRESSION
B.4 Poisson regression

B.4.1 Fixed priors

A Poisson regression model, with a Poisson single-datum likelihood function according to Eq. (2.15), and regularising zero-centred Gaussian prior probability distributions for the unknown regression coefficients \( \beta \), is coded below. Herein standardised data is assumed for the independent variables. Note that we have included (but currently commented out) the alternative model specification for operating with exposures \( \tau \) and a rate parameter \( \lambda \). It activates the calculation of the WAIC-estimate for a model’s out-of-sample deviance.

Listing B.8: HMC sampling with Stan in R: model specification for Poisson regression.

```r
# Stan model: all of the following code needs to be embedded in a  
# modelString = "...", command in R

data{
  int<lower=1> N;
  int y[N];
  real zX0[N];
  real zX1[N]; // standardised independent variables!
  ...;
  real zXk[N];
}

parameters{
  real zb0; // standardised parameters!
  real zb1;
  ...;
  real zbk;
}

model{
  vector[N] theta;
  zbk ~ normal( 0 , 1 ); // regularising zero-centred Gaussian priors
  ...;
  zb0 ~ normal( 0 , 1 );
  for ( i in 1:N ) {
    theta[i] = exp(zb0 * zX0[i] + zb1 * zX1[i] + ... + zbk * zXk[i]);
    // lambda[i] = (1/tau[i]) * exp(zb0 * zX0[i] + zb1 * zX1[i]
    // + ... + zbk * zXk[i]);
  }
  y ~ poisson( theta );
  // y ~ poisson( lambda );
}

generated quantities{
```
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```stan
vector[N] theta;
real dev;
dev = 0;
for ( i in 1:N ) {
    theta[i] = exp(zb0 * zX0[i] + zb1 * zX1[i] + ... + zb2 * zXk[i]);
    lambda[i] = (1/tau[i]) * exp(zb0 * zX0[i] + zb1 * zX1[i] + ... + zbk * zXk[i]);
}
dev = dev + (-2)*poisson_lpmf( y | theta );
//dev = dev + (-2)*poisson_lpmf( y | lambda );
}
```

B.4.2 Adaptive priors

We here give the code for a varying-intercept Poisson regression model. A Gauss adaptive prior probability distribution is used for the group-level intercept parameter. The following code assumes standardised data for the independent variables. It activates the calculation of the WAIC-estimate for a model’s out-of-sample deviance.

Listing B.9: HMC sampling with Stan in R: model specification for varying-intercept Poisson regression.

```
# Stan model: all of the following code needs to be embedded in a
# modelString = "..." command in R

data{
    int<lower=1> N;
    int<lower=1> N_gp; // number of groups
    int y[N];
    int gp[N]; // group variable
    real zX0[N];
    real zX1[N]; // standardised independent variables!
    ...;
    real zXk[N];
}

parameters{
    vector[N_gp] zb0;
    real zbconst;
    real zb1; // standardised parameters!
    ...;
    real zbk;
    real<lower=0> gpSigma;
}

model{
```
vector[N] theta;
gpSigma ~ cauchy( 0 , 1 );
zbconst ~ normal( 0 , 10 );
zbk ~ normal( 0 , 1 ); // regularising zero-centred Gauss priors
...
zb1 ~ normal( 0 , 1 );
zb0 ~ normal( 0 , gpSigma ); // zero-centred adaptive Gauss prior
for ( i in 1:N ) {
    theta[i] = zbconst + zb0[gp[i]] * zX0[i] + zbl * zX1[i] + ... + zbk * zXk[i]); // take care of linebreak!
    //lambda[i] = -log(tau[i]) + zbconst + zb0[gp[i]] * zX0[i] //+ zbl * zX1[i] + ... + zbk * zXk[i]);
}
y ~ poisson_log( theta ); // log link function
//y ~ poisson_log( lambda );

generated quantities{
    vector[N] theta;
    real dev;
    dev = 0;
    for ( i in 1:N ) {
        theta[i] = zbconst + zb0[gp[i]] * zX0[i] + zbl * zX1[i] + ... + zbk * zXk[i]); // linebreak!
        //lambda[i] = -log(tau[i]) + zbconst + zb0[gp[i]] * zX0[i] //+ zbl * zX1[i] + ... + zbk * zXk[i]);
    }
    dev = dev + (-2)*poisson_log_lpmf( y | theta );
    //dev = dev + (-2)*poisson_log_lpmf( y | lambda );
}
Appendix C

Glossary of technical terms (GB – D)

A
act: Handlung
algorithm: Algorithmus, Rechenregel
ANOVA (analysis of variance): Varianzanalyse
autocorrelation: Autokorrelation

B
Bayes’ theorem: Satz von Bayes
behaviour: Verhalten
binomial coefficient: Binomialkoeffizient
bivariate: bivariat, zwei variable Größen betreffend
bounded rationality: begrenzte Rationalität, begrenzte Vernunft

C
choice: Wahl, Auswahl
cluster: Klumpen, Anhäufung
common sense: gesunder Menschenverstand
complete ignorance: gänzliche Unkenntnis
conditional probability: bedingte Wahrscheinlichkeit
conjunction: Konjunktion, Mengenschnitt
consequence: Konsequenz, Auswirkung
contingency table: Kontingenztafel
convenience sample: Gelegenheitsstichprobe
covariance matrix: Kovarianzmatrix

D
data: Daten
data-generating process: Daten generierender Prozess
data matrix: Datenmatrix
decision: Entscheidung
degree-of-belief: Glaubwürdigkeitsgrad, Plausibilität
degrees of freedom: Freiheitsgrade
degree of plausibility: Plausibilitätsgrad
dependent variable: abhängige Variable

design matrix: Regressormatrix, Modellmatrix

deviance: abweichendes Verhalten

deviation: Abweichung

disjunction: Disjunktion, Mengenvereinigung

dispersion: Streuung

distribution: Verteilung

divergence: Divergenz, Auseinanderstreben

E

estimation: Schätzung

evidence: Anzeichen, Hinweis, Anhaltspunkt, Indiz

echangeability: Austauschbarkeit

expectation value: Erwartungswert

exposure: Ausgesetztsein

F

fact-based reasoning: Fakten basiertes Argumentieren

fallacy: Trugschluss, Fehlschluss, Täuschung

G

group: Gruppe

H

heteroscedasticity: Heteroskedastizität, inhomogene Varianz

homoscedasticity: Homoskedastizität, homogene Varianz

hypothesis: Hypothese, Behauptung, Vermutung

I

ignorance: Unkenntnis

information: Information

information criterion: Informationskriterium

information entropy: Informationsentropie

interaction: Wechselwirkung

interaction effect: Wechselwirkungseffekt

intercept: Achsenabschnitt

J

joint distribution: gemeinsame Verteilung

K

knowledge: Wissen, Kenntnis, Erkenntnis, Wissensstand

L

Lagrange function: Lagrange-Funktion
Lagrange multiplier: Lagrange-Multiplikator, integrierender Faktor
linear regression analysis: lineare Regressionsanalyse
link function: Verknüpfungsfunktion
location parameter: Lokationsparameter
logical complement: logisches Gegenteil
loss function: Verlustfunktion

M
main effect: Haupteffekt
marginal distribution: Randverteilung
marginal frequencies: Randhäufigkeiten
marginalisation: Marginalisierung
maximum entropy distribution: Verteilung maximaler Entropie
measurement: Messung, Datenaufnahme
model comparison: Modellvergleich
multi-collinearity: Multikollinearität

N
non-knowledge: Nichtwissen
normalisation condition: Normierungsbedingung

O
observable: beobachtbar, messbar
observation: Beobachtung
odds: Wettchancen
operationalisation: Operationalisieren, latente Variable messbar gestalten
outlier: Ausreißer
over-fitting: übergenaues Anpassen

P
parameter: Parameter, wählbare Stellgröße
parsimony: Sparsamkeit
pooling: Zusammenlegen, gemeinsames Nutzen
population: Grundgesamtheit
precision: Präzisionsparameter
prediction: Vorhersage
predictor: erklärende Variable
premiss: Voraussetzung, Prämisse
primitive: Grundbaustein
probability: Wahrscheinlichkeit
probability density function (pdf): Wahrscheinlichkeitsdichte
probability function: Wahrscheinlichkeitsfunktion
proposition: Vorschlag, Antrag, Aussage, Behauptung, Prämisse
psychological value: psychologischer Wert

R
rare event: seltenes Ereignis
rate parameter: Ratenparameter
regression analysis: Regressionsanalyse
regression coefficient: Regressionskoeffizient
regression model: Regressionsmodell
regression toward the mean: Regression zur Mitte
re-scaling: Reskalierung, Größenordnungsänderung
retrodiction: Nachersage, Rekonstruktion (von Daten)
risk: Risiko (berechenbar)
rule of succession: Regel des nachfolgenden Wertes

S
sample: Stichprobe
sample mean: Stichprobenmittelwert
sample size: Stichprobenumfang
sample variance: Stichprobenvarianz
sampling distribution: Stichprobenkenngrößenverteilung
scale-invariant: skaleninvariant
scale parameter: Skalenparameter
scientific endeavour: wissenschaftliche Bemühung
scientific method: Wissenschaftliche Methode
shape parameter: Formparameter
shrinkage: Schrumpfen
slope: Steigung
standardisation: Standardisierung
state of Nature: Zustand der Außenwelt
statistical (in)dependence: statistische (Un)abhängigkeit
statistical model: statistisches Modell
statistical variable: Merkmal, Variable
sufficient statistic: suffizientes statistisches Maß
surprise: Überraschung, unerwartetes Ereignis

T
target population: Zielgruppe
transformation: Transformation, Umwandlung, Veränderung
translation: Translation, Verschiebung

U
uncertainty: Unsicherheit (nicht berechenbar)
under-fitting: ungenügendes Anpassen
univariate: univariat, eine einzige variable Größe betreffend
unit: (Maß-)Einheit
utility function: Nutzenfunktion

V
value: Wert
variance: Varianz
variation: Variation
Bibliography

[1] B P Abbott et al (LIGO Scientific Collaboration and Virgo Collaboration) (2016) Observation of gravitational waves from a binary black hole merger *Physical Review Letters* **116** 061102 (116) and Preprint arXiv:1602.03837v1 [gr-qc]

[2] J Albert (2009) *Bayesian Computation with R* 2nd Edition (Dordrecht: Springer) ISBN–13: 9780387922973

[3] M Allais (1953) Le comportement de l’homme rationnel devant le risque: critique des postulats et axioms de l’Ecole Américaine *Econometrica* **21** 503–546

[4] S Andreon and B Weaver (2015) *Bayesian Methods for the Physical Sciences — Learning from Examples in Astronomy and Physics* (Cham: Springer) ISBN–13: 9783319152868

[5] F J Anscombe and R J Aumann (1963) A definition of subjective probability *The Annals of Mathematical Statistics* **34** 199–205

[6] T Bayes (1763) An essay towards solving a problem in the doctrine of chances *Philosophical Transactions* **53** 370–418

[7] J O Berger (1985) *Statistical Decision Theory and Bayesian Analysis* 2nd Edition (New York: Springer) ISBN–10: 0387960988

[8] D Bernoulli (1738) Specimen theoriae novae de mensura sortis *Papers of the Imperial Academy of Sciences in St. Petersburg* English translation: (1954) Exposition of a new theory on the measurement of risk *Econometrica* **22** 23–36

[9] W M Briggs (2012) It is time to stop teaching frequentism to non-statisticians Preprint arXiv:1201.2590v1 [stat.OT]

[10] B P Carlin and S Chib (1995) Bayesian model choice via Markov chain Monte Carlo methods *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **57** 473–484

[11] S Chib (1995) Marginal likelihood from the Gibbs output *Journal of the American Statistical Association* **90** 1313–1321

[12] P Coles (2006) *From Cosmos to Chaos — The Science of Unpredictability* (Oxford: Oxford University Press) ISBN–13: 9780199588145

133
[13] R T Cox (1946) Probability, frequency, and reasonable expectation. *American Journal of Physics* **14** 1–13

[14] P Dalgaard (2008) *Introductory Statistics with R* 2nd Edition (New York: Springer) ISBN–13: 9780387790534

[15] C Darwin (1859) *The Origin of Species* (London: John Murray)

[16] E Dekel, B L Lipman and A Rustichini (1998) Standard state-space models preclude unawareness. *Econometrica* **66** 159–173

[17] M J Denwood (2016) runjags: an R package providing interface utilities, model templates, parallel computing methods and additional distributions for MCMC models in JAGS *Journal of Statistical Software* **71** 1–25

[18] S Duane, A D Kennedy, B J Pendleton and D Roweth (1987) Hybrid Monte Carlo *Physics Letters B* **195** 216–222

[19] The Economist (2013) Trouble at the lab URL (cited on June 16, 2018): www.economist.com/news/briefing/21588057-scientists-think-science-self-correcting-alarming-degree-it-not-trouble

[20] A Einstein (1915) Die Feldgleichungen der Gravitation. *Sitzungsberichte der Preußischen Akademie der Wissenschaften (Berlin)* 844–847

[21] D Ellsberg (1961) Risk, ambiguity, and the Savage axioms. *The Quarterly Journal of Economics* **75** 643–669

[22] H van Elst (2015) Foundations of descriptive and inferential statistics Preprint arXiv:1302.2525v3 [stat.AP]

[23] H van Elst (2015) An introduction to business mathematics Preprint arXiv:1509.04333v2 [q-fin.GN]

[24] H van Elst (2015) *Gravitation’s management of the Universe* (blog entry: November 16, 2015) URL (cited on August 25, 2018): blog.karlshochschule.de/2015/11/16/gravitations-management-of-the-universe/

[25] R P Feynman (1985) "Surely You're Joking, Mr. Feynman!" (New York: Bantam) ISBN–10: 0553346687

[26] B de Finetti (1930) Funzione caratteristica di un fenomeno aleatorio *Atti della Academia Nazionale dei Lincei Rendiconti, Class di Scienze Fisiche, Matematiche e Naturali* **4** 86–133

[27] B de Finetti (1937) La prévision: ses lois logiques, ses sources subjectives. *Annales de l’Institut Henri Poincaré* **7** 1–68

[28] R A Fisher (1935) *The Design of Experiments* (Edinburgh: Oliver and Boyd) (1971) 9th Edition ISBN–10: 0028446909
[29] F Galton (1886) Regression towards mediocrity in hereditary stature. *The Journal of the Anthropological Institute of Great Britain and Ireland* **15** 246–263

[30] C F Gauß (1809) Theoria motus corporum celestium in sectionibus conicis solem ambientum

[31] A E Gelfand and A F M Smith (1990) Sampling based approaches to calculating marginal densities. *Journal of the American Statistical Association* **85** 398–409

[32] A Gelman (1998) Some class-participation demonstrations for decision theory and Bayesian statistics. *The American Statistician* **52** 167–174

[33] A Gelman (2006) Prior distributions for variance parameters in hierarchical models (Comment on article by Browne and Draper). *Bayesian Analysis* **3** 515–534

[34] A Gelman and D B Rubin (1995) Avoiding model selection in Bayesian social research. *Sociological Methodology* **25** 165–173

[35] A Gelman, J B Carlin, H S Stern, D B Dunson, A Vehtari and D B Rubin (2014) *Bayesian Data Analysis* 3rd Edition (Boca Raton, FL: Chapman & Hall) ISBN–13: 9781439840955

[36] S Geman and D Geman (1984) Stochastic relaxation, Gibbs distributions, and the Bayesian restoration of images. *IEEE Transactions on Pattern Analysis and Machine Intelligence* **6** 721–741

[37] I Gilboa (2009) *Theory of Decision under Uncertainty* (Cambridge: Cambridge University Press) ISBN–13: 9780521571324

[38] J Gill (1999) The insignificance of null hypothesis significance testing. *Political Research Quarterly* **52** 647–674

[39] J Gill (2015) *Bayesian Methods: A Social and Behavioral Sciences Approach* 3rd Edition (Boca Raton, FL: Chapman & Hall) ISBN–13: 9781439862483

[40] M Gönen, W O Johnson, Y Lu and P H Westfall (2005) The Bayesian two-sample $t$ test. *The American Statistician* **59** 252–257

[41] E Greenberg (2013) *Introduction to Bayesian Econometrics* 2nd Edition (Cambridge: Cambridge University Press) ISBN–13: 9781107015319

[42] M Gross and L McGoey (editors) (2015) *Routledge International Handbook of Ignorance Studies* (Abingdon: Routledge) ISBN–13: 9780415718967

[43] W K Hastings (1970) Monte Carlo sampling methods using Markov chains and their applications. *Biometrika* **57** 97–109

[44] R Hatzinger, K Hornik, H Nagel and M J Maier (2014) $R$ — *Einführung durch angewandte Statistik* 2nd Edition (München: Pearson Studium) ISBN–13: 9783868942507

[45] S W Hawking and G F R Ellis (1973) *The Large Scale Structure of Space-Time* (Cambridge: Cambridge University Press) ISBN–13: 9780521099066
[46] D Helbing (2013) Globally networked risks and how to respond Nature 497 51–59

[47] E T Jaynes (1957) Information theory and statistical mechanics Physical Review 106 620–630

[48] E T Jaynes (2003) Probability Theory — The Logic of Science (Cambridge: Cambridge University Press) ISBN–13: 9780521592710

[49] W H Jefferys and J O Berger (1992) Ockham’s razor and Bayesian analysis American Scientist 80 64–72

[50] H Jeffreys (1939) The Theory of Probability (Oxford: Oxford University Press) (1961) 3rd Edition ISBN–13 (1998 Reissue): 9780198503682

[51] D Kahneman (2011) Thinking, Fast and Slow (London: Penguin) ISBN–13: 9780141033570

[52] D Kahneman and A Tversky (1972) Subjective probability: a judgment of representativeness Cognitive Psychology 3 430–454

[53] D Kahneman and A Tversky (1979) Prospect Theory: an analysis of decision under risk Econometrica 47 263–292

[54] R E Kass and A E Raftery (1995) Bayes Factors Journal of the American Statistical Association 90 773–795

[55] J M Keynes (1921) A Treatise on Probability (London: Macmillan) ISBN–10 (2008 Reprint): 1603861181

[56] F H Knight (1921) Risk, Uncertainty and Profit (Boston, MA: Houghton Mifflin) Library of Economics and Liberty URL (cited on May 12, 2018): http://www.econlib.org/library/Knight/knRUP.html

[57] J K Kruschke (2013) Bayesian estimation supersedes the t test Journal of Experimental Psychology: General 142 573–603

[58] J K Kruschke (2015) Doing Bayesian Data Analysis — A Tutorial with R, JAGS, and Stan 2nd Edition (Amsterdam: Academic Press) ISBN–13: 9780124058880

[59] J K Kruschke, H Aguinis and H Joo (2012) The time has come: Bayesian methods for data analysis in the organizational sciences Organizational Research Methods 15 722–752

[60] J K Kruschke and T M Liddell (2017) The Bayesian New Statistics: hypothesis testing, estimation, meta-analysis, and power analysis from a Bayesian perspective Psychonomic Bulletin & Review 24 1–29 (Brief Report)

[61] S Kullback and R A Leibler (1951) On information and sufficiency The Annals of Mathematical Statistics 22 79–86

[62] P S Laplace (1774) Mémoire sur la probabilité des causes par les événements Mémoires de l'Académie Royale des Sciences Presentés par Divers Savans 6 621–656
[63] P M Lee (2012) *Bayesian Statistics — An Introduction* 4th Edition (Chichester: Wiley) ISBN–13: 9781118332573

[64] H Lesch and J Müller (2003) *Big Bang, zweiter Akt — Auf den Spuren des Lebens im All* 2nd Edition (München: Goldmann) ISBN–10: 3442153433

[65] T Lodewyckx, W Kim, M D Lee, F Tuerlinckx, P Kuppens and E-J Wagenmakers (2011) A tutorial on Bayes factor estimation with the product space method *Journal of Mathematical Psychology* 55:331–347

[66] D J Lunn, A Thomas, N Best and D Spiegelhalter (2000) WinBUGS – A Bayesian modelling framework: concepts, structure, and extensibility *Statistics and Computing* 10:325–337

[67] A D Martin, K M Quinn and J H Park (2011) MCMCpack: Markov Chain Monte Carlo in R *Journal of Statistical Software* 42:1–21

[68] R McElreath (2016) *Statistical Rethinking — A Bayesian Course with Examples in R and Stan* (Boca Raton, FL: Chapman & Hall) ISBN–13: 9781482253443

[69] R McElreath (2016) *rethinking: Statistical Rethinking book package (R package version 1.59)*

[70] N Metropolis and S Ulam (1949) The Monte Carlo method *Journal of the American Statistical Association* 44:335–341

[71] N Metropolis, A W Rosenbluth, M N Rosenbluth, A H Teller and E Teller (1953) Equations of state calculations by fast computing machines *Journal of Chemical Physics* 21:1087–1092

[72] C W Misner, K S Thorne and J A Wheeler (1973) *Gravitation* (New York: Freeman and Co.) ISBN–10: 0716703440

[73] R D Morey and J N Rouder (2018) BayesFactor: Computation of Bayes factors for common designs (R package version 0.9.12-4.2) URL (cited on June 30, 2018): https://CRAN.R-project.org/package=BayesFactor

[74] J A Nelder and R W M Wedderburn (1972) Generalized linear models *Journal of the Royal Statistical Society: Series A (General)* 135:370–384

[75] J von Neumann and O Morgenstern (1944) *Theory of Games and Economic Behavior* (Princeton, NJ: Princeton University Press) ISBN–13: 9780691130613

[76] A Ng (2018) *Machine Learning Yearning — Technical Strategy for AI Engineers, in the Era of Deep Learning* (Draft Version)

[77] R Nuzzo (2014) Scientific method: statistical errors — P values, the ‘gold standard’ of statistical validity, are not as reliable as many scientists assume *Nature* 506:150–152

[78] D Papineau (2018) *Thomas Bayes and the crisis in science* (blog entry: June 28, 2018) URL (cited on July 2, 2018): https://www.the-tls.co.uk/articles/public/thomas-bayes-science-crisis/
[79] V Pareto (1896) Cours d’Économie Politique (Geneva: Droz)

[80] J H Park (2018) CRAN Task View: Bayesian Inference URL (cited on March 25, 2018): https://CRAN.R-project.org/view=Bayesian

[81] R Penrose (1989) The Emperor’s New Mind: Concerning Computers, Minds, and the Laws of Physics (Oxford: Oxford University Press) ISBN–13 (2016 Reprint): 9780198784920

[82] M Peterson (2017) An Introduction to Decision Theory 2nd Edition (Cambridge: Cambridge University Press) ISBN–13: 9781316606209

[83] M Plummer (2016) rjags: Bayesian Graphical Models using MCMC (R package version 4–6) URL (cited on March 25, 2018): https://CRAN.R-project.org/package=rjags

[84] M Plummer (2017) JAGS Version 4.3.0 user manual URL (cited on June 23, 2018): sourceforge.net/projects/mcmc-jags/files/Manuals/

[85] M Plummer, N Best, K Cowles and K Vines (2006) CODA: Convergence Diagnosis and Output Analysis for MCMC [R News 6] 7–11

[86] H Rinne (2008) Taschenbuch der Statistik 4th Edition (Frankfurt/Main: Harri Deutsch) ISBN–13: 9783817118274

[87] D Rumsfeld (2002) U.S. Department of Defense news briefing on February 12, 2002 URL (cited on December 3, 2017): www.defense.gov/transcripts/transcript.aspx?transcriptid=2636

[88] P Saha (2002) Principles of Data Analysis Online lecture notes URL (cited on August 15, 2013): www.physik.uzh.ch/~psaha/pda/ ISBN–10: 1902918118

[89] L J Savage (1954) The Foundations of Statistics (New York: Wiley) Reprint: (1972) 2nd revised Edition (New York: Dover) ISBN–13: 9780486623498

[90] C E Shannon (1948) A mathematical theory of communication The Bell System Technical Journal 27 379–423

[91] N Silver (2012) The Signal and the Noise — The Art and Science of Prediction (London: Penguin) ISBN–13: 9780141975658

[92] D S Sivia and J Skilling (2006) Data Analysis — A Bayesian Tutorial 2nd Edition (Oxford: Oxford University Press) ISBN–13: 9780198568322

[93] D J Spiegelhalter, N G Best, B P Carlin and A Van Der Linde (2002) Bayesian measures of model complexity and fit Journal of the Royal Statistical Society: Series B (Statistical Methodology) 64 583–639

[94] Stan Development Team (2017) Stan Modeling Language — User’s Guide and Reference Manual (Stan Version 2.17.0) URL (cited on June 23, 2018): mc-stan.org/users/documentation/
[95] Stan Development Team (2018) *RStan: the R interface to Stan (R package version 2.17.3)* URL (cited on June 14, 2018): [https://CRAN.R-project.org/package=rstan](https://CRAN.R-project.org/package=rstan)

[96] S M Stigler (1986) *The History of Statistics — The Measurement of Uncertainty before 1900* (Cambridge, MA: Harvard University Press) ISBN–10: 067440341x

[97] Student [W S Gosset] (1908) The probable error of a mean *Biometrika* **6** 1–25

[98] E Svetlova and H van Elst (2012) How is non-knowledge represented in economic theory? *Preprint* [arXiv:1209.2204v1 [q-fin.GN]]

[99] E Svetlova and H van Elst (2014) Decision-theoretic approaches to non-knowledge in economics *Preprint* [arXiv:1407.0787v1 [q-fin.GN]]

[100] N N Taleb (2007) *The Black Swan — The Impact of the Highly Improbable* (London: Penguin) ISBN–13: 9780141034591

[101] R H Thaler and C R Sunstein (2008) *Nudge — Improving Decisions about Health, Wealth and Happiness* (London: Penguin) ISBN–13: 9780141040011

[102] R Trotta (2008) Bayes in the sky: Bayesian inference and model selection in cosmology *Contemporary Physics* **49** 71–104 [arXiv:0803.4089v1 [astro-ph]]

[103] A Tversky and D Kahneman (1983) Extensional versus intuitive reasoning: the conjunction fallacy in probability judgment *Psychological Review* **90** 293–315

[104] S V asisht (2017) *The replication crisis in science* (blog entry: December 29, 2017) URL (cited on July 2, 2018): [https://thewire.in/science/replication-crisis-science](https://thewire.in/science/replication-crisis-science)

[105] A Vehtari, A Gelman and J Gabry (2017) Practical Bayesian model evaluation using leave-one-out cross-validation and WAIC *Statistics and Computing* **27** 1413–1432

[106] A Wald (1950) *Statistical Decision Functions* (New York: Wiley)

[107] S Watanabe (2010) Asymptotic equivalence of Bayes cross validation and Widely Applicable Information Criterion in singular learning theory *Journal of Machine Learning Research* **11** 3571–3594

[108] J D Watson and F H C Crick (1953) Molecular structure of nucleic acids: a structure for Deoxyribose Nucleic Acid *Nature* **171** 737–738

[109] M H F Wilkins, A R Stokes and H. R. Wilson (1953) Molecular structure of nucleic acids: molecular structure of Deoxypentose Nucleic Acids *Nature* **171** 738–740