B. J. K. Kleijn

The frequentist theory of Bayes procedures

February 26, 2018

Springer
Preface

This book grew out of a set of lecture notes that were written for the course in Bayesian statistics, taught at University of Amsterdam in the spring of 2007 and in years thereafter. The course was aimed (initially) at first-year MSc.-students in statistics, mathematics and related fields. The goal was for students to understand the basic properties of Bayesian statistical methods; to be able to apply this knowledge to statistical questions and to know the extent (and limitations) of conclusions based thereon. All material was presented side-by-side with relevant frequentist methods for comparison. Considered were the basic properties of the Bayesian procedure, Bayesian forms of estimation, testing and uncertainty quantification, as well as the choice of the prior by objective and subjective criteria. Presently this material is covered in part I of this book. In addition part I considers the frequentist asymptotic theory of estimation of smooth parameters and efficiency, followed by the Bernstein-von-Mises theorem and the asymptotic identification of credible sets with confidence sets in that context.

It should be stressed that the material presented in part I covers only the most basic Bayesian concepts; further reading is recommended. Various books providing overviews of Bayesian statistics are recommended, depending on the background and interest of the reader: a highly theoretical treatment can be found in Le Cam (1986) [69], which develops a general, mathematical framework for statistics and decision theory, dealing with Bayesian methods as an important area of its application. For a more down-to-earth version of this work, applied only to smooth parametric models, the interested reader is referred to Le Cam and Yang (1990) [71]. A general reference of a more decision-theoretic inclination with a clear focus on Bayesian statistics, is the book by Berger (1985) [8]; a reference of a similar nature is Bernardo and Smith (1993) [13]. Recommendable is also Robert’s “The Bayesian choice” (2001) [79], which offers a very useful explanation on computational aspects of Bayesian statistics. Berger, Bernardo and Smith and Robert devote a great deal of attention to philosophical arguments in favour of the Bayesian approach to statistics, while staying rather brief with regard to mathematical considerations and focusing almost exclusively on parametric models. Finally, Ripley (1996) [80] discusses Bayesian methods with a very pragmatic focus on pattern classification. The
latter reference relates all material with applications in mind but does so based on a firm statistical and decision-theoretic background.

Part ?? concerns non-parametric statistics and is built on asymptotic arguments almost exclusively. On this subject, an early publication in book-form is Ghosh and Ramamoorthi [44] who give both the theory and examples as they existed at the time in the field of non-parametric Bayesian statistics. Recently Ghosal and van der Vaart [43] have published an impressive volume, that provides an overview of the non-parametric models and methods that have appeared in the intervening years. The present work has the rather more modest goal of formulating the modern, asymptotic theory of the posterior for the frequentist with mathematical precision and in full generality.

An attempt has been made to make part I of this book as self-contained as possible: in particular, appendix A summarizes the necessary basics of measure theory. Nevertheless the reader is expected to have been exposed to some frequentist statistics, preferably not just in practical setting but also from a more mathematical perspective. Throughout part I no familiarity with asymptotic and non-parametric statistics is assumed on the part of the reader. In part ?? some such familiarity is assumed, but the reader is not assumed to be at home with the details of locally convex spaces, which are summarized in appendix ??, Where possible, definitions, lemmas and theorems have been formulated such that they cover parametric and nonparametric models alike.

For corrections to early versions of these notes the author thanks Chris Muris. For the solutions to many exercises, the author thanks Audrius Jukonis and Mike Derksen.

*Bas Kleijn*
Amsterdam, February 2018
## Contents

### Part I  Parametric Bayesian statistics

1  **Introduction** ........................................................... 3
   1.1 Frequentist statistics .................................................. 3
   1.2 Frequentist estimation ................................................ 8
   1.3 Bayesian statistics ................................................... 11
   1.4 The frequentist analysis of Bayesian methods .................... 14

2  **Bayesian basics** ....................................................... 17
   2.1 Bayes’s rule, prior and posterior distributions ................. 17
      2.1.1 Bayes’s rule .................................................... 18
      2.1.2 Bayes’s billiard ................................................ 22
      2.1.3 The Bayesian view of the model .............................. 24
      2.1.4 A frequentist’s view of the posterior ...................... 27
      2.1.5 From prior to posterior ...................................... 29
   2.2 Bayesian point estimators .......................................... 30
      2.2.1 Posterior predictive and posterior mean .................... 30
      2.2.2 Small-ball and formal Bayes estimators .................... 34
      2.2.3 The Maximum-A-Posteriori estimator ....................... 36
   2.3 Confidence sets and credible sets ................................ 38
      2.3.1 Frequentist confidence intervals ............................ 38
      2.3.2 Bayesian credible sets ....................................... 41
   2.4 Tests and Bayes factors ............................................ 43
      2.4.1 Neyman-Pearson tests ....................................... 43
      2.4.2 Randomized tests and the Neyman-Pearson lemma .......... 46
      2.4.3 Test sequences and minimax optimality .................... 48
      2.4.4 Bayes factors ................................................ 50
   2.5 Decision theory and classification ............................... 52
      2.5.1 Decision theory ............................................... 53
      2.5.2 Bayesian decision theory .................................... 57
      2.5.3 Frequentist versus Bayesian classification ............... 60
Part I

Parametric Bayesian statistics
Use the template `part.tex` together with the Springer document class SVMono (monograph-type books) or SVMult (edited books) to style your part title page and, if desired, a short introductory text (maximum one page) on its verso page in the Springer layout.
Chapter 1
Introduction

The goal of statistical inference is to understand, describe and estimate (aspects of) the randomness of measured data. Qua
ti natu rally this invites the assumption that the data represents a sample from an unknown but fixed probability distribution.

1.1 Frequentist statistics

Any frequentist inferential procedure relies on three basic ingredients: the data, a model and an estimation procedure. The central assumption in frequentism is that the data has a definite but unknown, underlying distribution to which all inference pertains. The data is a measurement or observation which we denote by $Y$, taking values in a corresponding samplespace.

**Definition 1.1.** The samplespace for an observation $Y$ is a measurable space $\mathcal{Y}$ with $\sigma$-algebra $\mathcal{B}$ (see definition A.2) containing all values that $Y$ can take upon measurement.

Measurements and data can take any form, ranging from categorical data (sometimes referred to as nominal data where the samplespace is simply a (usually finite) set of points or labels with no further mathematical structure), ordinal data (also known as ranked data, where the samplespace is endowed with an total ordering), to interval data (where in addition to having an ordering, the samplespace allows one to compare differences or distances between points), to ratio data (where we have all the structure of the real line). Moreover $Y$ can collect the results of a number of measurements, so that it takes its values in the form of a vector (think of an experiment involving repeated, stochastically independent measurements of the same quantity, leading to a so-called independent and identically distributed (or i.i.d.) sample). The data $Y$ may even be functional data, taking its values in a space of functions or in other infinite-dimensional spaces, for example, in the statistical study of continuous-time time-series.
The samplespace \( \mathcal{Y} \) is assumed to be a measurable space to enable the consideration of probability measures on \( \mathcal{Y} \), formalizing the uncertainty in measurement of \( Y \). As was said in the opening words of this chapter, frequentist statistics hinges on the assumption that there exists a probability measure \( P_0 : \mathcal{B} \to [0, 1] \) on the samplespace \( \mathcal{Y} \) representing the "true distribution of the data":

\[
Y \sim P_0
\]  

(1.1)

Hence from the frequentist perspective, statistics revolves around the central question: “What does the data make clear about \( P_0 \)?”, which may be considered in parts by questions like, “From the data, what can we say about the mean of \( P_0 \)?”, “Based on the data that we have, how sharp can we formulate hypotheses concerning the value of the variance of \( P_0 \)?”, etcetera.

The second ingredient of a statistical procedure is a model, which contains all explanations under consideration of the randomness in \( Y \).

**Definition 1.2.** A (frequentist) statistical model \( \mathcal{P} \) is a collection of probability measures \( P : \mathcal{B} \to [0, 1] \) on the samplespace \( (\mathcal{Y}, \mathcal{B}) \). The distributions \( P \) are called model distributions. For every sample space \( (\mathcal{Y}, \mathcal{B}) \), the collection of all probability distributions is called the full model (sometimes referred to as the full non-parametric model), denoted \( \mathcal{M}^+_1(\mathcal{Y}, \mathcal{B}) \).

The model \( \mathcal{P} \) contains the candidate distributions for \( Y \) that the statistician finds "reasonable" explanations of the uncertainty he observes (or expects to observe) in \( Y \). As such, it constitutes a choice of the statistician analyzing the data rather than a given. From a more mathematical perspective we observe that a model \( \mathcal{P} \) on \( (\mathcal{Y}, \mathcal{B}) \) is a subset of the space \( \mathcal{M}(\mathcal{Y}, \mathcal{B}) \) of all finite, signed measures \( \mu : \mathcal{B} \to \mathbb{R} \) (that is, all countably additive, real-valued set functions) that are of finite total variation. Equipped with the total-variational norm (see appendix A, definition A.6), \( \mu \mapsto \|\mu\| \), \( \mathcal{M}(\mathcal{Y}, \mathcal{B}) \) is a Banach space [30], in which the full model can be characterized by,

\[
\mathcal{M}^+_1(\mathcal{Y}, \mathcal{B}) = \left\{ P \in \mathcal{M}(\mathcal{Y}, \mathcal{B}) : P \geq 0, P(\mathcal{Y}) = 1 \right\}.
\]

Often, we describe models as families of probability densities rather than distributions.

**Definition 1.3.** If there exists a \( \sigma \)-finite measure \( \mu : \mathcal{B} \to [0, \infty] \) such that for all \( P \in \mathcal{P}, P \ll \mu \), we say that the model is dominated (notation: \( \mathcal{P} \ll \mu \)).

The Radon-Nikodym theorem (see theorem A.7) guarantees that we may represent a dominated probability measure \( P \) in terms of a probability density function \( p = dP/d\mu : \mathcal{Y} \to [0, \infty) \) that satisfies \( \int_A p(y) \, d\mu(y) = P(A) \) for all \( A \in \mathcal{B} \). For dominated models, it makes sense to adopt a slightly different mathematical perspective: if \( \mu \) dominates \( \mathcal{P} \), we map \( \mathcal{P} \) to the space of all \( \mu \)-integrable functions \( L_1(\mu) \) by means of the Radon-Nikodym mapping.

**Example 1.1.** Suppose that \( \mathcal{Y} \) is countable (and let \( \mathcal{B} \) be the powerset of \( \mathcal{Y} \): then the measure \( \mu \) that puts mass one at every point in \( \mathcal{Y} \), also known as the counting
measure on $\mathcal{F}$, is $\sigma$-finite and dominates every other (finite) measure on $\mathcal{F}$. Consequently, any model on $(\mathcal{F}, \mathcal{B})$ can be represented in terms of elements $p$ in the Banach space $L_1(\mu)$, more commonly denoted as $\ell_1$,

$$\ell_1 = \{(f_1, f_2, \ldots) \in [0,1]^\infty : \sum_{i \geq 1} |f_i| < \infty\}.$$ 

where it is noted that $p_i \geq 0$ and $\|p\| = \sum p_i = 1$ for all $P \in \mathcal{M}_1^+(\mathcal{F}, \mathcal{B})$.

In case the sample space is not discrete, the full model is not dominated by a $\sigma$-finite measure. However, suppose that a $\sigma$-finite measure $\mu$ on the sample space is given. The Radon-Nikodym mapping maps every $\mu$-dominated model $P$ to a subset of,

$$\mathcal{M}_1^+(\mu) = \{p \in L_1(\mu) : p \geq 0, \int_{\mathcal{F}} p(y) d\mu(y) = 1\}.$$

**Lemma 1.1.** The mapping between a model $\mathcal{P}$ dominated by a $\sigma$-finite measure $\mu$ and its $L_1(\mu)$-representation is an isometry: for all $p_1, p_2 \in \mathcal{P}$,

$$\|P_1 - P_2\| = \frac{1}{2} \int_{\mathcal{F}} \left| p_1(y) - p_2(y) \right| d\mu(y) = \int_{\mathcal{F}} (p_1(y) - p_2(y))^+ d\mu(y).$$

Note that for the dominating measure is not unique and hence, that the $L_1$-representation of $\mathcal{P}$ depends on the particular choice of dominating measure $\mu$.

The most common way of representing a statistical model is a description in terms of a parameterization.

**Definition 1.4.** A model $\mathcal{P}$ is **parameterized** with parameter space $\Theta$, if there exists a surjective map $\Theta \to \mathcal{P} : \theta \mapsto P_\theta$, called the parameterization of $\mathcal{P}$.

Parametrizations are motivated by the context of the statistical question and the parameter $\theta$ usually has a clear interpretation when viewed in this context. The formulation of parametric model descriptions is the modelling step of statistics: to the statistician, it transforms the data from a mere list of numbers to an informative (but noisy) representation of an underlying truth.

**Definition 1.5.** A parameterization of a statistical model $\mathcal{P}$ is said to be **identifiable**, if the map $\Theta \to \mathcal{P} : \theta \mapsto P_\theta$ is injective.

Injectivity of the parameterization means that for all $\theta_1, \theta_2 \in \Theta$, $\theta_1 \neq \theta_2$ implies that $P_{\theta_1} \neq P_{\theta_2}$. In other words, no two different parameter values $\theta_1$ and $\theta_2$ give rise to the same distribution. Clearly, in order for $\theta \in \Theta$ to serve as a useful representation for the candidate distributions $P_\theta$, identifiability is a first requirement. Other common conditions on the map $\theta \mapsto P_\theta$ are continuity (for example, with respect to the total-variational norm, or through requiring continuity of all maps $\theta \mapsto P_\theta g$, with $g$ any bounded measurable function), differentiability (the definition of which may involve technical subtleties in case $\Theta$ is infinite-dimensional) and other smoothness conditions.
Remark 1.1. Although strictly speaking ambivalent, it is commonplace to refer to both \( \mathcal{P} \) and the parameterizing space \( \Theta \) as “the model”. This practice is not unreasonable in view of the fact that, in practice, almost all models are parameterized in an identifiable way, so that there exists a bijective correspondence between \( \Theta \) and \( \mathcal{P} \). Here, reference to the model always concerns \( \mathcal{P} \) while \( \Theta \) is always called the parameter space.

An assumption often made in frequentist statistics is that the true distribution of the data is a model distribution.

**Definition 1.6.** A model \( \mathcal{P} \) is said to be well-specified if it contains the true distribution of the data \( P_0 \), i.e.

\[
P_0 \in \mathcal{P}.
\] (1.2)

If (1.2) does not hold, the model is said to be mis-specified.

Clearly if \( \mathcal{P} \) is parameterized by \( \Theta \), (1.2) implies the existence of a point \( \theta_0 \in \Theta \) such that \( P_{\theta_0} = P_0 \); if, in addition, the model is identifiable, the parameter value \( \theta_0 \) is unique.

If the full non-parametric model is used, (1.2) holds trivially. However, for smaller models, (1.2) has the status of an assumption on the unknown quantity of interest \( P_0 \) and may as such be hard to justify. The reason for (the somewhat odd and certainly very contentious) assumption (1.2) lies in the interpretation of statistical conclusions: an estimate of a parameter is of value if that parameter can be attributed to the “true” distribution of the data. If, on the other hand, one assumes that the model is mis-specified, parameter estimates may reflect aspects of the true distribution but cannot be associated with the true distribution of the data directly any more.

The model we use in a statistical procedure constitutes a choice rather than a given: presented with a particular statistical problem, different statisticians may choose to use different models. The only condition is that (1.2) is satisfied, which is why we have to choose the model in a “reasonable way” given the nature of \( Y \). When choosing the model, two considerations compete: on the one hand, small models are easy to handle mathematically and statistically and parameters usually have clear interpretations, on the other hand, for large models, assumption (1.2) is more realistic since they have a better chance of containing \( P_0 \) (or at least approximate it more closely). The amount of data available plays a crucial role: if we have a limited sample, simple models have a better chance of leading to sensible results, while an abundance of data enables more sophisticated forms of statistical analysis. In this respect the most important distinction is made in terms of the dimension of the model.

**Definition 1.7.** A model \( \mathcal{P} \) is said to be parametric of dimension \( d \), if there exists an identifiable parameterization \( \Theta \rightarrow \mathcal{P} : \theta \mapsto P_\theta \), where \( \Theta \subset \mathbb{R}^d \) with non-empty interior \( \Theta \neq \emptyset \).

The requirement regarding the interior of \( \Theta \) in definition 1.7 ensures that the dimension \( d \) really concerns \( \Theta \) and not just the dimension of the space \( \mathbb{R}^d \) (in which \( \Theta \) could otherwise be a lower-dimensional subset).
Example 1.2. The normal model for a single, real measurement $Y$, is the collection of all normal distributions on $\mathbb{R}$, i.e.

$$\mathcal{D} = \{N(\mu, \sigma^2) : (\mu, \sigma) \in \Theta\}$$

where the parameterizing space $\Theta$ equals $\mathbb{R} \times (0, \infty)$. The map $(\mu, \sigma) \mapsto N(\mu, \sigma^2)$ is surjective and injective, i.e. the normal model is a two-dimensional, identifiable parametric model. Moreover, the normal model is dominated by the Lebesgue measure on the samplespace $\mathbb{R}$ and can hence be described in terms of Lebesgue-densities:

$$p_{\mu, \sigma}(y) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}.$$ 

Note that for any fixed $y \in \mathcal{D}$, the dependence $\Theta \rightarrow \mathbb{R} : (\mu, \sigma) \mapsto p_{\mu, \sigma}(y)$ is continuous on all of $\Theta$. So if $(\mu_n, \sigma_n)$ converges to $(\mu, \sigma)$ in $\Theta$, then $p_{\mu_n, \sigma_n}(y)$ converges to $p(y) := p_{\mu, \sigma}(y)$. Then total-variational distance between the distributions $P_n$ and $P$ (associated with the densities $p_n$ and $p$ respectively) satisfies,

$$\|P_n - P\| = \frac{1}{2} \int_{\mathcal{D}} |p_n(y) - p(y)| \, d\mu(y) \rightarrow 0.$$ 

by lemma 1.1 and Scheffé’s lemma (see corollary A.2). Conclude that the parametrization $\Theta \rightarrow \mathcal{D} : (\mu, \sigma) \mapsto P_{\mu, \sigma}$ is continuous with respect to the total-variational metric on $\mathcal{D}$.

Definition 1.8. If there is no finite-dimensional $\Theta$ that parameterizes $\mathcal{D}$, then $\mathcal{D}$ is called a non-parametric model.

For instance, the full model $\mathcal{M}(\mathcal{Y}, \mathcal{B})$ is non-parametric unless the samplespace contains a finite number of points.

Example 1.3. Let $\mathcal{Y}$ be a finite set containing $n \geq 1$ points $y_1, y_2, \ldots, y_n$ and let $\mathcal{B}$ be the power-set $2^\mathcal{Y}$ of $\mathcal{Y}$. Any probability measure $P : \mathcal{B} \rightarrow [0, 1]$ on $(\mathcal{Y}, \mathcal{B})$ is absolutely continuous with respect to the counting measure on $\mathcal{Y}$ (see example A.2). The density of $P$ with respect to the counting measure is a map $p : \mathcal{Y} \rightarrow \mathbb{R}$ such that $p \geq 0$ and

$$\sum_{i=1}^{n} p(y_i) = 1.$$ 

As such, $P$ can be identified with an element of the so-called simplex $S_n$ in $\mathbb{R}^n$, defined as follows

$$S_n = \left\{ p = (p_1, \ldots, p_n) \in \mathbb{R}^n : p_i \geq 0, \sum_{i=1}^{n} p_i = 1 \right\}.$$ 

This leads to an identifiable parameterization $S_n \rightarrow \mathcal{D} : p \mapsto P$ of the full non-parametric model on $(\mathcal{Y}, \mathcal{B})$, of dimension $n - 1$. Note that $S_n$ has empty interior in $\mathbb{R}^n$, but can be brought in one-to-one correspondence with a compact set in $\mathbb{R}^{n-1}$ with non-empty interior by the embedding:
\[
\left\{ (p_1, \ldots, p_{n-1}) \in \mathbb{R}^{n-1} : p_i \geq 0, \sum_{i=1}^{n-1} p_i \leq 1 \right\} \rightarrow S_n : \\
(p_1, \ldots, p_{n-1}) \mapsto \left( p_1, \ldots, p_{n-1}, 1 - \sum_{i=1}^{n-1} p_i \right).
\]

### 1.2 Frequentist estimation

The third ingredient of a frequentist inferential procedure is an estimation method. Clearly not all statistical problems involve an explicit estimation step and of those that do, not all estimate the distribution \( P_0 \) directly. Nevertheless, one may regard the problem of point-estimation in the model \( \mathcal{P} \) as prototypical.

**Definition 1.9.** A point-estimator (or estimator) for \( P_0 \) is a map \( \hat{P} : \mathcal{Y} \rightarrow \mathcal{P} \), representing our “best guess” \( \hat{P} \in \mathcal{P} \) for \( P_0 \) based on the data \( Y \) (and other known quantities).

Note that a point-estimator is a statistic: since a point-estimator must be calculable in practice, it may depend only on information that is known to the statistician after he has performed the measurement realized as \( Y = y \). Also note that a point-estimator is a stochastic quantity: \( \hat{P} = \hat{P}(Y) \) depends on \( Y \) and is hence random. Upon measurement of \( Y \) resulting in a realisation \( Y = y \), the realisation of the estimator is an estimate \( \hat{P}(y) \), a definite point in \( \mathcal{P} \). If the model is parameterized, one may define a point-estimator \( \hat{\theta} : \mathcal{Y} \rightarrow \Theta \) for \( \theta_0 \), from which we obtain \( \hat{P} = \hat{P}(\hat{\theta}) \) as an estimator for \( P_0 \). In that case the continuity requirement we impose on the map \( \theta \mapsto P_\theta \) guarantees that \( \theta \rightarrow \theta_0 \) implies \( P_\theta \rightarrow P_{\theta_0} \). If the model is identifiable, estimation of \( \theta_0 \) in \( \Theta \) is equivalent to estimation of \( P_0 \) in \( \mathcal{P} \).

Aside from estimates for the distribution \( P_0 \), one is often interested in estimating only certain aspects of \( P_0 \).

**Example 1.4.** Suppose that a bank tries to assess market risk for an asset: they have the asset on the books for price \( x \) but tomorrow’s market will say that it is worth a price \( X \), distributed according to an unknown \( P_0 \). To assess the risk of holding the position until tomorrow, the absolute return \( X - x \) is of importance. Of course, the bank would prefer to have a reliable estimate for \( P_0 \) (and thus for the distribution of \( X - x \)) but that question is often too hard to answer and reliability cannot be guaranteed. Instead, the bank will resort to a simplification by focussing on the aspect of the distribution \( P_0 \) that they find most important for their risk assessment. A popular notion in this context is a quantity called value-at-risk: given a time-horizon (in this case, tomorrow) and a significance level \( \alpha \in (0, 1) \) (often chosen equal to 0.05 or 0.01), value-at-risk \( q \) is defined as the minimal \( q \) at which,

\[
P_0(X - x < q) \geq \alpha.
\]
To interpret $q$, note that losses exceeding value-at-risk occur on only an expected fraction $\alpha$ of all trading days. In statistical terms, $q$ is a quantile of $P_0$. Estimation of the quantile $q$ suffices: we estimate only an aspect of the distribution $P_0$.

Another example occurs in parametric models: if the dimension $d$ of a parametric model is greater than one, we may choose to estimate only one component of $\theta$ (called the parameter of interest) and disregard other components (called nuisance parameters). More generally, we may choose to estimate certain properties of $P_0$ (e.g. its expectation, variance) rather than $P_0$ itself and in many cases, direct estimation of the property of interest of $P_0$ is more efficient than estimation through $\hat{P}$.

Example 1.5. Consider a model $\mathcal{P}$ consisting of distributions on $\mathbb{R}$ with finite expectation and define the functional $e : \mathcal{P} \to \mathbb{R}$ by the expectation $e(P) = \mathbb{E}X$. Suppose that we are interested in the expectation $e_0 = e(P_0)$ of the true distribution. Obviously, based on an estimator $\hat{P}$ for $P_0$ we may define an estimator,

$$
\hat{e} = \int_{\mathbb{R}} x \, d\hat{P}(x)
$$

(1.3)

to estimate $e_0$. For instance, assume that $X$ is integrable under $P_0$ and $Y = (X_1, \ldots, X_n)$ collects the results of an i.i.d. experiment with $X_i \sim P_0$ marginally (for all $1 \leq i \leq n$), then the empirical expectation of $X$, defined simply as the sample-average of $X$,

$$
P_nX = \frac{1}{n} \sum_{i=1}^{n} X_i,
$$

provides an estimator for $e_0$. (Note that the sample-average is also of the form (1.3) if we choose as our point-estimator for $P_0$ the empirical distribution $\hat{P} = P_n$.) The law of large numbers guarantees that $P_nX$ converges to $e_0$ almost-surely as $n \to \infty$, and (if $X$ is quadratically integrable) the central limit theorem asserts that this convergence proceeds at rate $n^{-1/2}$ (and that the limit distribution is zero-mean normal with $P_0(X - \mathbb{E}X)^2$ as its variance). Many parameterizations $\theta \mapsto P_\theta$ are such that (components of) $\theta$ coincide with expectations. Often, other properties of $P_0$ can also be related to expectations: for example, if $X \in \mathbb{R}$, the probabilities $F_0(s) = P_0(X \leq s) = P_0\{X \leq s\}$ ($s \in \mathbb{R}$) can be estimated by,

$$
P_n(s) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\{X_i \leq s\},
$$

i.e. as the empirical expectation of the function $x \mapsto \mathbb{1}\{x \leq s\}$. This leads to a step-function with $n$ jumps of size $1/n$ at samplepoints, which estimates the distribution function $F_0$. Generalizing, any property of $P_0$ that can be expressed in terms of an expectation of a $P_0$-integrable function of $X$, $P_0g$, is estimable by the corresponding empirical expectation, $P_ng$. (With regard to the estimator $P_n$, the convergence $P_n(s) \to F_0(s)$ does not only hold pointwise but even uniform in $s$, i.e. $\sup_{s \in \mathbb{R}} |P_n(s) - F_0(s)| \to 0$ almost-surely, c.f. the Glivenko-Cantelli theorem.)
To estimate a probability distribution (or any of its properties or parameters),
many different estimators may exist. Therefore, the use of any particular estimator
constitutes (another) choice made by the statistician analyzing the problem. Whether
such a choice is a good or a bad one depends on optimality criteria, which are either
dictated by the particular nature of the problem (see section 2.5 which extends the
purely inferential point of view), or based on more generically desirable properties
of the estimator (note the use of the rather ambiguous qualification “best guess” in
definition 1.9).

Example 1.6. To illustrate what we mean by “desirable properties”, note the follow-
ing. When estimating $P_0$ one may decide to use an estimator $\hat{P}$ because it has the
property that it is close to the true distribution of $Y$ in total variation. To make this
statement specific, the property that make such an estimator $\hat{P}$ attractive is that there
exist small constants $\varepsilon > 0$ and $\alpha > 0$, such that for all $P \in \mathcal{P},$

$$P(\|\hat{P}(Y) - P\| < \varepsilon) > 1 - \alpha,$$

i.e. if $Y \sim P$, then $\hat{P}$ lies close to $P$ with high $P$-probability. Note that we formulate
this property “for all $P$ in the model”: since $P_0 \in \mathcal{P}$ is unknown, the only way to
guarantee that this property holds under $P_0$, is to prove that it holds for all $P \in \mathcal{P},$
provided that (1.2) holds. (By contrast, for Bayesians any claim concerning points
$P$ in the model is acceptable if it is true almost-everywhere in $\mathcal{P}$ with respect to the
prior measure).

A popular method of estimation that satisfies common optimality criteria in many
(but certainly not all, see [70]) problems is maximum-likelihood estimation.

Definition 1.10. Suppose that the model $\mathcal{P}$ is dominated by a $\sigma$-finite measure $\mu$
and parametrized through $\mu$-densities by $\theta \mapsto p_\theta \in L_1(\mu)$. The likelihood princi-
ple (see [79] for an elaborate overview and spirited argument in favour) says that
all information implied by data $Y$ concerning the parameter $\theta$ is contained in the
likelihood-function $\theta \mapsto p_\theta(Y)$ (note that this defines a random function $\theta \mapsto [0, \infty]$).
Accordingly, one can define $\hat{\theta} \in \Theta$ as an estimator for the true parameter value $\theta_0$
by maximization,

$$p_{\hat{\theta}}(Y) = \sup_{\theta \in \Theta} p_\theta(Y).$$

So $\hat{\theta}$ is the point in the parameter space for which the likelihood-function evaluated
in $Y$, $\Theta \rightarrow [0, \infty] : \theta \mapsto p_\theta(Y)$ attains its maximum. This defines the maximum-
likelihood estimator (or MLE) $\hat{\theta}$ for $\theta_0$. (Note that the Bayesian posterior we define
later can be written in terms of the likelihood function, thus defining another way to
estimate on the basis of the likelihood principle.)

Remark 1.2. The MLE $\hat{P} = P_{\hat{\theta}}$ does not depend on the dominating measure $\mu$ chosen
to define the densities $p_\theta = dP_\theta/d\mu$.

A word of caution is in order: mathematically, the above “definition” of the MLE
begs questions of existence and uniqueness: regarding $\theta \mapsto p_\theta(Y)$ as a (random)
map on the parameter space, there may not be any point in $\mathcal{P}$ where the likelihood takes on its supremal value (with $P_0$-probability one), nor is there any guarantee that such a maximal point is unique (with $P_0$-probability one).

The above is only a very brief and rather abstract overview of the basic framework of frequentist statistics, highlighting the central premise that a true underlying distribution $P_0$ for $Y$ exists. It makes clear, however, that frequentist inference concerns itself primarily with the stochastics of the random variable $Y$ and not with the context in which $Y$ resides. Other than the fact that the model has to be chosen “reasonably” based on the nature of $Y$, frequentist inference does not involve any information regarding the background of the statistical problem in its procedures unless one chooses to use such information explicitly (see, for example, remark 2.6 on penalized maximum-likelihood estimation). In Bayesian statistics the use of background information is an integral part of the procedure unless one chooses to disregard it: by the definition of a prior measure, the statistician may express that he believes in certain points of the model more strongly than others. This thought is elaborated on further in section 1.3 (e.g. example 1.8).

Similarly, results of estimation procedures are sensitive to the context in which they are used: two statistical experiments may give rise to the same model formally, but the estimator used in one experiment may be totally unfit for use in the other experiment.

Example 1.7. For example, if we interested in a statistic that predicts the rise or fall of a certain share-price on the stock market based on its value over the past week, the estimator we use does not have to be a very conservative one: we are interested primarily in its long-term performance and not in the occasional mistaken prediction. However, if we wish to predict the rise or fall of white-bloodcell counts in an HIV-patient based on last week’s counts, overly optimistic predictions can have disastrous consequences.

Although in the above example, data and models are very similar in these statistical problems, the estimator used in the medical application should be much more conservative than the estimator used in the stock-market problem. The purely statistical aspects of both questions are the same, but the context in which inference is expressed calls for differentiated approaches. Such considerations form the motivation for statistical decision theory, as explained further in section 2.5.

1.3 Bayesian statistics

The subject here is an alternative approach to statistical questions known as Bayesian statistics, after Rev. Thomas Bayes, the author of “An essay towards solving a problem in the doctrine of chances” published posthumously in 1763 [4]. Bayes considered a number of probabilistic questions in which data and parameters are treated on equal footing. The Bayesian procedure itself is explained in detail in chapter 2
and further chapters explore its properties. In this section we have the more modest goal of illustrating the conceptual differences with frequentist statistical analysis.

In Bayesian statistics, data and model form two factors of the same space, i.e. no formal distinction is made between measured quantities \( Y \) and parameters \( \theta \). One may envisage the process of generating a measurement outcome \( Y = y \) as two draws, one draw from \( \Theta \) (or \( \mathcal{P} \)) to select a value of \( \theta \) (or distribution \( P \)) and a subsequent draw from a model distribution \( P_\theta \) to arrive at \( Y = y \). This perspective may seem rather strange in view of the definitions made in section 1.1, but in [4], Bayes gives examples in which this perspective is perfectly reasonable (see subsection 2.1.2). An element \( P_\theta \) of the model is interpreted simply as the distribution of \( Y \) given the parameter value \( \theta \), i.e. as the conditional distribution of \( Y | \theta \). The joint distribution of \( (Y, \theta) \) then follows upon specification of the marginal distribution of \( \theta \) on \( \Theta \), which is called the prior. Based on the joint distribution for the data \( Y \) and the parameters \( \theta \), straightforward conditioning on \( Y \) gives rise to a conditional distribution \( \Pi(\cdot|Y) \) for the parameters \( \theta | Y \) called the posterior distribution on the model \( \Theta \). Hence, given the model, the data and a prior distribution, the Bayesian procedure leads to a posterior distribution that incorporates the information provided by the data. All statistical questions are then answered using the posterior. For example, what a frequentist would call point-estimation of the underlying distribution with the posterior mean,

\[
P^{\Pi|Y}(A) = \int_\Theta P_\theta(A) d\Pi(\theta|Y),
\]

(for all measurable \( A \)), is called prediction by Bayesians, who refer to \( P^{\Pi|Y} \) as the posterior predictive distribution.

Often in applications, the nature of the data and the background of the problem suggest that certain values of \( \theta \) are more “likely” than others, even before any measurements are done. The model \( \mathcal{P} \) describes possible probabilistic explanations of the data and, in a sense, the statistician believes more strongly in certain explanations than in others. This is illustrated by the following example, which is due to L. Savage (1961) [81].

**Example 1.8.** Consider the following three statistical experiments:

1. A lady who drinks milk in her tea claims to be able to tell which was poured first, the tea or the milk. In ten trials, she determines correctly whether it was tea or milk that entered the cups first.
2. A music expert claims to be able to tell whether a page of music was written by Haydn or by Mozart. In ten trials conducted, he correctly determines the composer every time.
3. A drunken friend says that he can predict the outcome of a fair coin-flip. In ten trials, he is right every time.

Let us analyze these three experiments in a frequentist fashion, e.g. we assume that the trials are independent and possess a definite Bernoulli distribution, c.f. (1.1). In all three experiments, \( \theta_0 \in \Theta = [0, 1] \) is the per-trial probability that the person gives the right answer. We test their respective claims posing the hypotheses:
The total number of successes out of ten trials is a sufficient statistic for \( \theta \) and we use it as our test-statistic, noting that its distribution is binomial with \( n = 10, \theta = \theta_0 \) under \( H_0 \). Given the data \( Y \) with realization \( y \) of ten correct answers, applicable in all three examples, we reject \( H_0 \) at \( p \)-value \( 2^{-10} \approx 0.1\% \). So there is strong evidence to support the claims made in all three cases. Note that there is no difference in the frequentist analyses: formally, all three cases are treated exactly the same.

Yet intuitively (and also in every-day practice), one would be inclined to treat the three claims on different footing: in the second experiment, we have no reason to doubt the expert’s claim, whereas in the third case, the friend’s condition makes his claim less than plausible. In the first experiment, the validity of the lady’s claim is hard to guess beforehand. The outcome of the experiments would be as expected in the second case and remarkable in the first. In the third case, one would either consider the friend extremely lucky, or begin to doubt the fairness of the coin being flipped.

The above example convincingly makes the point that in our intuitive approach to statistical issues, we include all knowledge we have, even resorting to strongly biased estimators if the model does not permit a non-biased way to incorporate it. The Bayesian approach to statistics allows us to choose priors that reflect this subjectivity: from the outset, we attach more prior mass to parameter-values that we deem more likely, or that we believe in more strongly. In the above example, we would choose a prior that concentrates more mass at high values of \( \theta \) in the second case and at low values in the third case. In the first case, the absence of prior knowledge would lead us to remain objective, attaching equal prior weights to high and low values of \( \theta \). Although the frequentist’s testing procedure can be adapted to reflect subjectivity, the Bayesian procedure incorporates it rather more naturally through the choice of a prior.

Subjectivist Bayesians view the above as an advantage; objectivist Bayesians and frequentists view it as a disadvantage. Subjectivist Bayesians argue that personal beliefs are an essential part of statistical reasoning, deserving of a explicit role in the formalism and interpretation of results. Objectivist Bayesians and frequentists reject this thought because scientific reasoning should be devoid of any personal beliefs or interpretation. So the above freedom in the choice of the prior is also the Achilles’s heel of Bayesian statistics: fervent frequentists and objectivist Bayesians take the point of view that the choice of prior is an undesirable source of ambiguity, rather than a welcome way to incorporate “expert knowledge” as in example 1.8. After all, if the subjectivist Bayesian does not like the outcome of his analysis, he can just go back and change the prior to obtain a different outcome. Similarly, if two subjectivist Bayesians analyze the same data they may reach completely different conclusions, depending on the extent to which their respective priors differ.

To a certain extent such ambiguity is also present in frequentist statistics, since frequentists have the freedom to choose biased point-estimators. For example, the use of either a maximum-likelihood or penalized maximum-likelihood estimator leads to differences, the size of which depends on the relative sizes of likelihood and
penalty. (Indeed, through the maximum-a-posteriori Bayesian point-estimator (see definition 2.12), one can demonstrate that the log-prior-density can be viewed as a penalty term in a penalized maximum-likelihood procedure, c.f. remark 2.6.) Yet the natural way in which subjectivity is expressed in the Bayesian setting is more explicit. Hence the frequentist or objectivist Bayesian sees in this a clear sign that Bayesian statistics lacks universal value unless one imposes that the prior should not express any bias (see section 3.2).

A second difference in philosophy between frequentist and Bayesian statisticians arises as a result of the fact that the Bayesian procedure does not require that we presume the existence of a “true, underlying distribution” $P_0$ of $Y$ (compare with (1.1)). The subjectivist Bayesian views the model with (prior or posterior) distribution as his own, subjective explanation of the uncertainty in the data. For that reason, subjectivists prefer to talk about their (prior or posterior) “belief” concerning parameter values rather than implying objective validity of their assertions. On the one hand, such a point of view makes intrinsic ambiguities surrounding statistical procedures explicit; on the other hand, one may wonder about the relevance of strictly personal belief in a scientific tradition that emphasizes universality of reported results.

The philosophical debate between Bayesians and frequentists has raged with varying intensity for decades, but remains undecided to this date. In practice, the choice for a Bayesian or frequentist estimation procedure is usually not motivated by philosophical considerations, but by far more practical issues, such as ease of computation and implementation, common custom in the relevant field of application, specific expertise of the researcher or other forms of simple convenience. More recent developments [3] suggest that the philosophical debate will be put to rest in favour of more practical considerations as well. In later chapters it is demonstrated how Bayesian and frequentist statistical limits are related in the large-sample asymptotic regime.

1.4 The frequentist analysis of Bayesian methods

Since this point has the potential to cause great confusion, we emphasize the following: this text presents Bayesian statistics from a hybrid perspective, i.e. we consider Bayesian techniques but analyze them in frequentist setting and with frequentist methods.

We take the frequentist point of view with regard to the data, e.g. assumption (1.1); we distinguish between sample space and model and we do not adhere to subjectivist interpretations of results (although their perspective is discussed in the main text). On the other hand, we endow the model with a prior probability measure and calculate the posterior distribution, i.e. we use concepts and definitions from Bayesian statistics. This enables us to assess Bayesian methods on equal footing with frequentist statistical methods and extends the range of interesting questions. Moreover, it resolves the inherent ambiguity haunting the subjectivist interpretation of statistical results. Note, however, that the derivation of expression (2.12) for the
1.4 The frequentist analysis of Bayesian methods

posterior, for example, is the result of subjectivist Bayesian assumptions on data
and model. Since these assumptions are at odds with the frequentist perspective, we
shall take (2.12) as a definition rather than a derived form (see subsection 2.1.4).

Much of the material covered in this book does not depend on any particular
philosophical point of view, especially when the subject matter is purely mathe-
matical. Nevertheless, it is important to realize when philosophical issues may come
into play and there will be points where this is the case. In particular when dis-
cussing asymptotic properties of Bayesian procedures, adoption of assumption (1.1)
is instrumental, basically because discussing convergence requires a limit-point.

Exercises

1.1. Let $Y \in \mathcal{Y}$ be a random variable with unknown distribution $P_0$. Let $\mathcal{P}$ be a
model for $Y$, dominated by a $\sigma$-finite measure $\mu$ and parametrized by $\Theta \to \mathcal{P}: \theta \mapsto P_0$. Assume that the maximum-likelihood estimator $\hat{\theta}$ (see definition 1.10) is
well-defined, $P_0$-almost-surely. Show that if $\nu$ is a $\sigma$-finite measure dominating $\mu$ and we calculate the likelihood using $\nu$-densities, then the associated MLE is equal
to $\hat{\theta}$. Conclude that the MLE does not depend on the dominating measure used, c.f.
remark 1.2.

1.2. Prove lemma 1.1.

1.3. Let $\mathcal{Y} = \mathbb{R}$ with $\sigma$-algebra $\mathcal{B}$. Show that if $\mathcal{B}$ is the usual Borel $\sigma$-algebra, then
$\mathcal{M}_1^+(\mathcal{Y}, \mathcal{B})$ is not dominated. Also show, that if $\mathcal{B}$ is generated by the collection of
all half-open intervals $(x, y]$, where $x, y \in \mathbb{R}$, $x < y$, then $\mathcal{M}_1^+(\mathcal{Y}, \mathcal{B})$ is dominated.

1.4. Although customarily the model is defined first and estimators follow, it is possible to
reverse the order: suppose that we have a certain fixed estimator in mind, how should we choose the model in order for the fixed estimator to perform?

More explicitly, consider a data vector $Y = (X_1, \ldots, X_n)$ that forms an i.i.d. sample
from a unknown distribution $P_0$ on $\mathbb{R}$. We are interested in estimation of the quantity
$\psi = P_0 g(X)$, assumed to be finite, where $g : \mathbb{R} \to \mathbb{R}$ is a given measurable function
defined on the sample space for $X$. Examples: if $g$ is the identity map, then $\psi$ is the expectation of $X$; if $g = (X - P_0 X)^2$, then $\psi$ is the variance of $X$; if $g = 1\{X \leq x\}$
for some $x \in \mathbb{R}$, then $\psi = F_0(x)$, the value of the distribution function associated
with $P_0$ at $x$. In such cases, estimation of $\psi$ by the sample mean $\hat{\psi}_n := \frac{1}{n} \sum X_i$
appears sensible for large $n$.

a. Based on the limit $n \to \infty$, characterize the largest model $\mathcal{P}$ in which estimation
of $\psi$ by $\hat{\psi}_n$ makes sense. What can be said of $\mathcal{P}$ if $g$ is a bounded function?
b. Show that $\hat{\psi}_n$ is consistent: $\lim_{n \to \infty} \hat{\psi}_n = \psi$, $P_0$-almost-surely.

To analyze the behaviour of $\hat{\psi}_n$ in some more detail, consider the following question.

c. Restrict the model $\mathcal{P}$ further to demonstrate that $\hat{\psi}_n$ converges to $\psi$ at rate $n^{-1/2}$,
\textit{i.e.} for every sequence $M_n \to \infty$, 

\[ P_0^n \left( n^{1/2} | \hat{\psi}_n - \psi | > M_n \right) \to 0, \]

as \( n \to \infty \).

d. Compare the property under c. above with example 1.6 and state in words how the quality of \( \hat{\psi}_n \) as an estimator for \( \psi \) improves as \( n \to \infty \).

1.5. In the three experiments of example 1.8, describe a test for hypotheses \( H_0 \) and \( H_1 \) at level \( \alpha \in (0, 1) \), for example the likelihood ratio test. Calculate the \( p \)-value of the realization of 10 successes and 0 failures (in 10 Bernoulli trials according to \( H_0 \)).
Chapter 2  
Bayesian basics

In this chapter, we consider the basic definitions and properties of Bayesian statistical and decision-theoretic methods. We derive the posterior distribution from data, model and prior and we discuss how the posterior should be viewed if one assumes the frequentist point of view of section 2.1. In section 2.2 we consider point estimators derived from the posterior and in section 2.3 we discuss confidence sets and credible sets. Section 2.4 discusses the Neyman-Pearson theory of hypothesis testing, as well as a brief introduction to the Le Cam’s theory of asymptotically optimal test sequences and, of course, posterior odds and Bayes factors. Section 2.5 concludes the chapter with a discussion of minimax risk and Bayes risk, and the differences that occur in decision theory. Throughout the chapter the explicit goal is to consider frequentist methods side-by-side with the Bayesian procedures, for comparison and reference.

2.1 Bayes’s rule, prior and posterior distributions

In this section, we introduce the basic definitions and procedures in Bayesian statistics. Formalizing the Bayesian procedure can be done in several ways. We start this section with considerations that are traditionally qualified as being of a “subjectivist” nature: in subsection 2.1.1 we derive the relation between data, model and prior on the one hand, and the posterior on the other based on Bayes’s Rule without reference to the frequentist’s “true distribution of the data”. We take due care with regard to the support of the prior (see subsection 2.1.3) and consider a prototypical example usually referred to as Bayes’s Billiard in subsection 2.1.2. In subsection 2.1.4 we revert to the “frequentist” point of view through an assumption relating the “true distribution of the data” to the prior predictive distribution (see definition 2.4).
2.1.1 Bayes’s rule

The Bayesian framework does not just view the data $Y$ as a random variable but casts the parameter in that form as well. The parameter space $\Theta$ is assumed to be a measurable space, with $\sigma$-algebra $\mathcal{G}$ and, rather than just taking on fixed values $\theta$ as in the frequentist case, the parameter is represented by a random variable $\vartheta$ taking values in $\Theta$. We assume that on the product-space $\mathcal{Y} \times \Theta$ (with product $\sigma$-algebra $\sigma(\mathcal{B} \times \mathcal{G})$) we have a probability measure,

$$\Pi^* : \sigma(\mathcal{B} \times \mathcal{G}) \to [0,1].$$ (2.1)

The probability measure $\Pi^*$ provides a joint probability distribution for $(Y, \vartheta)$, where $Y$ is the observation and $\vartheta$ (the random variable associated with) the parameter of the model.

Implicitly the choice for the measure $\Pi^*$ defines the model in Bayesian context, by the possibility to condition the distribution of $Y$ on fixed values $\vartheta = \theta$ in $\Theta$. The conditional distribution for $Y|\vartheta$ (see appendix A.5) describes the distribution of the observation $Y$ given the parameter $\vartheta$. As such, the distributions for $Y|\vartheta = \theta$ can be identified with the elements $\mathcal{P}_\theta$ of what was referred to as a parametrized model $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ in chapter 1.

**Definition 2.1.** The distribution of the data $Y$ conditional on the parameter $\vartheta$ (c.f. definition A.15) is a regular conditional distribution,

$$\Pi_{Y|\vartheta} : \mathcal{B} \times \Theta \to [0,1],$$ (2.2)

which describes the model distributions.

(see definition A.16). Since conditional probabilities are defined almost-surely with respect to the marginal (see definition A.15), the Bayesian notion of a model is represented only up to null-sets of the marginal distribution of $\vartheta$, referred to in Bayesian context as the prior for the parameter $\vartheta$.

**Definition 2.2.** The marginal distribution $\Pi : \mathcal{G} \to [0,1]$ for $\vartheta$ is called the prior.

The prior is interpreted in the subjectivist’s philosophy as the “degree of belief” attached to subsets of the model a priori, that is, before any observation has been made or incorporated in the calculation. It is important to note that $\Pi^*$ is usually constructed by choice of a prior measure $\Pi$ for $\vartheta$ and model distributions $\theta \mapsto P_\theta$,

$$\Pi^*(A \times B) = \int_B \Pi(A|\vartheta = \theta) d\Pi(\theta) = \int_B P_\theta(A) d\Pi(\theta),$$

for all $A \in \mathcal{B}$ and $B \in \mathcal{G}$ (where $\theta \mapsto P_\theta(A)$ is assumed to be measurable for all $A \in \mathcal{B}$). Central to the Bayesian framework is the conditional distribution for $\vartheta$ given $Y$, called the posterior. The transition from prior to posterior represents the way in which “prior belief” is turned into “posterior belief” (concerning the parameter) based on the data. The posterior is interpreted as a data-amended version of the prior.
that is to say, the subjectivist’s original “degree of belief” corrected by observation of \( Y \) through conditioning. Below we define the posterior in conjunction with the marginal distribution for the data, the so-called prior predictive distribution.

**Definition 2.3.** The conditional distribution \( \Pi_{\theta|Y} : \mathscr{G} \times \mathcal{B} \rightarrow [0, 1] \) for \( \theta|Y \) is called the posterior distribution.

The definition of the posterior is almost-sure with respect to the marginal data distribution \( \Pi \) (see definition A.14 and the concluding remarks of subsection A.5).

**Definition 2.4.** The marginal distribution \( P^\Pi : \mathcal{B} \rightarrow [0, 1] \) for \( Y \) is called the prior predictive distribution. If, in the above, one replaces the prior by the posterior, the resulting distribution for \( Y \) is referred to as the posterior predictive distribution.

In the subjectivist philosophy, the prior predictive distribution describes a subjectivist’s expectations concerning the observation \( Y \) based only on model and prior, \textit{i.e.} before involving the data or realizations thereof. Given model and prior, the prior predictive distribution is of mixture form.

**Lemma 2.1.** The prior predictive \( P^\Pi \) can be expressed in terms of model distributions \( P_\theta \) and the prior, taking the form,

\[
P^\Pi(Y \in A) = \int_\Theta P_\theta(A) d\Pi(\theta), \tag{2.3}
\]

for all \( A \in \mathcal{B} \).

The Bayesian symmetry between observation and parameter invites an identity expressing its essence. Bayes’s Rule relates model distributions, prior, posterior and prior predictive distribution through \( \Pi(\theta \in B | Y \in A) = \Pi(Y \in A | \theta \in B) \Pi(\theta \in B), \) for all \( A \in \mathcal{B} \) and \( B \in \mathscr{G} \) (see proposition A.2). The following theorem restates this fact in terms of the concepts we have introduced above, in a property which is sometimes referred to as a disintegration of the joint measure on model times sample space: (2.4) should be viewed as a double-sided version of definition A.15.

**Theorem 2.1.** Posterior, prior predictive, model distributions and prior are related through Bayes’s Rule,

\[
\int_A \Pi(B | Y = y) dP^\Pi(y) = \int_B P_\theta(A) d\Pi(\theta), \tag{2.4}
\]

for all \( A \in \mathcal{B} \) and \( B \in \mathscr{G} \).

**Proof.** Equality (2.4) follows since both sides are equal to \( \Pi^\ast(A \times B) \), c.f. definition A.15.

Note that, given model and prior, property (2.4) characterizes the posterior, up to re-definition on null sets of the prior predictive distribution \( P^\Pi \). Consequently, we may turn this theorem around and use property (2.4) as the defining property of the posterior.
Definition 2.5. Given model and prior, any map \( \pi : G \times Y \to [0, 1] \) such that \( y \mapsto \pi(B, y) \) is measurable for all \( B \in G \) and such that \( \pi \) satisfies,
\[
\int_A \pi(B, y) dP^\Pi(y) = \int_B p_\theta(A) d\Pi(\theta),
\]
(2.5)
for all \( A \in B \) and \( B \in G \), is called a version of the posterior.

Unfortunately property (2.5) does not imply that \( \pi \) is a regular conditional probability, so we are left with an equivalence in which property 2 of definition A.16 remains as a condition.

Proposition 2.1. A map \( \pi : G \times Y \to [0, 1] \) is a regular version of the posterior iff \( \pi \) is \( B \)-measurable for all \( B \in G \) and satisfies (2.5), and \( B \mapsto \pi(B, y) \) is a (probability) measure on \( G \) for \( P^\Pi \)-almost-all \( y \in Y \).

By contrast, the following construction does imply regularity. Assuming that the model \( P \) is dominated, there exists an expression for the posterior in terms of model densities. Since most statistical models are defined as families of densities (e.g. Lebesgue-densities on \( \mathbb{R} \) or \( \mathbb{R}^n \)) this accessible form of the posterior is used often.

Theorem 2.2. Assume that the model \( P = \{ P_\theta : \theta \in \Theta \} \) is dominated by a \( \sigma \)-finite measure \( \mu \) on \( (Y, B) \) with densities \( p_\theta = dP_\theta / d\mu \). Then the posterior can be expressed as,
\[
\Pi(\theta \in B | Y) = \frac{\int_B p_\theta(Y) d\Pi(\theta)}{\int_\Theta p_\theta(Y) d\Pi(\theta)},
\]
(2.6)
for all \( B \in G \). This version of the posterior is regular.

Proof. Since the model is dominated, the prior predictive distribution has a density with respect to \( \mu \), because for every \( A \in B \),
\[
P^\Pi(A) = \int_\Theta P_\theta(A) d\Pi(\theta) = \int_A p_\theta(y) d\mu(y) d\Pi(\theta)
\]
\[
= \int_A \left( \int_\Theta p_\theta(y) d\Pi(\theta) \right) d\mu(y).
\]
in accordance with the Fubini and Radon-Nikodym theorems. The prior predictive density \( p^\Pi : Y \to \mathbb{R} \) is therefore equal to the denominator on the \( r.h.s. \) of (2.6). Let \( A \in B \) and \( B \in G \) be given. Substituting (2.6) into the \( l.h.s. \) of (2.4), we obtain,
\[
\int_A \Pi(B | Y = y) dP^\Pi(y) = \int_A \left( \int_B p_\theta(Y) d\Pi(\theta) / \int_\Theta p_\theta(Y) d\Pi(\theta) \right) dP^\Pi(y)
\]
\[
= \int_A \int_B p_\theta(y) d\Pi(\theta) d\mu(y) = \int_B p_\theta(A) d\Pi(\theta).
\]
According to theorem 2.1, (2.6) is a version of the posterior and property 3 of definition A.16 is satisfied. Property 1 of definition A.16 follows from Fubini’s theorem.
(which guarantees measurability of the r.h.s. of (2.6)). Since \( p_\Pi(p_\Pi > 0) = 1 \), the denominator in (2.6) is non-zero \( p_\Pi \)-almost-surely and the posterior is well-defined (as a map \( \mathcal{G} \to [0,1] \)), \( p_\Pi \)-almost-surely. In addition, for all \( y \) such that \( p_\Pi(y) > 0 \) and any sequence \( (B_n) \) of disjoint, \( \mathcal{G} \)-measurable sets,

\[
\Pi(\theta \in \bigcup_{n \geq 1} B_n | Y = y) = (p_\Pi(y))^{-1} \int_{\bigcup_{n \geq 1} B_n} p_\theta(y) d\Pi(\theta)
\]

\[
= (p_\Pi(y))^{-1} \sum_{n \geq 1} 1_{\theta \in B_n} p_\theta(y) d\Pi(\theta)
\]

\[
= \sum_{n \geq 1} (p_\Pi(y))^{-1} \int_{B_n} p_\theta(y) d\Pi(\theta) = \sum_{n \geq 1} \Pi(\theta \in B_n | Y = y),
\]

by monotone convergence. We have established that on an event of \( p_\Pi \)-measure one, this version of the posterior is well-defined and \( \sigma \)-additive, so that also property 2 of definition A.16 holds. Conclude that (2.6) is a regular version of the posterior.

In the rest of part I and most of part ??, we shall not concern ourselves with regularity of posteriors any more: in all parametric and most non-parametric settings explored here and in the literature, the model is dominated or it is a Polish space (see theorem A.9), either of which implies existence of regular posteriors. But in part ?? we shall also encounter topological circumstances (from rather compelling theoretical arguments based on certain weak model topologies) and questions regarding regularity will resurface there.

To demonstrate that it is easy to define a model (with prior) that theorem A.9 does not cover, consider the following example.

**Example 2.1.** Suppose that the samplespace is \( \mathbb{R} \) and the model \( \mathcal{P} \) consists of all measures of the form (see example A.3):

\[
P = \sum_{j=1}^{m} \alpha_j \delta_{x_j},
\]

(2.7)

for some \( m \geq 1 \), with \( \alpha_1, \ldots, \alpha_m \) satisfying \( \alpha_j \geq 0, \sum_{j=1}^{m} \alpha_j = 1 \) and \( x_1, \ldots, x_m \in \mathbb{R} \). A suitable prior for this model exists (if one is willing to allow \( m = \infty \)): distributions drawn from a so-called Dirichlet process prior (see section 3.6) are of the form (2.7) with probability one. There is no \( \sigma \)-finite dominating measure for this model (not even if we restrict to measures of the form (2.7) with \( m = 1 \)) and the model can not be represented by a family of densities, c.f. definition 1.3. Definition (2.6) cannot be used in this case. We have to resort to definition 2.3 in order to make sense of the posterior distribution and existence of a version of the posterior that displays regularity is a concern in this case.

This model \( \mathcal{P} \) can also be used as a parametrizing space for a so-called mixture model \( \mathcal{P}' \) of distributions on \( \mathbb{R} \). For a fixed probability distribution \( F \) with Lebesgue density \( f : \mathbb{R} \to \mathbb{R} \) and any probability distribution \( P \) on \( \mathbb{R} \), define the convolution \( f_P \) as follows,
\[ f_P(x) = \int f(x - y) dP(y), \]

for (Lebesgue-almost-all) \( x \in \mathbb{R} \). Note that \( f_P \) is a Lebesgue probability density on \( \mathbb{R} \) (due to Fubini’s theorem), describing the distribution of the random variable \( Z = X + Y \), for some \( (X, Y) \) that are independent and marginally, \( X \sim P \) and \( Y \sim F \).

If we let \( P \) be from the model \( \mathcal{P} \) above, convolution defines a map from \( \mathcal{P} \) to a new model \( \mathcal{P}' \) of densities, \( \mathcal{P} \to \mathcal{P}' : P \to f_P \), of the form,

\[ f_P(x) = \sum_{j=1}^{m} \alpha_j f(x_j - x), \]

where \( P \) is as in (2.7), a convex combination of \( m \) clusters in which the intra-cluster variability is described by the density \( f \); the model describes observation of a randomly selected cluster location \( X = x_j \) with random (e.g. noisy) displacement \( Y \sim F \).

### 2.1.2 Bayes’s billiard

To many who have been introduced to statistics from the frequentist point of view, treating the parameter \( \theta \) for the model as a random variable \( \vartheta \) seems somewhat unnatural because the frequentist role for the parameter is entirely different from that of the data. The following example demonstrates that in certain situations the Bayesian point of view is not unnatural at all.

**Example 2.2.** In the posthumous publication of “An essay towards solving a problem in the doctrine of chances” in 1763 [4], Thomas Bayes included an example of a situation in which the above, subjectivist perspective arises quite naturally. It involves a number of red balls and one white ball placed on a table and has become known in the literature as Bayes’s billiard.

We consider the following experiment: unseen by the statistician, someone places \( n \) red balls and one white ball on a billiard table of length 1. The statistician will be reported the number \( K \) of red balls that is closer to the cushion than the white ball (\( K \) plays the role of the data in this example) and is asked to give a distribution reflecting his beliefs concerning the position of the white ball \( X \) (\( X \) plays the role of the parameter) based on \( K \). Calling the distance between the white ball and the bottom cushion of the table \( X \) and the distances between the red balls and the bottom cushion \( Y_i \), \( i = 1, \ldots, n \), it is known to the statistician that their joint distribution is:

\[ (X; Y_1, \ldots, Y_n) \sim U[0, 1]^{n+1}, \]

\[ (2.8) \]

\textit{i.e.} all balls are placed independently and uniformly. This distribution gives rise both to the \textit{model} (for \( K \)) and to the \textit{prior} (for \( X \)). Prior knowledge concerning \( X \) \textit{(i.e.} without knowing the observed value \( K = k \)) offers little information: the best that can be said is that \( X \sim U[0, 1] \), \textit{i.e.} the prior is uniform. The question is how
this distribution for $X$ changes when we incorporate the observation $K = k$, that is, when we use the observation to arrive at posterior beliefs.

Since for every $i$, $Y_i$ and $X$ are independent c.f. (2.8), we have model distributions that give rise to,

$$P(Y_i \leq X | X = x) = P(Y_i \leq x) = x,$$

for any $x \in [0, 1]$. So for each of the red balls, determining whether it lies closer to the cushion than the white ball amounts to a Bernoulli experiment with parameter $x$. Since in addition the positions $Y_1, \ldots, Y_n$ are independent, counting the number

![Diagram showing posterior densities for the position $X$ of the white ball, given the number $k$ of red balls closer to the cushion of the billiard (out of a total of $n = 6$ red balls). For the lower values of $k$, the white ball is close to the cushion with high probability, since otherwise more red balls would probably lie closer to the cushion. This is reflected by the posterior density for $X|K = 1$, for example, by the fact that it concentrates much of its mass close to $x = 0$.]

$K$ of red balls closer to the cushion than the white ball amounts to counting “successes” in a sequence of independent Bernoulli experiments. We conclude that $K$ has a binomial distribution Bin$(n; x)$, i.e.,

$$P(K = k | X = x) = \frac{n!}{k!(n-k)!} x^k (1-x)^{n-k}.$$ 

It is possible to obtain the density for the distribution of $X$ conditional on $K = k$ from the above display using Bayes’s Rule:

$$p(x|K = k) = P(K = k | X = x) \frac{p(x)}{P(K = k)}, \quad (2.9)$$
but in order to use it, we need the two marginal densities \( p(x) \) (the prior density) and \( P(K = k) \) (the prior predictive density) in the fraction. From (2.8) it is known that \( p(x) = 1 \) and \( P(K = k) \) can be obtained by integrating,

\[
P(K = k) = \int_0^1 P(K = k | X = x) \, p(x) \, dx.
\]

Substituting in (2.9), we find:

\[
p(x | K = k) = \frac{P(K = k | X = x) \, p(x)}{\int_0^1 P(K = k | X = x) \, p(x) \, dx} = B(n, k) x^k (1 - x)^{n-k},
\]

where \( B(n, k) \) is a normalization factor. The \( x \)-dependence of the density in the above display reveals that \( X | K = k \) is distributed according to a Beta-distribution, \( B(k + 1, n - k + 1) \), so that the normalization factor \( B(n, k) \) must equal \( B(n, k) = \frac{\Gamma(n + 2)}{\Gamma(k + 1) \Gamma(n - k + 1)} \).

This provides the statistician with distributions reflecting his beliefs concerning the position of the white ball for all possible values \( k \) for the observation \( K \). Through conditioning on \( K = k \), the prior distribution of \( X \) is changed into the posterior for \( X \): if a relatively small number of red balls is closer to the cushion than the white ball (i.e. in case \( k \) is small compared to \( n \)), then the white ball is probably close to the cushion; if \( k \) is relatively large, the white ball is probably far from the cushion (see figure 2.1). The illustration on the cover of appears in [4] and is Bayes’s own version of his Billiard, complete with Beta-density drawn along the bottom edge.

### 2.1.3 The Bayesian view of the model

Based on the definitions of subsection 2.1.1 a remark is in order with regard to the notion of the model in Bayesian statistics: if, for a subset \( \mathcal{P}_1 \subset \mathcal{P} \), the prior assigns mass zero, then for all practical purposes \( \mathcal{P}_1 \) does not play a role since omission of \( \mathcal{P}_1 \) from \( \mathcal{P} \) does not influence the posterior. As long as the model is parametric, i.e. \( \Theta \subset \mathbb{R}^d \), we can always use priors that dominate the Lebesgue measure, ensuring that any \( \mathcal{P}_1 \) of prior measure zero has Lebesgue measure zero in \( \Theta \) and can therefore be thought of as negligibly small. However, in non-parametric models null-sets of the prior and posterior may be much larger than expected intuitively.

**Example 2.3.** Taking the above argument to the extreme, consider a normal location model \( \mathcal{P} = \{ N(\theta, 1) : \theta \in \mathbb{R} \} \) with a prior \( \Pi = \delta_{\theta_1} \) (see example A.3), for some \( \theta_1 \in \mathbb{R} \), defined on the Borel \( \sigma \)-algebra \( \mathcal{B} \). Then the model is dominated by the Lebesgue measure and the posterior takes the form:

\[
\Pi(\theta \in A|Y) = \int_A p_\theta(Y) \, d\Pi(\theta) \bigg/ \int \int p_\theta(Y) \, d\Pi(\theta) = \frac{p_{\theta_1}(Y)}{p_{\theta_1}(Y)} \Pi(A) = \Pi(A).
\]
for any $A \in \mathcal{B}$. In other words, the posterior equals the prior, concentrating all its mass in the point $\theta_1$. Even though we started out with a model that suggests estimation of location, effectively the model consists of only one point due to the degeneracy of the prior. In subjectivist terms, the prior belief is fully biased towards $\theta_1$, leaving no room for amendment by the data when we condition to obtain the posterior.

This example raises the question which part of the model proper $P$ plays a role in the Bayesian approach. From a topological perspective it is helpful to make the following definition.

**Definition 2.6.** In addition to $(\Theta, \mathcal{G}, \Pi)$ being a probability space, let $(\Theta, T)$ be a topological space and assume that $\mathcal{G}$ contains the Borel $\sigma$-algebra $\mathcal{B}$ corresponding to the topology $T$. The support $\text{supp}(\Pi)$ of the prior $\Pi$ is defined as the smallest closed set $S$ such that $\Pi(\Theta \setminus S) = 0$.

It is tempting to equate the support of a prior to the set described by the following intersection.

$$S = \bigcap \{ G \in \mathcal{G} : \text{closed}, \Pi(\Theta \setminus G) = 0 \}.$$  \hfill (2.10)

Perhaps somewhat surprisingly, the validity of this identification is hard to establish: for any $(\Theta, \mathcal{G})$ as in definition 2.6, $S$ is measurable, in fact, $S$ is (an intersection of closed sets so $S$ is) closed. Since the Borel $\sigma$-algebra is generated by the open sets (see definition A.1 and the example that follows) $S \in \mathcal{B} \subset \mathcal{G}$. To show that $\Pi(\Theta \setminus S) = 0$ requires extra conditions on the space $\Theta$; the following lemma covers a large (but not exhaustive) class of models.

**Lemma 2.2.** In addition to $(\Theta, \mathcal{G}, \Pi)$ being a probability space, let $(\Theta, T)$ be a topological space and assume that $\mathcal{G}$ contains the Borel $\sigma$-algebra $\mathcal{B}$ corresponding to the topology $T$. If $T$ is second countable, $S = \text{supp}(\Pi)$.

**Proof.** Consider the complement $V = \Theta \setminus S$. We can write,

$$V = \bigcup \{ U \in \mathcal{G} : \text{open}, \Pi(U) = 0 \}.$$  

The set $V$ is open and contains every open subset of $\Pi$-measure zero. Because the topology is second countable, $V$ can be written as a countable union of open sets $\{ U_k : k \geq 1 \}$ of $\Pi$-measure zero. Therefore, $\Pi(V) = \Pi(\cup_{k \geq 1} U_k) \leq \sum_{k \geq 1} \Pi(U_k) = 0$ and we conclude that $\Pi(S) = 1$.

This implies, for example, that the support of $\Pi$ is of the form (2.10) if $(\Pi, T)$ is a separable metrizable space (the interested reader should describe the countable basis for $T$ in that case).

**Example 2.4.** In example 2.3, the model $\mathcal{P}$ consists of all normal distributions of the form $N(\theta, 1)$, $\theta \in \mathbb{R}$, but the support of the prior $\text{supp}(\Pi)$ equals the singleton $\{ N(\theta_1, 1) \} \subset \mathcal{P}$. 
Note that the support of the prior is defined based on a topology, the Borel $\sigma$-algebra of which must belong to the domain of the prior measure. In parametric models this assumption is rarely problematic but in non-parametric models, finding such a prior may be difficult and the support may be an ill-defined concept. Therefore we may choose to take a less precise but more generally applicable perspective: the model is viewed as the support of the prior $\Pi$, but only up to $\Pi$-null-sets (c.f. the $\Pi$-almost-sure nature of the identification (2.2)). That means that we may add to or remove from the model at will, as long as we make sure that the changes have prior measure equal to zero: the model itself is a $\Pi$-almost-sure concept.

To demonstrate how the notion of the support of a probability measure can collide with the above remark concerning prior null-sets in non-parametric models, the following example.

**Example 2.5.** Consider again the full model $\mathcal{P}$ on a countable samplespace $\mathcal{X} = \{i : i \geq 1\}$, as in example 1.1, and represent it as the $\ell_1$-subset, 

$$\mathcal{M} = \{p \in \ell_1 : p_i \geq 1, \sum_{i \geq 1} p_i = 1\}.$$ 

Also define the subsets $\mathcal{M}_k \subset \mathcal{M}$, $(k \geq 1)$, $\mathcal{M}_k = \{p \in \mathcal{M} : p_i = 0, i \geq k\}$, and $\mathcal{N} = \{p \in \mathcal{M} : p_i > 0, i \geq 1\}$. Note that $\mathcal{N}$ can be thought of as describing a generic point in $\mathcal{M}$ (and this is made rigorous when one remarks that $\mathcal{N}$ is residual in $\mathcal{M}$ in the Baire sense [54]). For all $k \geq 1$, place priors $\Pi_k$ of full support on the finite-dimensional simplices that the $\mathcal{M}_k$ describe (and embed in $\mathcal{M}$). Define a prior $\Pi$ on $\mathcal{M}$ based on a sequence $(\lambda_k)$ such that $\lambda_k > 0$ for all $k \geq 1$ and $\sum_{k \geq 1} \lambda_k = 1$,

$$\Pi(A) = \sum_{k \geq 1} \lambda_k \Pi_k(A).$$

It is noted that the normed space $\ell_1$ is separable, so the support $S$ of $\Pi$ is well-defined and coincides with (2.10). To find $S$, let $\varepsilon > 0$ and $p \in \mathcal{M}$ be given. There exists a $k \geq 1$ such that $\sum_{i > k} p_i < \frac{1}{2}\varepsilon$. Therefore, there exists a $q \in \mathcal{M}_k$ and an $\ell_1$-neighbourhood $U$ of $q$ in $\mathcal{M}_k$ such that for all $q' \in U$, $\|p - q'\| < \varepsilon$. Therefore,

$$\Pi\left(\{q \in \mathcal{M} : \|p - q\| < \varepsilon\}\right) \geq \lambda_k \Pi_k(U) > 0.$$ 

Conclude that $S = \mathcal{M}$, that is, $\Pi$ is of full support. Nevertheless, $\mathcal{N} \cap \mathcal{M}_k = \emptyset$ for all $k \geq 1$, so $\Pi(\mathcal{N}) = 0$. The set $\mathcal{N}$ is a null-set of $\Pi$: any Bayesian analysis with this prior involves support $\mathcal{M}$ but $\mathcal{M} \setminus \mathcal{N}$ is called the model with equal validity from the Bayesian perspective.

The conceptual confusion about where a prior places its mass in a topological sense lies at the heart of the first examples of Bayesian non-parametric asymptotic inconsistency [38].
2.1 Bayes’s rule, prior and posterior distributions

2.1.4 A frequentist’s view of the posterior

So far, we have not discussed the details of the data $Y$, we have treated $Y$ completely abstractly. In this section we consider, firstly, the relation between the frequentist distribution of $Y$ (the “true” $P_0$) and the Bayesian distribution of $Y$ (the marginal $P^{\Pi}$). Secondly, we consider samples of independent, repeated measurements of a random variable $X$. We shall see that the Bayesian way to describe data and statistical experiments is in contradiction with the frequentist assumption. The section concludes with a sort of recipe listing the steps involved in the Bayesian analysis of a data set. These steps are illustrated with a very simple parametric example.

The derivation of the posterior in subsection 2.1.1 does not refer to the any “true, underlying distribution of the data” but it does involve a marginal distribution for $Y$, the prior predictive distribution of definition 2.4. If one adopts the frequentist framework to analyze Bayesian tools like the posterior, a discrepancy arises since $P_0$ and $P^{\Pi}$ are two distributions for the data $Y$ that are not equal (for a striking instance of the discrepancy, see remark 2.1 below). To the frequentist, $P^{\Pi}$ is a side-product of the Bayesian construction that has no realistic interpretation. There is, however, a clear technical issue: all definitions and derivations in subsection 2.1.1 are almost-sure with respect to the prior predictive distribution. To ensure that all of this continues to make sense after we adopt assumption (1.1) we require that $P^{\Pi}$ dominates $P_0$:

$$P_0 \ll P^{\Pi}. \quad (2.11)$$

In that case, null-sets of $P^{\Pi}$ are also null-sets of $P_0$, so that all $P^{\Pi}$-almost-sure statements and definitions are also $P_0$-almost-sure. In particular, expression (2.6) for the posterior in a dominated model satisfies the regularity condition not only $P^{\Pi}$- but also $P_0$-almost-surely, if we assume (2.11). We shall adopt the frequentist philosophy to analyse Bayesian tools, i.e. we assume (1.1) and (2.11).

In many experiments or observations, the data consists of a sample of $n$ repeated, stochastically independent measurements of the same quantity (an i.i.d. sample). To accommodate this and other situations where the data is gathered sequentially, we assume that we observe data $X^n$ taking values in measurable spaces $(X_n, B_n)$ for all $n \geq 1$, and we consider parametrized models $\Theta \rightarrow P_n : \theta \mapsto P_{\theta,n}$. The frequentist assumes that there is some sequence of probability measures $(P_{0,n})$ such that $X^n \sim P_{0,n}$ for all $n \geq 1$, and often, that there exists a $\theta_0 \in \Theta$, such that, $P_{0,n} = P_{\theta_0,n}$ for all $n \geq 1$.

In the case of i.i.d. data from a measurable space $(X, \mathcal{B})$, $X^n = (X_1, \ldots, X_n) \in X^n$ with $\Theta$ some collection $\mathcal{P}$ of probability measures $P$ on $(X, \mathcal{B})$ and parametrization $\mathcal{P} \rightarrow \mathcal{P}_n : P \mapsto P^n$. Assuming a well-specified model $\mathcal{P}$ implies the existence of some $P_0 \in \mathcal{P}$ such that $P_{0,n} = P^n_0$ for all $n \geq 1$.

For Bayesians $(\Theta, \mathcal{G}, \Pi)$ is a measurable space and $\Theta \rightarrow \mathcal{P}_n : \theta \mapsto P_{\theta,n}(B)$ must be measurable for all $B \in \mathcal{B}_n$. But because Bayesians do not entertain the concept of a ‘true’ distribution of the data, they express assumptions concerning the data only through model distributions. Particularly for the i.i.d. assumption, the Bayesian assumes conditional independence of the observations, given $\vartheta = \theta$:
\[ \Pi_{X_i \mid \theta}(X_1 \in A_1, \ldots, X_n \in A_n \mid \theta = \theta) = \prod_{i=1}^{n} \Pi_{Y_i \mid \theta}(X_i \in A_i \mid \theta = \theta) = \prod_{i=1}^{n} P_\theta(A_i), \]

for all \((A_1, \ldots, A_n) \in \mathcal{A}^n\) and \(\Pi\)-almost all \(\theta\). Similarly we see that the prior predictive distribution for i.i.d. data takes the form:

\[ P_\Pi(X_1 \in A_1, \ldots, X_n \in A_n) = \int \prod_{i=1}^{n} P_\theta(A_i) d\Pi(\theta). \]

The posterior is now a solution for Bayes’s Rule in the following form,

\[ \int_A \Pi(B \mid X_1 = x_1, \ldots, X_n = x_n) dP_\Pi(x_1, \ldots, x_n) = \int_B \prod_{i=1}^{n} P_\theta(A_i) d\Pi(\theta), \]

where \(A = A_1 \times \ldots \times A_n, B \in \mathcal{G}\). Assuming that the model \(\mathcal{P} = \{P_\theta : \theta \in \Theta\}\) for the marginal distributions is dominated by a \(\sigma\)-finite measure \(\mu\) on \(\mathcal{X}\), the above can also be expressed in terms of \(\mu\)-densities \(p_\theta = dP_\theta/d\mu\). Using theorem 2.2 we obtain the following expression for the posterior distribution:

\[ \Pi_n(\theta \in B \mid X_1, X_2, \ldots, X_n) = \int_B \prod_{i=1}^{n} p_\theta(X_i) d\Pi(\theta) \Bigg/ \int_\Theta \prod_{i=1}^{n} p_\theta(X_i) d\Pi(\theta), \quad (2.12) \]

for any \(B \in \mathcal{G}\). In a dominated model, the Radon-Nikodym derivative (see theorem A.7) of the posterior with respect to the prior is the likelihood function, normalized to be a probability density function:

\[ \frac{d\Pi(\cdot \mid X_1, \ldots, X_n)}{d\Pi}(\theta) = \prod_{i=1}^{n} p_\theta(X_i) \Bigg/ \int_\Theta \prod_{i=1}^{n} p_\theta(X_i) d\Pi(\theta), \quad (2.13) \]

\(P_\Pi\)-almost-surely, and under (2.11), also \(P_0\)-almost-surely. The latter fact explains why such strong relations exist between Bayesian and maximum-likelihood methods. Indeed, the proportionality of the posterior density and the likelihood provides a useful qualitative picture of the posterior as a measure that concentrates on regions in the model where the likelihood is relatively high. This may serve as a direct, Fisherian motivation for the use of Bayesian methods in a frequentist context, c.f. section 1.4.

Remark 2.1. Note that the prior predictive distribution for i.i.d. data is itself not a product distribution but a mixture of product distributions! This illustrates the discrepancy between \(P_0\) and \(P_\Pi\) quite clearly: while the true distribution of the data describes an i.i.d. random vector, the prior predictive distribution describes a random vector that is just exchangeable (in accordance with De Finetti’s theorem (see theorem A.2.2)).

Remark 2.2. For the frequentist to use Bayesian tools, e.g. a posterior calculated using (2.12), he has to assume condition (2.11). In the context of i.i.d. samples, that requirement takes the form,
2.1 Bayes’s rule, prior and posterior distributions

\[ P_n^0 \ll P_n^{\Pi}, \text{ (for all } n \geq 1). \]

2.1.5 From prior to posterior

To summarize, the Bayesian procedure consists of the following steps,

(i) Based on the background of the data \( Y \), the statistician chooses a model \( \mathcal{P} \) of “reasonable” candidate distributions for the data (usually with some parameterization \( \Theta \rightarrow \mathcal{P} : \theta \rightarrow P_\theta \)).

(ii) A prior measure \( \Pi \) on \( \mathcal{P} \) is chosen, reflecting “belief” concerning these candidates, see chapter 3, (usually as a probability measure on \( \Theta \)).

(iii) Based on definition 2.3, on expression (2.6) or in the case of an i.i.d. sample, on (2.12), we calculate the posterior as a function of the data \( Y \).

(iv) We observe a realization of the data \( Y = y \) and use it to calculate a realization of the posterior.

The statistician may then infer properties of the parameter \( \theta \) from the posterior \( \Pi(\cdot | Y = y) \). One important point: when reporting the results of any statistical procedure, one is obliged to reveal all relevant details concerning the procedure followed and the data. So when making inference on \( \theta \), the statistician should report on the nature of the sample used and his choice of model, and in the Bayesian case, should always report his choice of prior as well, with a clear motivation.

Example 2.6. To illustrate the above “recipe” with a concrete example, consider the one-dimensional parametric model \( \mathcal{P} \) consisting of exponential distributions:

\[ \mathcal{P} = \{ \text{Exp}(\theta) : \theta \in \Theta = (0, \infty) \}. \]

Lebesgue measure dominates the model and densities take the form \( p_\theta(x) = \theta \exp(-\theta x) \), for \( x \geq 0 \). Assume that the data consists of \( n \) observations, (conditionally) independent and identically distributed. As a prior on the model, we take another exponential distribution with density \( \pi(\theta) = \exp(-\theta) \) (for \( \theta \in \Theta \)). The posterior density relative to Lebesgue measure on \( \Theta \) takes the form,

\[
d\Pi(\theta | X_1, \ldots, X_n) = C(X_1, \ldots, X_n) \left( \prod_{i=1}^{n} \theta e^{-\theta X_i} 1_{\{X_i \geq 0\}} \right)e^{-\theta} d\theta
\]

where \( C(X_1, \ldots, X_n) \) denotes the (data-dependent) normalization factor that makes the posterior a probability measure. We calculate,

\[
d\Pi(\theta | X_1, \ldots, X_n) = C(X_1, \ldots, X_n) \theta^n e^{-\theta(1+\sum X_i)} 1_{\{X_i \geq 0\}} d\theta
\]

(where \( X_{(1)} = \min X_i \)). Since,

\[
\int_{0}^{\infty} \theta^n e^{-\alpha \theta} d\theta = \frac{n!}{\alpha^{n+1}},
\]
we see that $C(X_1, \ldots, X_n)$ must be equal to $(1 + \sum X_i)^{n+1}/n!$. So for any measurable $A \subset \Theta$, the posterior probability is given by:

$$
\Pi(\vartheta \in A|X_1, \ldots, X_n) = \frac{1}{n!} \left(1 + \sum_{i=1}^n X_i\right)^{n+1} \int_A \theta^n e^{-\theta(1+\sum_{i=1}^n X_i)} d\theta.
$$

Note that the posterior density collapses to zero (and no longer describes a probability distribution!) if $X_i < 0$ for some $1 \leq i \leq n$. As Bayesians, we insist that the data must be compatible with the model, we require that $\Pi^*(X_i \geq 0) = P^\Pi(X_i \geq 0) = 1$. As frequentists we involve the underlying distribution $P_0$, requiring that $P_0(X \geq 0) = 1$ so that the posterior is well-defined $P_0^\Pi$-almost-surely. More generally, $P^\Pi$ dominates Lebesgue measure, so $P_0 \ll P^\Pi$ as long as $P_0$ has a density with respect to Lebesgue measure.

### 2.2 Bayesian point estimators

When considering questions of statistical estimation, the outcome of a frequentist procedure is of a different nature than the outcome of a Bayesian procedure: a point-estimator (the frequentist outcome) gives a point in the model whereas the posterior (the Bayesian outcome) is a distribution on the model. A first question, then, concerns the manner in which to compare the two. We assume the frequentist philosophy to analyse Bayesian methodology (c.f. subsection 2.1.4) and, in this section, we derive point-estimators from the posterior distribution in various ways: we consider the posterior predictive distribution, as well as the parametric posterior mean and the maximum-a-posteriori estimator. In later sections we approach the matter from the opposite perspective: every point-estimator has a sampling distribution, which can be compared with the posterior because both are distributions on the model or the parameter space. This is the view that gives rise to the Bernstein-von Mises theorem of chapter 4.

#### 2.2.1 Posterior predictive and posterior mean

We think of a Bayesian point-estimator as a point in the model around which posterior mass is accumulated most, a point around which the posterior distribution is concentrated in some way. As such, any reasonable Bayesian point-estimator should represent the “location” of the posterior distribution. However there is no unique definition for the “location” of a distribution and, accordingly, there are many different ways to define Bayesian point-estimators.

**Remark 2.3.** Arguably, there are distributions for which even the existence of a “location” is questionable. For instance, consider the convex combination of point-masses $P = \frac{1}{2}\delta_{-1} + \frac{1}{2}\delta_{+1}$ on $(\mathbb{R}, \mathcal{B})$. Reasonable definitions of location, like the
mean and the median of $P$, all assign as the location of $P$ the point $0 \in \mathbb{R}$. Yet small neighbourhoods of 0 do not receive any $P$-mass, so 0 can hardly be viewed as a point around which $P$ concentrates its mass. The problem is not of a mathematical nature, it is conceptual: when we think of the “location” of a distribution we normally think of unimodal distributions which have unambiguous “locations”. However, it is common practice to formulate the notion for all distributions by the same definitions.

One quantity that is often used to represent a distribution’s location is its expectation. This motivates the first and most Bayesian definition of a posterior-based point-estimator: the posterior predictive distribution.

**Definition 2.7.** Consider a statistical problem involving data $Y$ taking values in a samplespace $(\mathcal{Y}, \mathcal{B})$ and a model $(\mathcal{P}, \mathcal{G})$ with prior $\Pi$. Assume that all the maps $\mathcal{P} \to [0, 1] : P \mapsto P(B), (B \in \mathcal{B})$ are measurable with respect to $\mathcal{G}$ and that the posterior $\Pi(P|Y)$ is a regular conditional distribution. The posterior predictive distribution is a data-dependent set-function $\hat{P} : \mathcal{B} \to [0, 1]$ defined by,

$$\hat{P}(B) = \int_{\mathcal{P}} P(B) \, d\Pi(P|Y),$$

(2.14)

for every event $B \in \mathcal{B}$.

**Proposition 2.2.** The posterior predictive distribution $\hat{P} : \mathcal{B} \to [0, 1]$ is a probability measure, almost surely.

**Proof.** (Assuming that the posterior is a regular conditional distribution) $\hat{P}$ is defined $P^\Pi$-almost-surely as a map $\mathcal{B} \to [0, 1]$. Let $F \in \mathcal{B}$ denote the event that $\hat{P}$ is well-defined and let $y \in F$ be given. Clearly, for all $B \in \mathcal{B}$, $0 \leq \hat{P}(B) \leq 1$. Let $\{B_i\}_{i \geq 1} \subset \mathcal{B}$ be any sequence of disjoint events. Since $(P, i) \mapsto P(B_i)$ is non-negative and measurable, Fubini’s theorem applies in the third equality below:

$$\hat{P}\left(\bigcup_{i \geq 1} B_i\right) = \int_{\mathcal{P}} P\left(\bigcup_{i \geq 1} B_i\right) \, d\Pi(P|Y = y) = \int_{\mathcal{P}} \sum_{i \geq 1} P(B_i) \, d\Pi(P|Y = y)$$

$$= \sum_{i \geq 1} \int_{\mathcal{P}} P(B_i) \, d\Pi(P|Y = y) = \sum_{i \geq 1} \hat{P}(B_i),$$

(or by monotone convergence), which proves $\sigma$-additivity of $\hat{P}$ for all $y \in F$, that is, $P^\Pi$-almost-surely.

**Remark 2.4.** The qualification “almost surely” in the formulation of proposition 2.2 has distinct explanations for Bayesians and for frequentists: for the Bayesian, the data $Y$ is marginally distributed according to the prior predictive distribution, so it is with respect to null sets of $P^\Pi$ that “almost surely” is to be interpreted in that case. By contrast, the frequentist assumes that $Y \sim P_0$, so he is forced to adopt assumption (2.11) and the interpretation of “almost surely” refers to null sets of $P_0$ in that case. This dual purpose of the phrase “almost surely” re-occurs in many places below.
Although we refer to $\hat{P}$ as a point-estimator (see definition 1.9), strictly speaking, we have not shown that $\hat{P} \in \mathcal{P}$ and indeed, generically, $\hat{P} \notin \mathcal{P}$ as the following proposition shows.

**Proposition 2.3.** Let $(\mathcal{Y}, \mathcal{B})$ be a Polish sample space with model $\mathcal{P}$. Endow $\mathcal{P}$ with the total-variational norm as a metric, assume that the model is pre-compact in the corresponding metric topology and let $\Pi$ be a Borel prior on $\mathcal{P}$. Then $\hat{P}$ lies in the closed convex hull of $\mathcal{P}$, almost-surely.

**Proof.** Let $\varepsilon > 0$ be given. Let $\mathcal{P}$ denote the completion of $\mathcal{P}$. Since $\mathcal{P}$ is a compact metrizable space, $\mathcal{P}$ is Polish. The posterior extends trivially from a Borel probability measure on the subspace $\mathcal{P}$ to such a measure on $\mathcal{P}$, so the posterior has a almost-surely unique regular version (see theorem A.9). Therefore, (2.14) is a well-defined probability measure, on an event $F \in \mathcal{B}$ of $P\Pi$-probability one. Since $\mathcal{P}$ is pre-compact by assumption, for every $\varepsilon > 0$, there exists an $N \geq 1$ and $\{P_1, \ldots, P_N\} \subset \mathcal{P}$ such that the total-variation balls $B_{\varepsilon} = \{P' \in \mathcal{P} : \|P - P\| < \varepsilon\}$ form a finite cover of $\mathcal{P}$, i.e. $\mathcal{P} = \bigcup_{i=1}^{N} B_{\varepsilon}$. Through definition of $C_{i+1} = B_{\varepsilon} \setminus C_{i}$ (for all $i \geq 1$, with $C_1 = B_1$) this cover is turned into a finite measurable partition $\{C_1, \ldots, C_N\}$ of $\mathcal{P}$. For $y \in F$ and $1 \leq i \leq N$, define $\lambda_i = \Pi(C_i | Y = y)$ and note that,

$$
\|\hat{P} - \sum_{i=1}^{N} \lambda_i P_i\| = \sup_{B \in \mathcal{B}} \left| \sum_{i=1}^{N} \int_{C_i} (P(B) - P_i(B)) d\Pi(P | Y = y) \right|
\leq \sup_{B \in \mathcal{B}} \sum_{i=1}^{N} \int_{C_i} |P(B) - P_i(B)| d\Pi(P | Y = y)
\leq \sum_{i=1}^{N} \left( \sup_{B \in \mathcal{B}} \int_{C_i} |P(B) - P_i(B)| d\Pi(P | Y = y) \right) \leq \varepsilon.
$$

We have shown that there exist elements in the convex hull co($\mathcal{P}$) of $\mathcal{P}$ that are arbitrarily close to $\hat{P}$ in total variation and conclude that $\hat{P}$ lies in its closure $\overline{\text{co}}(\mathcal{P})$.

Two remarks regarding the pre-compactness requirement in proposition 2.3: firstly, if the model is (such that it has as its completion) a Polish space, any prior is a Radon measure (on the completion), so for any $\varepsilon$ there is a compact subset (of the completion) $\mathcal{P}'$ such that $\Pi(\mathcal{P}') > 1 - \varepsilon$. Conditional on $\mathcal{P}'$ the (pre-)compactness condition is satisfied and the resulting approximate posterior predictive distribution $\hat{P}'$ lies in the (compact, hence closed) convex hull of $\mathcal{P}'$. Secondly, in part ??, we shall see that there are uniform topologies weaker than the total-variational topology, in which all models are pre-compact: with a regular posterior, the above proof continues to hold so the posterior predictive distribution always lies in the closed convex hull of the model (albeit with a wider notion of what closure means).

In many practical situations, the model $\mathcal{P}$ is parametric with measurable parameterization $\Theta \rightarrow \mathcal{P} : \theta \mapsto P_0$. In case $\Theta$ is convex, a different form of “averaging over the model” applies.
Definition 2.8. Let the model \( \mathcal{P} \) be parametric with measurable parameterization \( \Theta \to \mathcal{P} : \theta \mapsto P_{\theta} \). Assume that \( \Theta \) is a Borel measurable, convex subset \( \Theta \) of \( \mathbb{R}^d \). Let \( \Pi \) be a Borel prior defined on \( \Theta \) with a posterior \( \Pi(\cdot | Y) \). If \( \vartheta \) is integrable with respect to the posterior, the posterior mean is defined

\[
\hat{\theta}_1(Y) = \int_{\Theta} \theta \, d\Pi(\theta | Y) \in \Theta, \tag{2.15}
\]

almost-surely.

In the above definition the posterior is has an almost-surely unique regular version because the completion of \( \Theta \) is a Polish subspace of \( \mathbb{R}^d \). For the same reason, approximate

Example 2.7. In example 2.6 the posterior takes the form:

\[
\Pi(\vartheta \in A | X_1, \ldots, X_n) = \frac{1}{n!} \left( 1 + \sum_{i=1}^{n} X_i \right)^{n+1} \int_{A} \theta^n e^{-\theta (1 + \sum_{i=1}^{n} X_i)} d\theta.
\]

Assuming that \( P_0(X \geq 0) = 1 \), we omit the indicator for \( X_{(1)} \geq 0 \) and write the posterior mean of definition 2.8 as follows:

\[
\hat{\theta}_1(Y) = \int_{\Theta} \theta \, d\Pi(\theta | Y) = \frac{1}{n!} \left( 1 + \sum_{i=1}^{n} X_i \right)^{n+1} \int_{0}^{\infty} \theta^n e^{-\theta (1 + \sum_{i=1}^{n} X_i)} d\theta
\]

\[
= \frac{1}{n!} \left( 1 + \sum_{i=1}^{n} X_i \right)^{-1} \int_{0}^{\infty} \zeta^{n+1} e^{-\zeta} d\zeta = (n+1)! \left( 1 + \sum_{i=1}^{n} X_i \right)^{-1} \tag{2.16},
\]

where we have used that \( \int_{0}^{\infty} \zeta^{n+1} e^{-\zeta} d\zeta = \Gamma(n+2) = (n+1)! \).

In definition 2.8 convexity of \( \Theta \) is a condition (rather than an afterthought, as with definition 2.7): if \( \Theta \) is not convex there is no guarantee that \( \hat{\theta}_1 \in \Theta \), in which case \( P_{\hat{\theta}_1} \) is not defined since \( \hat{\theta}_1 \) does not lie in the domain of the parameterization. It is tempting to think that there is no difference between the posterior predictive and the posterior mean if the model is parametric. This is not the case, however, as demonstrated by the following (counter)example.

Example 2.8. Consider a normal location model in two dimensions for an observation \( Y \), where the location \( \mu \in \mathbb{R}^2 \) lies on the unit circle and the covariance \( \Sigma \) is fixed and known:

\[
\mathcal{P} = \{ P_\theta = N(\mu(\theta), \Sigma) : \mu(\theta) = (\cos \theta, \sin \theta), \theta \in [0, 2\pi] \}.
\]

This is an identifiable, one-dimensional parametric model with convex parameterizing space \( \Theta = [0, 2\pi] \). Assume that \( \Xi \) is the uniform distribution on \( \Theta \) (\( \Xi \) plays the role of the posterior; it does not matter what shape the posterior really has, all we need is a counterexample). We define the corresponding measure \( \Xi' \) on \( \mathcal{P} \) by applying \( \Xi \) to the pre-image of the parameterization. By rotational symmetry of \( \Xi \) and Fubini’s theorem, the expectation of \( Y \) under \( \hat{P} \) is...
\[ \int Y \, d\mathcal{P} = \int_{\mathcal{P}} PY \, d\mathcal{Z}(P) = \int_{\Theta} P\theta Y \, d\Xi(P) = \frac{1}{2\pi} \int_0^{2\pi} \mu(\theta) \, d\theta = (0, 0). \]

Note that none of the distributions in \( \mathcal{P} \) has the origin as its expectation. We can also calculate the expectation of \( Y \) under \( \mathcal{P} \) in this situation:

\[ \hat{\theta}_1(Y) = \int_{\Theta} \theta \, d\Xi(\theta) = \frac{1}{2\pi} \int_0^{2\pi} \theta \, d\theta = \pi, \]

which leads to \( P\theta Y = P\eta Y = (-1, 0) \). Clearly, the posterior predictive distribution does not equal the model distribution corresponding to the posterior mean. In fact, the above illustrates that the posterior predictive distribution does not belong to the model necessarily: \( \hat{\mathcal{P}} \notin \mathcal{P} \).

The fact that the expectations of \( \hat{\mathcal{P}} \) and \( \hat{\mathcal{P}} \) in example 2.8 differ makes it clear that \( \hat{\mathcal{P}} \neq \mathcal{P} \hat{\theta} \) unless special circumstances apply: if we consider a parameterization \( \theta \mapsto P\theta \) from a (convex) parameterizing space \( \Theta \) (like example 2.1) with posterior measure \( \Pi(d\theta) \) onto a space of probability measures \( \mathcal{P} \) (with induced posterior \( \Pi(d\mathcal{P}) \)), it makes a difference whether we consider definition (2.14), or calculate \( \mathcal{P} \hat{\theta} \).

### 2.2.2 Small-ball and formal Bayes estimators

Since there are multiple ways of defining the location of a distribution, there are multiple ways of obtaining point-estimators from the posterior distribution. A straightforward alternative for the posterior averages of the previous subsection, is given in the following definition which requires that the model is one-dimensional.

**Definition 2.9.** Let \( \Theta \) be a closed, non-empty subset of \( \mathbb{R} \) and let \( \mathcal{P} = \{ P\theta : \theta \in \Theta \} \) be a parametric model with Borel prior \( \Pi \) on \( \Theta \) and posterior \( \Pi(\cdot|Y) \). The **posterior median** is defined by,

\[ \tilde{\theta}(Y) = \inf \{ s \in \Theta : \Pi(\theta \leq s|Y) \geq 1/2 \}, \]

almost-surely.

Thus the posterior median represents the smallest value for \( \theta \) such that the posterior mass to its left is greater than or equal to 1/2. This definition simplifies drastically in case the posterior has a continuous, (strictly) monotone distribution function: in that case the above definition reduces to the perhaps more familiar definition as the (unique) point \( \hat{\theta} \in \Theta \) where \( \Pi(\theta \leq \hat{\theta}|Y) = 1/2 \). In some situations, the posterior median offers an advantage over the posterior mean since its definition does not depend on integrability requirements and because of robustness against perturbation of the tails of the posterior.

Another alternative is decision-theoretic in essence (see section 2.5), that is, one takes the perspective in which an assessment of loss is inherent. Suppose that we
2.2 Bayesian point estimators

Consider estimation in a metric model \((\mathcal{P}, d)\) and we quantify errors in estimation as follows: if the true distribution of the data is \(P_0\) and we estimate that it is \(P\), then we incur a loss (to be specified further by the context of the problem) that is a monotone increasing function \(\ell : [0, \infty) \rightarrow [0, \infty)\) of the distance \(d(P_0, P)\). If we assume that the posterior concentrates its mass around \(P_0\) (as well as possible) then the estimator that minimizes the expected loss relative to the posterior optimizes the so-called Bayesian risk function,

\[
r(\Pi, \theta') = \int_{\Theta} P_0(\theta') d\Pi(\theta),
\]

for given prior \(\Pi\) and estimator \(\theta'\).

**Definition 2.10.** Let \(\mathcal{P}\) be a model with metric \(d : \mathcal{P} \times \mathcal{P} \rightarrow \mathbb{R}\) and a Borel prior \(\Pi\) on \(\mathcal{P}\). Any monotone increasing function \(\ell : [0, \infty) \rightarrow [0, \infty)\) is called a loss-function if it is such that \(\ell(0) = 0\). (Often \(\ell\) is assumed to be convex or (semi-)continuous.) Provided it exists, the formal Bayes estimator is a minimizer \(\tilde{P}\) of the function,

\[
\mathcal{P} \rightarrow \mathbb{R} : Q \mapsto \int_{\mathcal{P}} \ell(d(Q, P)) d\Pi(\theta),
\]

over the model \(\mathcal{P}\), defined almost-surely.

Note that definition 2.10 retains its form when expressed in terms of a formal Bayes estimator \(\tilde{\theta}\) for a parameter \(\theta \in \Theta\).

**Theorem 2.3.** Let the model \(\mathcal{P}\) be dominated and parametrized by a metric space \((\Theta, d)\). If the formal Bayes estimator \(\tilde{\theta}\) is well-defined, it minimizes the Bayesian risk function:

\[
r(\Pi, \tilde{\theta}) = \inf_{\theta' \in \Theta} r(\Pi, \theta').
\]

**Proof.** Rewrite the Bayesian risk function for the formal Bayes estimator:

\[
r(\Pi, \tilde{\theta}) = \int_{\Theta} P_0(\theta) \ell(d(\tilde{\theta}(\theta))) d\Pi(\theta) = \int_{\Theta} \int_{\Theta} \ell(d(\theta, \tilde{\theta}(\theta))) dP_0(\theta) d\Pi(\theta)
\]

\[
= \int_{\Theta} \left( \int_{\Theta} \ell(d(\theta, \tilde{\theta}(\theta))) p_\theta(y) d\Pi(\theta) d\mu(y) \right) dP_0(\theta)
\]

\[
= \int_{\Theta} \int_{\Theta} \ell(d(\theta, \tilde{\theta}(\theta))) d\Pi(\theta | Y = y) d\mu(y).
\]

where we use the Radon-Nikodym theorem (see theorem A.7), Fubini’s theorem (see theorem A.6) and the definition of the posterior, c.f. (2.12). Using the prior predictive distribution (2.3), we rewrite the Bayesian risk function further:

\[
r(\Pi, \tilde{\theta}) = \int_{\Theta} \int_{\Theta} \ell(d(\theta, \tilde{\theta}(\theta))) d\Pi(\theta | Y = y) dP_\Pi(y).
\]

By assumption, the formal Bayes estimator \(\tilde{\theta}\) exists. Since \(\tilde{\theta}\) satisfies
Bayesian basics

\[
\int_\Theta \ell(d(\theta, \hat{\theta}(y))) \, d\Pi(\theta | Y = y) = \inf_{\theta' \in \Theta} \int_\Theta \ell(d(\theta, \theta')) \, d\Pi(\theta | Y = y)
\]

for \( P^\Pi \)-almost all \( y \in \mathcal{Y} \), we obtain

\[
\begin{align*}
    r(\Pi, \hat{\theta}) &= \int_\mathcal{Y} \inf_{\theta' \in \Theta} \int_\Theta \ell(d(\theta, \theta')) \, d\Pi(\theta | Y = y) \, dP^\Pi(y) \\
    &\leq \inf_{\theta' \in \Theta} \int_\mathcal{Y} \int_\Theta \ell(d(\theta, \theta')) \, d\Pi(\theta | Y = y) \, dP^\Pi(y) = \inf_{\theta' \in \Theta} r(\Pi, \theta').
\end{align*}
\]

One estimator of this type is defined in the following intuitively reasonable way.

**Definition 2.11.** Let the data \( Y \) with model \( \mathcal{P} \), metric \( d \) and prior \( \Pi \) be given. Suppose that the \( \sigma \)-algebra on which \( \Pi \) is defined contains the Borel \( \sigma \)-algebra. For given \( \varepsilon > 0 \), the small-ball estimator is defined to be the maximizer \( \hat{\theta} \) of the function

\[
P \mapsto \int_\mathcal{Y} \inf_{\theta' \in \Theta} \int_\Theta \ell(d(\theta, \theta')) \, d\Pi(\theta | Y = y) \, dP^\Pi(y)
\]

over the model, where \( B_d(P, \varepsilon) \) is the \( d \)-ball in \( \mathcal{P} \) of radius \( \varepsilon \) centred on \( P \). Provided that such a maximizer exists and is unique, it is defined almost-surely.

Note that this is simply the formal Bayes estimator for the loss function \( \ell(d) = 1\{d \geq \varepsilon\} \). Existence of a small-ball estimator \( \hat{\theta} \) therefore implies optimality in the sense that,

\[
\Pi(d(\hat{\theta}, \hat{\theta}) \geq \varepsilon | Y) = \inf_{Q \in \mathcal{P}} \Pi(d(P, \bar{P}) \geq \varepsilon | Y).
\]

**Remark 2.5.** Similarly to definition 2.11, for a fixed value \( p \) such that \( 1/2 < p < 1 \), we may define a Bayesian point estimator as the centre point of the smallest \( d \)-ball with posterior mass greater than or equal to \( p \) (if it exists and is unique).

Suitable conditions for the existence of small-ball estimators form the subject of exercise 2.12.

### 2.2.3 The Maximum-A-Posteriori estimator

If the posterior is dominated by a \( \sigma \)-finite measure \( \nu \), the posterior density with respect to \( \nu \) can be used as a basis for defining Bayesian point estimators.

**Definition 2.12.** Let \( \mathcal{P} \) be a model with prior \( \Pi \). Assume that the posterior is absolutely continuous with respect to a \( \sigma \)-finite measure \( \nu \) on \( \mathcal{P} \), with \( \nu \)-density \( \theta \mapsto \pi(\theta | Y) \). The maximum-a-posteriori estimator (or MAP-estimator, or posterior mode) \( \hat{\theta}_2 \) for \( \theta \) is defined as the point in the model where the posterior density takes on its maximal value:

\[
\pi(\hat{\theta}_2 | Y) = \sup_{\theta \in \Theta} \pi(\theta | Y).
\]

Provided that such a point exists and is unique, the MAP-estimator is defined almost-surely.
2.2 Bayesian point estimators

The MAP-estimator has a serious weak point: a different choice of dominating measure $\nu$ leads to a different MAP estimator! A MAP-estimator is therefore not fully specified unless we indicate which dominating measure was used to define the posterior density. It is with respect to this dominating measure that we define our estimator, so a motivation for the dominating measure used is inherently necessary. Often the Lebesgue measure is used without further comment, or objective measures (see section 3.2) are used. Another option is to use the prior measure as the dominating measure, in which case the MAP estimator equals the maximum-likelihood estimator.

Remark 2.6. There is an interesting connection between (Bayesian) MAP-estimation and (frequentist) maximum-likelihood estimation. Referring to formula (2.12) we see that in an i.i.d. experiment with parametric model, the MAP-estimator maximizes:

$$\Theta \to \mathbb{R} : \theta \mapsto n \prod_{i=1}^{n} p_{\theta}(X_i) \pi(\theta),$$

where it is assumed that the model is dominated and that the prior has a density $\pi$ with respect to the Lebesgue measure $\nu$. If the prior had been uniform, the last factor would have dropped out and maximization of the posterior density is maximization of the likelihood. Therefore, differences between ML and MAP estimators are entirely due to non-uniformity of the prior. Subjectivist interpretation aside, prior non-uniformity has an interpretation in the frequentist setting as well, through what is called penalized maximum likelihood estimation (see, for example, van de Geer (2000) [40]): Bayes’s rule applied to the posterior density $\pi_n(\theta|X_1, \ldots, X_n)$ gives:

$$\log \pi_n(\theta|X_1, \ldots, X_n) = \log \prod_{i=1}^{n} p_{\theta}(X_i) + \log \pi(\theta) + D(X_1, \ldots, X_n),$$

where $D$ is a ($\theta$-independent) normalization constant. The first term equals the log-likelihood and the logarithm of the prior plays the role of a penalty term when maximizing over $\theta$. Hence, maximizing the posterior density over the model $\Theta$ can be identified with maximization of a penalized likelihood over $\Theta$. So defining a penalized MLE $\hat{\theta}_n$ with the logarithm of the prior density $\theta \mapsto \log \pi(\theta)$ in the role of the penalty, the MAP-estimator coincides with $\hat{\theta}_n$. The above offers a direct connection between Bayesian and frequentist methods of point-estimation. As such, it provides an frequentist interpretation of the prior as a penalty in the ML procedure.

All Bayesian point estimators defined above as maximizers or minimizers over the model suffer from the usual existence and uniqueness issues associated with extrema. However, there are straightforward methods to overcome such issues. We illustrate using the MAP-estimator. Questions concerning the existence and uniqueness of MAP-estimators should be compared to those of the existence and uniqueness of $M$-estimators in frequentist statistics. Although it is hard to formulate conditions of a general nature to guarantee that the MAP-estimator exists, often one can use the following lemma to guarantee existence.
Lemma 2.3. Consider a parameterized model $\Theta \to \mathcal{P}$: $\theta \mapsto P_\theta$. If the parameter space $\Theta$ is compact and the posterior density $\theta \mapsto \pi(\theta | Y)$ is upper-semicontinuous, then the MAP-estimator exists almost surely.

To prove uniqueness one has to be aware of various possible problems among which, for instance, identifiability of the model (see section 1.1, in particular definition 1.5).

Example 2.9. Assuming that $P_0(X \geq 0) = 1$, the posterior density in example 2.6 has the form:

$$
\pi(\theta | X_1, \ldots, X_n) = \frac{1}{n!} \left(1 + \sum_{i=1}^n X_i\right)^{n+1} \theta^n e^{-\theta(1+\sum_{i=1}^n X_i)},
$$

$P_0^a$-almost-surely, where $\theta > 0$. Setting the $\theta$-derivative to zero, we find that the MAP-estimator is given by:

$$
\hat{\theta}_2(Y) = n \left(1 + \sum_{i=1}^n X_i\right)^{-1}.
$$

The MAP-estimator is similar to the maximum likelihood estimator (equal to $n(\sum X_i)^{-1}$) and the posterior mean (equal to $(n+1)(1+\sum X_i)^{-1}$, see 2.16). Although it is possible technically that these three estimators differ substantially, in many (e.g. unimodal or convergent) cases the maximum of the posterior density lies in the bulk that determines the posterior mean as well, and MAP and posterior mean are close. If, in addition, the influence of the prior is relatively small because the likelihood function peaks very sharply at its maximum, the maximum-likelihood estimator is expected to be close too. Note that differences between these three estimators become negligible in the limit $n \to \infty$.

2.3 Confidence sets and credible sets

Besides point-estimation, frequentist statistics has several other inferential techniques at its disposal. The two most prominent are the analysis of confidence intervals and the testing of statistical hypotheses. In the next section, we consider frequentist testing of hypotheses, in this section, we discuss frequentist confidence sets and their Bayesian counterparts, called credible sets.

2.3.1 Frequentist confidence intervals

Assume that we have a model $\mathcal{P}$ parametrized by an identifiable parameter $\theta$ in a parameter set $\Theta$, assuming that the true distribution of the data $Y \sim P_0$ belongs to the model, that is, $P_0 = P_{\theta_0}$ for some $\theta_0 \in \Theta$. The inferential goal is to use the data
2.3 Confidence sets and credible sets

Let $\Theta \rightarrow \mathcal{P} : \theta \mapsto P_{\theta}$ be an identifiable parametrization and assume that $Y \sim P_{\theta_0}$ for some $\theta_0 \in \Theta$. Choose a confidence level $\alpha \in (0, 1)$. Let $C_\alpha(Y)$ be a subset of $\Theta$ dependent only on the data $Y$. Then $C_\alpha$ is a confidence set for $\theta$ of confidence level $\alpha$, if it solves the equation,

$$P_{\theta_0}(\theta_0 \in C_\alpha) \geq 1 - \alpha. \quad (2.20)$$

The condition that $C_\alpha$ be dependent on the data $Y$ is meant to express the requirement that $C_\alpha$ can be calculated once the data has been observed. The confidence set may also depend on other quantities that are known to the statistician, so $C_\alpha$ is a statistic (see definition 1.9). The dependence of $C_\alpha$ on the data $Y$ makes $C_\alpha$ a random subset of the model. (Compare this to point estimators which are random points in the model.) The measurability of the event $\{Y : \theta_0 \in C_\alpha(Y)\}$ is a non-trivial technical matter that has to be addressed at the model-specific level.

Clearly confidence sets are not unique and small confidence sets are more informative than large ones: if, for some confidence level $\alpha$, we have two different procedures of finding confidence sets, leading to sets $C_\alpha$ and $D_\alpha$ of confidence level $\alpha$ respectively, and $C_\alpha \subset D_\alpha$, $P_0$-almost-surely for all $\theta$, then $C_\alpha$ is preferred over $D_\alpha$.

Example 2.10. Let $X^n = (X_1, \ldots, X_n)$ be an i.i.d. sample from a normal distribution $N(\mu_0, \sigma^2)$, with known variance $\sigma^2 > 0$ and unknown $\mu_0 \in \mathbb{R}$. As is well-known, the sample average is normally distributed,

$$\bar{\mu}_n = \frac{1}{n} \sum_{i=1}^n X_i \sim N(\mu_0, \sigma_x^2) \quad (2.21)$$

with a variance $\sigma_x^2 = \sigma^2/n$. We rephrase as follows:

$$P_0^\mu \left( \frac{\bar{X} - \mu_0}{\sigma_x} \leq x \right) = \Phi(x),$$

for all $x \in \mathbb{R}$, where $\Phi$ denotes the distribution function of the standard normal distribution. Consequently,

$$P_0^\mu \left( \frac{\bar{X} - \sigma x}{\sqrt{n}} \leq \mu_0 \leq \frac{\bar{X} + \sigma x}{\sqrt{n}} \right) = \Phi(x) - \Phi(-x).$$

Fixing some confidence level $\alpha > 0$, we solve for $x_{\alpha/2}$ in the equation $\Phi(x_{\alpha/2}) - \Phi(-x_{\alpha/2}) = 1 - \alpha$ to arrive at the conclusion that the interval,

$$C_\alpha = \left[ \frac{\bar{X} - \sigma x_{\alpha/2}}{\sqrt{n}}, \frac{\bar{X} + \sigma x_{\alpha/2}}{\sqrt{n}} \right]$$

is a level-$\alpha$ confidence set for the parameter $\mu$. 

Like in the example 2.10, confidence intervals for a parameter $\theta$ are often derived from estimators for $\theta$; in the case of example 2.10 the sample average estimates $\mu$ and it is the distribution of the sample average around $\mu$ that determines the confidence interval.

**Definition 2.14.** Let $\Theta \to \mathcal{P} : \theta \mapsto P_{\theta}$ be an identifiable model and assume that $Y \sim P_{\theta_0}$ for some $\theta_0 \in \Theta$. Let $\hat{\theta} : \mathcal{Y} \to \Theta$ be an estimator for $\theta$. The distribution of $\hat{\theta}$ over $\Theta$ is called the sampling distribution of the estimator.

Note that the randomness in $\hat{\theta}$ occurs because it is a function of the data, which is distributed according to $P_{\theta_0}$ itself. Therefore the sampling distribution of $\hat{\theta}$ depends on the parameter $\theta_0$; in fact, it is exactly this dependence that allows us to draw statistical conclusions. In example 2.10, the location of the sampling distribution is $\mu_0$, so it may be assumed that the sample average $\hat{\mu}_n$ lies close to its expectation, the true mean $\mu_0$. Exactly how close is quantified by the variance of the sampling distribution of $\hat{\mu}_n$. A confidence set is an inferential instrument to express how much uncertainty remains concerning the true value of a parameter after estimation.

In case we have a very large sample, the analysis is sometimes more conveniently done based on limits, in particular the weak limit in the central limit theorem. To that end, we also define sequences of confidence sets that reach the required confidence level only in the limit $n \to \infty$.

**Definition 2.15.** For every $n \geq 1$, let $X^n$ be data taking values in sample spaces $(\mathcal{Y}_n, \mathcal{B}_n)$, with a model $\mathcal{P}_n$ and identifiable parametrization $\Theta \to \mathcal{P}_n : \theta \mapsto P_{\theta,n}$. Assume that for some $\theta_0 \in \Theta$, $X^n \sim P_{\theta_0,n}$ for all $n \geq 1$, and choose a confidence level $\alpha \in [0,1)$. A sequence $(C_{\alpha,n})$ of sets such that $C_{\alpha,n}$ depends only on $X^n$, that solves,

$$\liminf_{n \to \infty} P_{\theta_0,n}(\theta_0 \in C_{\alpha,n}(X^n)) \geq 1 - \alpha,$$

is called an asymptotic confidence set of level $\alpha$. In case $\alpha = 0$, $\lim_n P_{\theta_0,n}(\theta_0 \in C_{0,n}) = 1$ and we say that the confidence sets $C_{0,n}$ are (asymptotically) consistent.

As it turns out, example 2.10 applies in an approximate form in all asymptotic cases where the central limit theorem applies, as the following example demonstrates.

**Example 2.11.** Let $\Theta \to \mathcal{P} : \theta \mapsto P_{\theta}$ be an identifiable, parametric model for measurements $X$ and assume that $X^n = (X_1, \ldots, X_n)$ is an i.i.d. sample from a distribution $P_{\theta_0}$ for some $\theta_0 \in \Theta$. Suppose that there exists a measurable function $f : \mathbb{R} \to \mathbb{R}$, such that $P_{\theta_0} f(X) = \theta$ and $P_{\theta_0} f(X)^2 < \infty$ for all $\theta \in \Theta$. Moreover, we assume that for some known constant $S > 0$, $\sigma^2(\theta) = P_{\theta_0} (f(X) - \theta)^2 \leq S^2$, for all $\theta \in \Theta$. Consider the sample-average $\hat{\theta}_n = \frac{1}{n} \sum f(X)$. According to the central limit theorem, estimators that are average averages for such $f$ have sampling distributions that converge weakly to normal distributions. Choose a confidence level $\alpha \in (0,1)$ and note that,

$$P_{\theta_0} \left( \frac{\sigma(\theta_0) x_{\alpha/2}}{\sqrt{n}} < \hat{\theta}_n - \theta_0 \leq \frac{\sigma(\theta_0) x_{\alpha/2}}{\sqrt{n}} \right) \to 1 - \alpha,$$

as $n \to \infty$. Define $C_{\alpha,n}$ by
2.3 Confidence sets and credible sets

\[ C_{\alpha,n} = \left[ \hat{\theta}_n - \frac{S \sigma_{1/2}}{\sqrt{n}}, \hat{\theta}_n + \frac{S \sigma_{1/2}}{\sqrt{n}} \right]. \]

Then \( P^n_{\theta_0}(\theta_0 \in C_{\alpha,n}) \to 1 - \alpha \), so for any \( \alpha' > \alpha \), \( P^n_{\theta_0}(\theta_0 \in C_{\alpha,n}) \geq 1 - \alpha' \) if \( n \) is large enough. Note that if we had not used \( S \) but \( \sigma(\theta_0) \) instead, the \( \theta_0 \)-dependence of \( \sigma(\theta_0) \) would violate the requirement that \( C_{\alpha,n} \) be a statistic: since the true value \( \theta_0 \) of \( \theta \) is unknown, so is \( \sigma(\theta_0) \). Substituting the (known) upper-bound \( S \) for \( \sigma(\theta_0) \) enlarges the \( \sigma(\theta_0) \)-interval that follows from (2.23), while eliminating the \( \theta_0 \)-dependence. In a practical situation one would not assume that there is some upper bound \( S > 0 \), but substitute \( \sigma(\theta_0) \) by an estimator \( \hat{\sigma}_n \) (a practice known as studentization, after the Student t-distribution one obtains upon plugging in \( \hat{\sigma} \) for finite \( n \geq 1 \) with \( X_i \) that are marginally normal; refer to the case of example 2.10 if \( \sigma^2 \) had not been known.) Since the asymptotics of the studentized version are equal to those of the version based on \( \sigma(\theta_0) \), studentization does not change the conclusions we based on (2.23), that is,

\[ C_{\alpha',n} = \left[ \hat{\theta}_n - \frac{\hat{\sigma} \sigma_{1/2}}{\sqrt{n}}, \hat{\theta}_n + \frac{\hat{\sigma} \sigma_{1/2}}{\sqrt{n}} \right]. \]

are asymptotic confidence intervals of any level \( \alpha' > \alpha \).

2.3.2 Bayesian credible sets

The Bayesian analogs of confidence sets are called credible sets and are derived from the posterior distribution. The rationale behind the definition of credible sets is exactly the same one that motivated confidence sets: we look for a subset \( D \) of the model that is as small as possible while receiving a certain minimal probability. Presently, however, the word ‘probability’ is not based on the sampling distribution of an estimator, but in line with the Bayesian notion, that is, ‘probability’ according to the posterior distribution.

Definition 2.16. Let \( (\Theta, \mathcal{G}) \) be a measurable space parameterizing an identifiable model \( \Theta \to \mathcal{P} : \theta \mapsto P_\theta \) for data \( Y \), with prior \( \Pi : \mathcal{G} \to [0, 1] \). Choose a level \( \alpha \in (0, 1) \). Let \( \mathcal{D}_{\alpha} \) be a subset of \( \Theta \). Then \( \mathcal{D}_{\alpha} \) is a level-\( \alpha \) credible set for \( \theta \), if it solves the equation,

\[ \Pi( \theta \in \mathcal{D}_{\alpha} \mid Y) \geq 1 - \alpha, \quad (2.24) \]

almost-surely.

To find credible sets in examples one starts by calculating the posterior distribution from the prior and the data and, based on that, derives a subset \( \mathcal{D}_{\alpha}(Y) \) such that (2.24) is satisfied. From a frequentist perspective, credible sets are statistics since they are defined based entirely on the posterior (which is a statistic itself). A credible set is sometimes referred to as a credible region, or, if \( D \) is an interval in a one-dimensional parameterspace, a credible interval. We can extend this definition to the
Definition 2.17. For every \( n \geq 1 \), let \( X^n \) be data taking values in sample spaces \( (\mathcal{X}_n, \mathcal{B}_n) \), with a model \( \mathcal{P}_n \) and identifiable parametrization \( \Theta \to \Theta_n : \theta \to P_{\theta,n} \). Choose a sequence of credible levels \( (\alpha_n) \), \( \alpha \in (0,1) \), \( \alpha_n \downarrow 0 \). A sequence of measurable subsets \( (D_{\alpha,n}) \) that solves,

\[
\Pi \left( \theta \in D_{\alpha,n} \mid X^n \right) = o(\alpha_n),
\]

almost-surely, is called a sequence of asymptotic credible sets of levels \( (\alpha_n) \).

Remark 2.7. In smooth, parametric models for i.i.d. data there is an close, asymptotic relation between Bayesian credible sets and frequentist confidence intervals centred on the maximum-likelihood estimator: the Bernstein-von Mises theorem implies that level-\( \alpha \) credible sets coincide with abovementioned level-\( \alpha \) confidence sets asymptotically! In situations where it is hard to calculate the ML estimator or to construct the corresponding confidence interval explicitly, it is sometimes relatively easy to obtain credible sets (based on a simulated sample from the posterior, as obtained from the MCMC procedure, for example). In such cases, one can calculate credible sets and conveniently interpret them as confidence intervals centred on the MLE, due to the Bernstein-von Mises theorem.

Definition 2.16 suffices to capture the concept of a credible set, but offers too much freedom in the choice of \( D \): given a level \( \alpha > 0 \), many sets will satisfy (2.24), just like confidence sets can be chosen in many different ways. Note that, also here, we prefer smaller sets over large ones: if, for some level \( \alpha \), two different level-\( \alpha \) credible sets \( F_{\alpha} \) and \( G_{\alpha} \) are given, both satisfying (2.24) and \( F_{\alpha} \subset G_{\alpha} \) then \( F_{\alpha} \) is preferred over \( G_{\alpha} \). If the posterior is dominated with density \( \theta \mapsto \pi(\theta \mid Y) \), we can be more specific. We define, for every \( k \geq 0 \), the level-sets,

\[
D(k) = \{ \theta \in \Theta : \pi(\theta \mid Y) \geq k \},
\]

and consider the following.

Definition 2.18. Let \( (\Theta, \mathcal{G}) \) a measurable space parameterizing a model \( \Theta \to \mathcal{P} : \theta \to P_\theta \) for data \( Y \in \mathcal{Y} \), with prior \( \Pi : \mathcal{G} \to [0,1] \). Assume that the posterior is dominated by a \( \sigma \)-finite measure \( \mu \) on \( (\Theta, \mathcal{G}) \), with density \( \pi(\cdot \mid Y) : \Theta \to \mathbb{R} \). Choose \( \alpha \in (0,1) \). A level-\( \alpha \) HPD-credible set (from highest posterior density) for \( \theta \) is the subset \( D_{\alpha} = D(k_{\alpha}) \), where \( k_{\alpha} \) equals:

\[
k_{\alpha} = \sup \{ k \geq 0 : \Pi(\theta \in D(k) \mid Y) \geq 1 - \alpha \}.
\]

In other words, \( D_{\alpha} \) is the smallest level-set of the posterior density that receives posterior mass greater than or equal to \( 1 - \alpha \). Note that HPD-credible sets depend on the choice of dominating measure: if we had chosen to use a different measure \( \mu \), HPD-credible sets would have changed as well!
2.4 Tests and Bayes factors

Having discussed confidence sets and credible sets in the previous section, we now turn to the related subject of hypothesis testing. We start with a discussion of the Neyman-Pearson framework and the famous lemma concerning the optimal test for testing one distribution versus another.

2.4.1 Neyman-Pearson tests

Assume that we have data \( Y \) and a parameterized model \( \mathcal{P} = \{ P_\theta : \theta \in \Theta \} \) such that \( Y \sim P_{\theta_0} \) for some \( \theta_0 \in \Theta \). For simplicity, we assume that \( \Theta \subset \mathbb{R} \) whenever the dimension of \( \Theta \) is of importance. We start with the central ideas and definitions that play a role in the Neyman-Pearson approach to statistical hypothesis testing. In this context, the hypotheses are presumptions one can make concerning the distribution of the data. Since the model contains all distributions the frequentist is willing to consider as candidates for \( P_0 \), the hypotheses are formulated in terms of a partition of the model (or its parameterization) into two disjoint subsets.

**Definition 2.19.** Testing of hypotheses proceeds through choice of a model subset \( \Theta_0 \) corresponding to the so-called null hypothesis \( H_0 \) and its complement \( \Theta_1 = \Theta \setminus \Theta_0 \), called the alternative hypothesis \( H_1 \). We distinguish between so-called simple hypotheses which consist of a single point in \( \Theta \) and composite hypotheses which consist of bigger subsets in \( \Theta \).

**Example 2.12.** As an example consider an i.i.d. real-valued sample \( X_1, \ldots, X_n \) from \( P_0 \) and let the model be a location family: we take some distribution \( Q \) and translate over \( \theta \in \Theta \subset \mathbb{R} \), \( P_\theta(A) = Q(A - \theta) \), for all \( A \). Let a \( \tilde{\theta} \in \Theta \) be a chosen point in the model and consider (simple) null-hypothesis \( H_0 \) and alternative \( H_1 \) concerning the true value \( \theta_0 \) of the parameter:

\[
H_0 : \quad \theta_0 = \tilde{\theta}, \quad H_1 : \quad \theta_0 \in \Theta \setminus \{ \tilde{\theta} \}, \tag{2.27}
\]

The procedure now requires that we use the data to investigate the hypotheses further.

An immediate warning is in order because there is a potential for the reader to trip over the following conceptual confusion: the null and alternative hypotheses do not play symmetric roles in the Neyman-Pearson procedure: the goal of Neyman-Pearson hypothesis testing is to find out whether or not the data contains “enough” evidence to reject the null hypothesis as a likely explanation when compared to explanations offered by the alternative. By no means does Neyman-Pearson testing equate to the corresponding classification problem, in which one would treat \( H_0 \) and \( H_1 \) symmetrically and make a choice for one or the other based on the data. (In subsection 2.4.3 we consider a symmetric form of testing, and for more on frequentist and Bayesian classification, see section 2.5 on decision theory.)
For the hypotheses (2.27), the most-used version of the Neyman-Pearson method seeks to find a so-called test statistic \( T(Y) \in \mathbb{R}^d \), displaying different behaviour depending on whether the data \( Y \) is distributed according to distributions in \( H_0 \) or \( H_1 \).

**Example 2.13.** If, in the situation of example 2.12, we specify that \( Q \) has a mean that equals 0, the hypotheses concern the mean of \( P_0 \), so it makes sense to use the sample average as our test statistic: if the mean of \( P_0 \) equals our chosen \( \tilde{\theta} \), the sample average may be expected to lie close to \( \tilde{\theta} \) with high probability, while a situation in which the mean of \( P_0 \) lies far away from \( \tilde{\theta} \) produces sample averages at some distance from \( \tilde{\theta} \) with high probability. Therefore the sample mean is a statistic that contains statistical information pertaining to the hypotheses. The amount of uncertainty left in this information, depends on the sampling distribution of the sample mean.

To make this precise, one also chooses a so-called critical set \( K \subset \mathbb{R}^d \) such that \( P_{\theta_0}(T \in K) \) is “small” and \( P_\theta(T \notin K) \) is “small” for all \( \theta \in \Theta \). What we mean by “small” probabilities in this context is a choice, the so-called significance level \( \alpha \in (0, 1) \) associated with the test. The significance level sets the standard for which probabilities are deemed “small”. That way, upon realization \( Y = y \), a distribution in the hypothesis \( H_0 \) makes an outcome \( T(y) \in K \) improbable (and hence, makes \( H_0 \) implausible). This set-up is formalised in the following definition.

**Definition 2.20.** Let \( \Theta \rightarrow \mathcal{P} : \theta \rightarrow P_\theta \) be an identifiable, parametrized model for a sample \( Y \). Formulate two hypotheses \( H_0 \) and \( H_1 \) by introducing a two-set partition \( \{ \Theta_0, \Theta_1 \} \) of the model \( \Theta \):

\[
H_0 : \quad \theta_0 \in \Theta_0, \quad H_1 : \quad \theta_0 \in \Theta_1.
\]

We say that a test for these hypotheses based on a test-statistic \( T \) with critical set \( K \) is of level \( \alpha \in (0, 1) \) if the power function \( \pi : \Theta \rightarrow [0, 1] \), defined by

\[
\pi(\theta) = P_{\theta}(T(Y) \in K),
\]

is uniformly small over \( \Theta_0 \):

\[
\sup_{\theta \in \Theta_0} \pi(\theta) \leq \alpha. \quad (2.28)
\]

From the above definition we arrive at the conclusion that if \( Y = y \) and \( T(y) \in K \), hypothesis \( H_0 \) is improbable enough to be rejected, since \( H_0 \) forms an “unlikely” explanation of observed data (at said significance level). The degree of “unlilkiness” can be quantified in terms of the so-called \( p \)-value, which is the lowest significance level at which the realised value of the test statistic \( T(y) \) would have led us to reject \( H_0 \).

Of course there is the possibility that our decision is wrong and \( H_0 \) is actually true but \( T(y) \in K \) nevertheless, so that our rejection of the null hypothesis is unwarranted. This is called a type-I error; a type-II error is made when we do not reject \( H_0 \) while \( H_0 \) is not true. The significance level \( \alpha \) represents a fixed upper bound for the
probability of a type-I error, c.f. (2.28). If we have several possible tests, all of which satisfy the Type-I error bound (2.28), the Neyman-Pearson approach calls for minimization of the Type-II error probability: of all the pairs \((T, K)\) satisfying (2.28), one prefers a pair that minimizes \(P_\theta(T(Y) \notin K)\), (ideally) for all \(\theta \in \Theta_1\). However, generically such uniformly most-powerful tests do not exist due to the possibility that different \((T, K)\) pairs satisfying (2.28) are most powerful over distinct subsets of the alternative.

We consider the Neyman-Pearson approach to testing in some more detail in the following example in the context of normally distributed data.

**Example 2.14.** Denote by \(P_\mu\) the normal distribution \(N(\mu, \sigma^2)\) with mean \(\mu \in \mathbb{R}\) and variance \(\sigma^2 > 0\). Let \(Y_n = (X_1, \ldots, X_n)\) be an i.i.d. sample from a normal distribution \(P_0 = P_{\mu_0}\), assuming that the variance \(\sigma^2 > 0\) is known, and unknown \(\mu_0 \in \mathbb{R}\). As we have seen in (2.21), the sample average is normally distributed, \(\hat{\mu}_n = \frac{1}{n} \sum X_i \sim N(\mu_0, \sigma^2/n)\). For any \(\mu\), we have,

\[
P_\mu \left( \frac{\sqrt{n} (\hat{\mu}_n - \mu)}{\sigma} \leq x \right) = \Phi(x),
\]

for all \(x \in \mathbb{R}\), where \(\Phi\) denotes the distribution function of the standard normal distribution. Re-write to obtain,

\[
P_\mu \left( -\frac{x \sigma}{\sqrt{n}} < \hat{\mu}_n - \mu \leq \frac{x \sigma}{\sqrt{n}} \right) = \Phi(x) - \Phi(-x),
\]

for \(x > 0\). By choosing some \(\bar{\mu}\) and a significance level \(\alpha\), we formulate null- and alternative hypotheses as in (2.27),

\[
H_0: \quad \mu_0 = \bar{\mu}, \quad H_1: \quad \mu_0 \neq \bar{\mu},
\]

and note that under the null-hypothesis,

\[
P_\mu \left( \bar{\mu} - \frac{x_{\alpha/2} \sigma}{\sqrt{n}} < \hat{\mu}_n \leq \bar{\mu} + \frac{x_{\alpha/2} \sigma}{\sqrt{n}} \right) = 1 - \alpha,
\]

if we choose the quantiles \(x_{\alpha/2}\) like in example 2.10. Hence the null-hypothesis makes it improbable to observe \(|\hat{\mu}_n - \bar{\mu}| > n^{-1/2} \sigma x_{\alpha/2}\), which gives rise to the following definition of the critical set \(K_\alpha\)

\[
K_\alpha = \mathbb{R} \setminus \left[ \bar{\mu} - \frac{x_{\alpha/2} \sigma}{\sqrt{n}}, \bar{\mu} + \frac{x_{\alpha/2} \sigma}{\sqrt{n}} \right],
\]

which enables us to formulate our decision on the null hypothesis, that is, to reject \(H_0\) or not:

(i) if the realised \(\hat{\mu}_n \in K_\alpha\), we reject \(H_0\) at significance level \(\alpha\), and,

(ii) if the realised \(\hat{\mu}_n \notin K_\alpha\), we do not see enough evidence in the data to reject \(H_0\) at significance level \(\alpha\).
Beware of a common pitfall regarding the interpretation: under case (ii), we do not draw the conclusion that $H_0$ is accepted. The data does not provide enough evidence to reject the null hypothesis but that does not imply that we accept it!

Note the behaviour of the procedure with varying sample-size: keeping the significance level fixed, the width of the critical sets $K_\alpha$ is of order $O(n^{-1/2})$, so smaller and smaller critical sets can be used as more information concerning the distribution $P_0$ (read, data) comes available. Conversely, if we keep the critical set fixed, the probability for a Type-I error decreases (exponentially) with growing sample-size. Analogous to example 2.11, it is common practice to use asymptotic tests because sampling distributions are rarely available in closed form: in cases where the sample-size is deemed to be large enough, asymptotic approximations to sampling distributions an be used (e.g. the central limit theorem when estimators are based on sample averages).

### 2.4.2 Randomized tests and the Neyman-Pearson lemma

According to the Neyman-Pearson approach, tests are only considered if they satisfy (2.28) and are optimal if, in addition, they maximize testing power over the alternative uniformly. Optimality in this sense is sometimes not achievable, so one wonders if, mathematically, anything can be said at all. The Neyman-Pearson lemma answers this question in the affirmative for problems where the null- and alternative hypotheses each contain a single distribution. In many models, (optimal) tests for composite hypotheses can be found.

To formulate the Neyman-Pearson lemma, however, we have to generalize the testing procedure slightly: as it turns out the existence of an optimal test can only be guaranteed if we allow for a randomization of our decision.

**Definition 2.21.** Let $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ be a parametrized model for data $Y$. Formulate two hypotheses $H_0$ and $H_1$ for $\theta$ based on the two-set partition $\{\Theta_0, \Theta_1\}$ of the model $\mathcal{P}$:

$$H_0 : \quad \theta_0 \in \Theta_0, \quad H_1 : \quad \theta_0 \in \Theta_1.$$ 

A **test function** $\phi$ is a map $\phi : \mathcal{P} \to [0, 1]$ used to formulate the following procedure called a randomized test: given a realisation $Y = y$ we reject $H_0$ with probability $\phi(y)$. The power function associated with the test function $\phi$ is given by $\pi : \Theta \to [0, 1] : \theta \mapsto P_\theta \phi$.

Note that if we use the test function $\phi(Y) = 1\{T(Y) \in K\}$, the randomized test reduces to the original (non-random) procedure of rejecting $H_0$ if $T(Y) \in K$. Clearly the probability for Type-I error when using the randomized procedure equals $\pi(\theta)$ (for $\theta \in \Theta_0$) and the probability for Type-II error equals $1 - \pi(\theta)$ (for $\theta \in \Theta_1$). Now return to the question regarding optimal Neyman-Pearson tests: we saw that the existence of an optimal test cannot be guaranteed as long as we look at composite hypotheses. However, if both null and alternative hypothesis are simple, no such
ambiguity is possible and a (randomized) optimal test exists by the famed Neyman-
Pearson lemma [65].

**Lemma 2.4.** Suppose the model is \( \mathcal{P} = \{ P_{\theta_0}, P_{\theta_1} \} \) and write \( p_{\theta_0} : \mathcal{Y} \mapsto \mathbb{R} \) and \( p_{\theta_1} : \mathcal{Y} \mapsto \mathbb{R} \) for the densities of \( P_{\theta_0} \) and \( P_{\theta_1} \) relative to some \( \sigma \)-finite measure \( \mu \). Choose a significance level \( \alpha \in (0, 1) \) and consider a test of the form,

\[
\phi(y) = \begin{cases} 
1 & \text{if } p_{\theta_1}(y) > cp_{\theta_0}(y) \\
\gamma(y) & \text{if } p_{\theta_1}(y) = cp_{\theta_0}(y) \\
0 & \text{if } p_{\theta_1}(y) < cp_{\theta_0}(y)
\end{cases},
\]

(2.29)

where the measurable function \( \gamma : \mathcal{Y} \mapsto [0, 1] \) and the constant \( c \in [0, \infty) \) form a solution to the equation:

\[ P_{\theta_0} \phi = \alpha, \]

The following two assertions concern the hypotheses,

\[ H_0 : \theta = \theta_0, \quad H_1 : \theta = \theta_1. \]

(i.) If a test of the form (2.29) has significance level \( \alpha \) then it is most powerful among all tests of level \( \alpha \).

(ii.) If a test \( \phi' \) is most powerful, then \( \phi' \) is of the form (2.29) for some \( \gamma(x) \) and some \( c \), almost-surely with respect to both \( P_{\theta_0} \) and \( P_{\theta_1} \).

**Proof.** Proof A proof can be found in Lehmann and Cassela (2005) [65].

The lemma is often used in conjunction with some condition on the model (or its
likelihood function) to extend this point-vs-point version to composite hypotheses
which are more interesting from a practical point of view.

**Example 2.15.** Suppose that we consider a random variable \( X \) drawn from a normal
distribution \( N(\theta, 1) \) where \( \theta \in \Theta = \{-1, 1\} \). Fixing a significance level \( \alpha \in (0, 1) \),
we consider a test of the form (2.29) for the hypotheses,

\[ H_0 : \theta = -1, \quad H_1 : \theta = +1. \]

(2.30)

A simple calculation shows that \( p_{+1}(X)/p_{-1}(X) = e^{2X} \), so, with \( \Phi \) denoting the
distribution function for the standard normal distribution,

\[ P_{-1} \phi(X) = P_{-1}(p_{+1}(X) > cp_{-1}(X)) = P_{-1}(e^{2X} > c) = P_{-1}(X > \frac{1}{2} \log c) = 1 - \Phi(\frac{1}{2} \log c + 1), \]

where we have used that \( X \) is distributed continuously (so that the middle term in
(2.29) does not play a role and any \( \gamma \) will do), and that \( P_{-1}(X \leq x) = \Phi(x + 1) \). So
to find \( c \), we solve \( 1 - \Phi(\frac{1}{2} \log c + 1) = \alpha \), so that the Neyman-Pearson procedure
for testing the hypotheses (2.30) has the form,

(i) if \( X > x_{1-\alpha} - 1 \), we reject \( H_0 \), and,
(ii) if \( X \leq x_{1 - \alpha} - 1 \), we do not see enough evidence in the data to reject \( H_0 \), at significance level \( \alpha \).

### 2.4.3 Test sequences and minimax optimality

Two points remain, the first being an asymptotic perspective on testing: just like we often study limits of sequences of estimators and conditions for their optimality, we are interested also in sequences of tests.

**Definition 2.22.** Let \( \mathcal{P} \) be a model for an i.i.d. sample \( X_1, X_2, \ldots \) taking values in \( \mathcal{X} \) and assume that the true distribution of the data lies in the model, \((X_1, \ldots, X_n) \sim P_0^n\) and \( P_0 \in \mathcal{P} \). Formulate two hypotheses \( H_0 \) and \( H_1 \) by introducing a two-set partition \( \{ \Theta_0, \Theta_1 \} \) of the parameter space \( \Theta \):

\[
H_0 : \theta_0 \in \Theta_0, \quad H_1 : \theta_0 \in \Theta_1.
\]

A test sequence \( (\phi_n)_{n \geq 1} \) is a sequence of statistics \( \phi_n : \mathcal{X}^n \to [0, 1] \), (for all \( n \geq 1 \)). For every \( n \geq 1 \), we reject \( H_0 \) with probability \( \phi_n(X_1, \ldots, X_n) \). The power function sequence of the test sequence \( (\phi_n) \) as a map \( \pi_n : \Theta \to [0, 1] \) on the model is defined by:

\[
\pi_n(\theta) = P_{\theta}^n \phi_n.
\]

Like in definition 2.20, the quality of the test sequence depends on the behaviour of the power sequence on \( \Theta_0 \) and \( \Theta_1 \) respectively. If we are interested exclusively in rejection of the null hypothesis, we could reason like in definition 2.20 and set a significance level \( \alpha \) to select only those test sequences that satisfy \( \sup_{\theta \in \Theta_0} \pi_n(P_\theta) \leq \alpha \). Subsequently, we prefer test sequences that have high power on the alternative in the limit \( n \to \infty \).

**Definition 2.23.** if we have two test sequences \( (\phi_n) \) and \( (\psi_n) \) and a point \( \theta \in \Theta_1 \) such that

\[
\lim_{n \to \infty} P_{\theta}^n \phi_n \geq \lim_{n \to \infty} P_{\theta}^n \psi_n,
\]

then \( (\phi_n) \) is said to be asymptotically more powerful than \( (\psi_n) \) at \( \theta \). If (2.31) holds for all \( \theta \in \Theta_1 \), the test sequence \( (\phi_n) \) is said to be uniformly asymptotically more powerful than \( (\psi_n) \). If one can show that this holds for all test sequences \( (\psi_n) \), then \( (\phi_n) \) is said to be uniformly asymptotically most powerful.

Note, however, that the above ordering of test sequences is not complete: it is quite possible that \( (\phi_n) \) is asymptotically more powerful than \( (\psi_n) \) on a subset of \( \Theta_1 \), whereas on its complement in \( \Theta_1 \), \( (\psi_n) \) is asymptotically more powerful. As a result, the existence of uniformly asymptotically most powerful test sequences can be problematic.

The second point that remains is to stress that the Neyman-Pearson criterion for tests is entirely geared at minimizing the probability of Type-I error (rejecting \( H_0 \).
when in fact \( H_0 \) contains the true distribution). As a result the procedure can only lead to one definite conclusion, rejection of the null hypothesis. More natural is a framework that treats null and alternative hypotheses symmetrically: we look for tests or test sequences that indicate whether the true value of the parameter resides in \( \Theta_0 \) or in \( \Theta_1 \). As a further generalization, we let \( \Theta_0 \) and \( \Theta_1 \) be arbitrary disjoint model subsets, rather than requiring that \( \Theta_0 \) and \( \Theta_1 \) partition the model. To formulate things in the asymptotic context immediately, we consider test sequences \((\phi_n)\) such that the quantity,

\[
\sup_{\theta \in \Theta_0} P_\theta^n \phi_n + \sup_{\theta \in \Theta_1} P_\theta^n (1 - \phi_n),
\]

is “small” in the limit \( n \to \infty \), possibly quantified by introduction of a significance level pertaining to both type-I and type-II errors simultaneously. Tests of this sort are used extensively in the formulation of Bayesian limit theorems.

Optimality of test sequences obtains as follows: we say that \((\phi_n)\) is minimax optimal if,

\[
\sup_{\theta \in \Theta_0} P_\theta^n \phi_n + \sup_{\theta \in \Theta_1} P_\theta^n (1 - \phi_n) = \inf_{\psi} \left( \sup_{\theta \in \Theta_0} P_\theta^n \psi + \sup_{\theta \in \Theta_1} P_\theta^n (1 - \psi) \right),
\]

for every \( n \geq 1 \). The infimum is taken over all measurable functions \( \psi : \mathcal{X}^n \to [0,1] \). Such tests exist as a consequence of the so-called minimax theorem (see theorem 2.4 in the next section): under certain convexity, continuity and compactness conditions, we can guarantee that:

\[
\inf_{\psi} \left( \sup_{\theta \in \Theta_0} P_\theta^n \psi + \sup_{\theta \in \Theta_1} P_\theta^n (1 - \psi) \right) = \sup_{\theta \in \Theta_0} \inf_{\theta' \in \Theta_1} \left( P_\theta^n \psi + P_{\theta'}^n (1 - \psi) \right),
\]

and, furthermore, that there exist tests \((\phi_n)\) satisfying (2.33). The difference between left and right sides in (2.34) is that for every \( n \geq 1 \) and all pairs \((\theta, \theta') \in \Theta_0 \times \Theta_1\) the test \( \psi \) on the right-hand side can be chosen equal to the (optimal) test based on the likelihood ratio \( p_{\theta}/p_{\theta'}(X_1, \ldots, X_n) \). After taking suprema and upper bounding, we prove the existence of a so-called minimax test sequence with explicitly known upper bound to the testing power.

**Lemma 2.5.** Let \( B, V \subset \mathcal{P} \) be model subsets such that their convex hulls \( \to B \) and \( \to V \) are separated by non-zero Hellinger distance:

\[
H(\to B, \to V) = \inf_{P \in B} \inf_{Q \in V} H(P, Q) > 0.
\]

Then, for every \( n \geq 1 \), there exists a test function \( \phi_n \) such that,

\[
\sup_{P \in B} P^n \phi_n + \sup_{Q \in V} Q^n (1 - \phi_n) \leq e^{-\frac{1}{4} n H(B,V)^2}.
\]

This lemma plays a central role in Bayesian limit theorems. Note that it does not refer to any underlying distribution \( P_0 \); it is a lemma that applies in Bayesian and frequentist approaches alike.
2.4.4 Bayes factors

Bayesian hypothesis testing is formulated in a far more straightforward fashion than frequentist methods based on the Neyman-Pearson approach. It treats null and alternative hypotheses symmetrically. The two hypotheses \( H_0 \) and \( H_1 \) correspond to a two-set partition \( \{ \Theta_0, \Theta_1 \} \) of the model \( \Theta \) and for each of the parts, we have both posterior and prior probabilities. Based on the proportions between those, we shall decide which hypothesis is the more likely one. We make the following definitions.

Definition 2.24. Let \((\Theta, \mathcal{G})\) a measurable space parameterizing a model \( \Theta \to \mathcal{P} : \theta \mapsto P_\theta \) for data \( Y \in \mathcal{Y} \), with prior \( \Pi : \mathcal{G} \to [0,1] \). Let \( \{ \Theta_0, \Theta_1 \} \) be a measurable partition of \( \Theta \) such that \( \Pi(\Theta_0) > 0 \) and \( \Pi(\Theta_1) > 0 \). The prior and posterior odds ratios are defined by \( \Pi(\Theta_0)/\Pi(\Theta_1) \) and \( \Pi(\Theta_0|Y)/\Pi(\Theta_1|Y) \) respectively. The Bayes factor in favour of \( \Theta_0 \) is defined to be

\[
B = \frac{\Pi(\Theta_0|Y)}{\Pi(\Theta_1|Y)} \frac{\Pi(\Theta_1)}{\Pi(\Theta_0)}.
\]

When doing Bayesian hypothesis testing, we have a choice of which ratio to use and that choice will correspond directly with a choice for subjectivist or objectivist philosophies. In the subjectivist’s view, the posterior odds ratio has a clear interpretation: if

\[
\frac{\Pi(\Theta_0|Y)}{\Pi(\Theta_1|Y)} > 1,
\]

then the probability of \( \theta \in \Theta_0 \) is greater than the probability of \( \theta \in \Theta_1 \) and, hence, the subjectivist decides to adopt \( H_0 \) rather than \( H_1 \). If, on the other hand, the Bayes factor in favour of \( \Theta_0 \) is smaller than 1, the subjectivist decides to adopt \( H_1 \) rather than \( H_0 \). (Note the difference with Neyman-Pearson frequentists who may reject \( H_0 \) but not adopt it.) The objectivist would object to this practice, saying that the relative prior weights of \( \Theta_0 \) and \( \Theta_1 \) can introduce a heavy bias in favour of one or the other in this approach (upon which the subjectivist would answer that that is exactly what he had in mind). Therefore, the objectivist would prefer to use a criterion that is less dependent on the prior weights of \( \Theta_0 \) and \( \Theta_1 \). We look at a very simple example to illustrate the point.

Example 2.16. Let \( \Theta \) be a dominated model that consists of only two points, \( \theta_0 \) and \( \theta_1 \) and let \( \Theta_0 = \{ \theta_0 \} \), \( \Theta_1 = \{ \theta_1 \} \), corresponding to simple null and alternative hypotheses \( H_0, H_1 \). Denote the prior by \( \Pi \) and assume that both \( \Pi(\{ \theta_0 \}) > 0 \) and \( \Pi(\{ \theta_1 \}) > 0 \). By Bayes rule, the posterior weights of \( \Theta_0 \) and \( \Theta_1 \) are

\[
\Pi(\theta \in \Theta_i|Y) = \frac{p_{\theta_i}(Y)\Pi(\Theta_i)}{p_{\theta_0}(Y)\Pi(\Theta_0) + p_{\theta_1}(Y)\Pi(\Theta_1)},
\]

for \( i = 0, 1 \). Therefore, the posterior odds ratio takes the form:

\[
\frac{\Pi(\theta \in \Theta_0|Y)}{\Pi(\theta \in \Theta_1|Y)} = \frac{p_{\theta_0}(Y)\Pi(\Theta_0)}{p_{\theta_1}(Y)\Pi(\Theta_1)},
\]
and the Bayes factor equals the likelihood ratio:

\[ B = \frac{p_{\Theta_0}(Y)}{p_{\Theta_1}(Y)}. \]

(Note the similarity with the Neyman-Pearson and optimal minimax tests for \( \Theta_0 \) versus \( \Theta_1 \), in that Bayes factors is defined in terms of the likelihood ratio \( p_{\Theta_0}(Y)/p_{\Theta_1}(Y) \).)

We see that the Bayes factor does not depend on the prior weights assigned to \( \Theta_0 \) and \( \Theta_1 \) (in this simple example), but the posterior odds ratio does. Indeed, suppose we stack the prior odds heavily in favour of \( \Theta_0 \), by choosing \( \Pi(\Theta_0) = 1 - \varepsilon \) and \( \Pi(\Theta_1) = \varepsilon \) (for some small \( \varepsilon > 0 \)). Even if the likelihood ratio \( p_{\Theta_0}(Y)/p_{\Theta_1}(Y) \) is much smaller than one (but greater than \( \varepsilon/(1-\varepsilon) \), the subjectivist’s criterion favours \( H_0 \). In that case, the data clearly advocates hypothesis \( H_1 \) but the prior odds force adoption of \( H_0 \). The Bayes factor \( B \) equals the likelihood ratio (in this example), so it does not suffer from the bias imposed on the posterior odds.

The objectivist prefers the Bayes factor to make a choice between two hypotheses: if \( B > 1 \) the objectivist adopts \( H_0 \) rather than \( H_1 \); if, on the other hand, \( B < 1 \), then the objectivist adopts \( H_1 \) rather than \( H_0 \). In example 2.16 the Bayes factor is independent of the choice of the prior. In general, the Bayes factor is not completely independent of the prior, but it does not depend on the relative prior weights of \( \Theta_0 \) and \( \Theta_1 \).

Lemma 2.6. Let \((\Theta, \mathcal{F})\) a measurable space parameterizing a model \( \Theta \to \mathcal{P} : \theta \mapsto P_{\theta} \) for data \( Y \in \mathcal{Y} \), with prior \( \Pi : \mathcal{F} \to [0, 1] \). Let \( \{\Theta_0, \Theta_1\} \) be a partition of \( \Theta \) such that \( \Pi(\Theta_0) > 0 \) and \( \Pi(\Theta_1) > 0 \). Then the Bayes factor \( B \) in favour of \( \Theta_0 \) does not depend on the prior odds ratio.

Proof. Proof For any prior such that \( \Pi(\Theta_0) > 0 \) and \( \Pi(\Theta_1) > 0 \),

\[ \Pi(A) = \Pi(A|\Theta_0) \Pi(\Theta_0) + \Pi(A|\Theta_1) \Pi(\Theta_1), \tag{2.36} \]

for all \( A \in \mathcal{F} \). In other words, \( \Pi \) is decomposed as a convex combination of two probability measures on \( \Theta_0 \) and \( \Theta_1 \) respectively. The Bayes factor is then rewritten (see lemma ??): \[ B = \frac{\Pi(\Theta_0|Y) \Pi(\Theta_1)}{\Pi(\Theta_1|Y) \Pi(\Theta_0)} = \frac{\Pi(Y|\Theta_0)}{\Pi(Y|\Theta_1)}, \]

where, in a dominated model,

\[ \Pi(Y|\Theta_i) = \int_{\Theta_i} p_\theta(Y) \, d\Pi(\theta|\Theta_i), \]

for \( i = 0, 1 \). In terms of the decomposition (2.36), \( B \) depends on \( \Pi(\cdot|\Theta_0) \) and \( \Pi(\cdot|\Theta_1) \), but not on \( \Pi(\Theta_0) \) and \( \Pi(\Theta_1) \).

So the difference between Bayes factors and posterior odds is exactly the bias introduced by non-zero prior odds; as such, it represents directly the difference between objectivist and subjectivist Bayesian philosophies.
Example 2.17. Consider a data vector \( Y = (X_1, \ldots, X_n) \) modelled as an \textit{i.i.d.} sample from a uniform distribution \( U[\theta, \theta + 1] \), with \( \theta \in \Theta = [-1, 1] \). We formulate hypotheses,

\[
H_0 : \theta \geq 0, \quad H_1 : \theta < 0.
\]

and, to show how prior odds influence posterior odds but not Bayes factors, we use a prior with a Lebesgue density of the form,

\[
\pi(\theta) = \lambda 1\{\theta < 0\} + (1 - \lambda) 1\{\theta \geq 0\},
\]

for some \( 0 < \lambda < 1 \) (where we note that \( \lambda = 0 \) or \( \lambda = 1 \) would \textit{not} be valid choices). Consequently, the prior odds for \( \Theta_0 \) versus \( \Theta_1 \) are \( 1 - \frac{1}{\lambda} \). The likelihood is given by,

\[
L_n(\theta; X_1, \ldots, X_n) = \prod_{i=1}^{n} 1\{\theta \leq X_i \leq \theta + 1\},
\]

and the posterior density (relative to the Lebesgue measure on \( \Theta = [-1, 1] \)) is proportional to,

\[
\pi(\theta|X_1, \ldots, X_n) \propto \lambda 1\{\theta < 0\} 1\{\theta \leq X_{(1)}\} 1\{X_{(n)} \leq \theta + 1\}
+ (1 - \lambda) 1\{\theta \geq 0\} 1\{\theta \leq X_{(1)}\} 1\{X_{(n)} \leq \theta + 1\},
\]

where \( X_{(1)} \) and \( X_{(n)} \) denote first and last order statistics of the sample respectively. To calculate the posterior odds we do not need the normalization factor in the posterior and we see immediately that,

\[
\frac{\Pi(\theta \geq 0 | X_1, \ldots, X_n)}{\Pi(\theta < 0 | X_1, \ldots, X_n)} = \frac{1 - \lambda}{\lambda} \int_{\theta}^{1} 1\{X_{(n)} - 1 \leq \theta \leq X_{(1)}\} d\theta
\]

Note the proportionality to the prior odds: the Bayes factor \( B \) is equal to only the latter fraction in the expression on the right-hand side of the above display and is insensitive to the subjective choice for \( \lambda \).

To conclude this section we make the following important remark.

Remark 2.8. The condition that both \( \Theta_0 \) and \( \Theta_1 \) receive prior mass strictly above zero is important since Bayes factors and odds ratios are based on conditioning of \( \vartheta \). Bayesian hypothesis testing is sensible \textit{only} if both \( \Theta_0 \) and \( \Theta_1 \) receive non-zero prior mass. This remark plays a role particularly when comparing a simple null hypothesis to an alternative, as illustrated in exercise 2.17.

2.5 Decision theory and classification

Many practical problems require that we make an observation and based on the outcome, make a decision of some kind. For instance when looking for the diagnosis for a patient, a doctor will observe variables like the patients temperature,
2.5 Decision theory and classification

blood-pressure and appearance, in addition to the results of chemical and physical scans to come to a decision regarding the affliction the patient is probably suffering from. Another example concerns the financial markets, where past stock- and option-prices are considered by analysts to decide whether to buy or sell stocks and derivatives. In a chemical plant, regulation of a chemical process amounts to a succession of decisions to control and optimize conditions, based on the measurement of thermo-dynamical quantities such as concentrations of chemicals involved in the reaction. In this section, we look at problems of this nature, first from a frequentist perspective and then with the Bayesian approach.

2.5.1 Decision theory

Practical problems like those described above usually involve optimality criteria that are prescribed by the context of the problem itself: for example, when a doctor makes the wrong diagnosis for a patient suffering from cancer the consequences can be most serious, whereas the misdiagnosis of a case of influenza is usually no more than unfortunate. In any useful statistical procedure meant to assist in medical diagnosis, such differences should be reflected in the decision-making procedure. That is certainly not the case for the methods that we have discussed thus far. Up to this point, we have used optimality criteria of a more general nature, like the accuracy of an estimation procedure, coverage probabilities for confidence intervals or the probability of Type-I and type-II errors in a testing procedure. The distinction lies in the nature of the optimality criteria: so far we have practiced what is called statistical inference, in which optimality is formulated entirely in terms of the stochastic description of the data. For that reason, it is sometimes said that statistical inference limits itself to those questions that “summarize the data”. By contrast, statistical decision theory formalizes the criteria for optimality by adopting the use of a so-called loss-function to quantify the consequences of wrong decisions in a way prescribed by the context of the statistical problem.

The distinction lies in the nature of the optimality criteria: so far we have practiced what is called statistical inference, in which optimality is formulated entirely in terms of the stochastic description of the data. For that reason, it is sometimes said that statistical inference limits itself to those questions that “summarize the data”. By contrast, statistical decision theory formalizes the criteria for optimality by adopting the use of a so-called loss-function to quantify the consequences of wrong decisions in a way prescribed by the context of the statistical problem. In statistical decision theory the nomenclature is slightly different from that introduced earlier. We consider a system that is in an unknown state $\theta \in \Theta$, where $\Theta$ is called the state-space. The observation $Y$ takes its values in the sample-space $\mathcal{Y}$, a measurable space with $\sigma$-algebra $\mathcal{B}$. The observation is stochastic, its distribution $P_{\theta} : \mathcal{B} \rightarrow [0, 1]$ being dependent on the state $\theta$ of the system. The observation does not reveal the state of the system completely or with certainty. Based on the outcome $Y = y$ of the observation, we take a decision $a \in \mathcal{A}$ (or perform an action $a$, as some prefer to say), where $\mathcal{A}$ is the called the decision-space. For each state $\theta$ of the system there may be an optimal or prescribed decision, but since observation of $Y$ does not give us the state $\theta$ of the system with certainty, the decision is stochastic and may be wrong. The goal of statistical decision theory is to arrive at a rule that decides in the best possible way given only the data $Y$.

The above does not add anything new to the approach we were already following: aside from the names, the concepts introduced here are those used in the usual prob-
lem of statistically estimating $a \in \mathcal{A}$. Decision theory distinguishes itself through its definition of optimality in terms of a so-called loss-function.

**Definition 2.25.** Any lower-bounded function $L : \Theta \times \mathcal{A} \to \mathbb{R}$ may serve as a loss-function. The utility-function is $-L : \Theta \times \mathcal{A} \to \mathbb{R}$.

(Although statisticians talk about loss-functions, people in applied fields often prefer to talk of utility-functions, which is why the above definition is given both in a positive and a negative version.) The interpretation of the loss-function is the following: if a particular decision $a$ is taken while the state of the system is $\theta$, then a loss $L(\theta, a)$ is incurred which can be either positive (loss) or negative (profit). To illustrate, in systems where observation of the state is direct (i.e. $Y = \theta$) and non-stochastic, the optimal decision $a(\theta)$ given the state $\theta$ is the value of $a$ that minimizes the loss $L(\theta, a)$. However, the problem we have set is more complicated because the state $\theta$ is unknown and can not be measured directly. All we have is the observation $Y$.

**Definition 2.26.** Let $\mathcal{A}$ be a measurable space with $\sigma$-algebra $\mathcal{H}$. A measurable $\delta : \mathcal{Y} \to \mathcal{A}$ is called a decision rule.

A decision-rule is an automated procedure to arrive at a decision $\delta(y)$, given that the observation is $Y = y$. We denote the collection of all decision rules under consideration by $\Delta$. Clearly our goal will be to find decision rules in $\Delta$ that “minimize the loss” in an appropriate sense. The above basic ingredients of decision-theoretic problems play a role in both the frequentist and Bayesian analysis. We consider the frequentist approach first and then look at decision theory from a Bayesian perspective.

In frequentist decision theory we assume that $Y \sim P_{\theta_0}$ for some state $\theta_0 \in \Theta$, and we analyze the expectation of the loss.

**Definition 2.27.** The risk-function $R : \Theta \times \Delta \to \mathbb{R}$ is defined as the expected loss under $Y \sim P_{\theta}$ when using $\delta$,

$$ R(\theta, \delta) = \int L(\theta, \delta(Y)) dP_{\theta} \quad (2.37) $$

Of interest to the frequentist is only the expected loss under the true distribution $Y \sim P_{\theta_0}$. But since $\theta_0$ is unknown, we are forced to consider all values of $\theta$, i.e. look at the risk-function $\theta \mapsto R(\theta, \delta)$ for each decision rule $\delta$.

**Definition 2.28.** Let the state-space $\Theta$, states $P_{\theta}$, $(\theta \in \Theta)$, decision space $\mathcal{A}$ and loss $L$ be given. Choose $\delta_1, \delta_2 \in \Delta$. The decision rule $\delta_1$ is $R$-better than $\delta_2$, if

$$ \forall \theta \in \Theta : \quad R(\theta, \delta_1) < R(\theta, \delta_2) \quad (2.38) $$

A decision rule $\delta$ is admissible if there exists no $\delta' \in \Delta$ that is $R$-better than $\delta$ (and inadmissible if such a $\delta'$ does exist).

It is clear that the definition of $R$-better decision-rules is intended to order decision rules: if the risk-function associated with a decision-rule is relatively small, then
that decision rule is preferable. Note, however, that the ordering we impose by definition 2.28 may be partial rather than complete; pairs $\delta_1, \delta_2$ of decision rules may exist such that neither $\delta_1$ nor $\delta_2$ is $R$-better than the other. This is due to the fact that $\delta_1$ may perform better (in the sense that $R(\theta, \delta_1) \leq R(\theta, \delta_2)$) for values of $\theta$ in some $\Theta_1 \subset \Theta$, while $\delta_2$ performs better in $\Theta_2 = \Theta \setminus \Theta_1$, resulting in a situation where (2.38) is true for neither. For that reason, it is important to find a way to compare risks (and thereby decision rules) in a $\theta$-independent way and thus arrive at a complete ordering among decision rules. This motivates the following definition.

**Definition 2.29.** (Minimax decision principle) Let the state-space $\Theta$, states $P_\theta$, ($\theta \in \Theta$), decision space $\mathcal{A}$ and loss $L$ be given. The function

$$\Delta \to \mathbb{R} : \delta \mapsto \sup_{\theta \in \Theta} R(\theta, \delta)$$

is called the minimax risk. Let $\delta_1, \delta_2 \in \Delta$ be given. The decision rule $\delta_1$ is minimax-preferred to $\delta_2$, if

$$\sup_{\theta \in \Theta} R(\theta, \delta_1) < \sup_{\theta \in \Theta} R(\theta, \delta_2).$$

If $\delta^M \in \Delta$ minimizes $\delta \mapsto \sup_{\theta} R(\theta, \delta)$ then $\delta^M$ is called a minimax decision-rule.

One of the foundations of statistical decision theory is the so-called minimax theorem which guarantees the existence of minimax decision rules under very general conditions.

**Theorem 2.4.** Assume that $\Delta$ and $\Theta$ are convex sets. Furthermore, assume that the map $\delta \mapsto R(\theta, \delta)$ is convex on $\Delta$ for every $\theta \in \Theta$ and that the map $\theta \mapsto R(\theta, \delta)$ is concave on $\Theta$ for every $\delta$. Finally, the topology on $\Delta$ is such that $\Delta$ is compact and $\delta \mapsto R(\theta, \delta)$ is continuous for all $\theta$. Then there exists a minimax decision rule $\delta^M$, i.e.

$$\sup_{\theta \in \Theta} R(\theta, \delta^M) = \inf_{\delta \in \Delta} \sup_{\theta \in \Theta} R(\theta, \delta) = \sup_{\theta \in \Theta} \inf_{\delta \in \Delta} R(\theta, \delta).$$

(2.39)

**Proof.** Proof See Strasser (1985) [88], p. 239.

Since many loss-functions used in practice satisfy the convexity requirements, the minimax theorem has broad applicability in statistical decision theory and many other fields, particularly econometrics.

Note that the minimax theorem holds only for convex $\Delta$. In other words, if we want to guarantee the existence of an minimax-optimal decision rule, we are forced to consider convex combinations of decision rules: as an example, suppose we entertain the possibility of using one of two different decision rules $\delta_1, \delta_2 : \mathcal{Y} \to \mathcal{A}$. After the data is realised as $Y = y$, $\delta_1$ and $\delta_2$ give rise to two decisions $\delta_1(y), \delta_2(y)$, which may differ. In that case, we flip a coin to decide which decision to use: the extra stochastic element introduced by the coin-flip has then randomized our decision rule. To formalize this and illustrate the connection with convexity, consider a measurable space $(\Omega, \mathcal{F})$ with data $Y : \Omega \to \mathcal{Y}$ and a decision rule $\delta : \Omega \to \text{co}(\mathcal{A})$. The decision rule $\delta$ is a randomized decision rule whenever $\sigma(\delta)$ is not a subset of $\sigma(Y)$,
i.e. $\delta$ is not just a function of $Y$. The product space $\mathcal{Y} \times \{0,1\}$ endowed with the product $\sigma$-algebra may serve as the measurable space $(\Omega, \mathcal{F})$ with $\delta : \Omega \to \text{co}(\mathcal{A})$ defined by,

$$(y,c) \mapsto \delta(y,c) = c \delta_1(Y) + (1 - c) \delta_2(y),$$

for all $y \in \mathcal{Y}$ and $c \in \{0,1\}$. Perhaps a bit counterintuitively (but certainly in accordance with the fact that minimization over a larger set produces a lower infimum), in some decision problems the minimax risk associated with such randomized decision rules lies strictly below the minimax risks of both non-randomized decision rules.

Example 2.18. (Decision theoretic $L_2$-estimation) The decision-theoretic approach can also be used to formulate estimation problems in a generalized way, if we choose the decision space $\mathcal{A}$ equal to the state-space $\Theta = \mathbb{R}$. Let $Y \sim N(\theta_0,1)$ for some unknown $\theta_0 \in \Theta$. Choose $L : \Theta \times \Theta \to \mathbb{R}$ equal to the quadratic difference

$$L(\theta,a) = (\theta - a)^2,$$

a choice referred to as an $L_2$-loss (or squared-error loss). Consider the decision-space

$$\Delta = \{ \delta_c : \mathcal{Y} \to \mathcal{A} : \delta_c(y) = cy, c \geq 0 \}.$$

Note that $\Delta$ plays the role of a family of estimators for $\theta_0$ here. The risk-function takes the form:

$$R(\theta,\delta_c) = \int L(\theta,\delta_c(Y)) dP_\theta = \int_\mathbb{R} (\theta - cy)^2 dN(\theta,1)(y)$$

$$= \int_\mathbb{R} (\theta - y) + (1 - c)\theta)^2 dN(\theta,1)(y)$$

$$= \int_\mathbb{R} (c^2(y - \theta)^2 + 2c(1 - c)\theta(y - \theta) - (1 - c)^2\theta^2) dN(\theta,1)(y)$$

$$= c^2 + (1 - c)^2\theta^2.$$ 

It follows that $\delta_1$ is $R$-better than all $\delta_c$ for $c > 1$, so that for all $c > 1$, $\delta_1$ is inadmissible. If we had restricted $c$ to be greater than or equal to 1, $\delta_1$ would have been admissible. However, since $c$ may lie in $[0,1)$ as well, admissibility in the uniform sense of (2.38) does not apply to any $\delta_c$. To see this, note that $R(\theta,\delta_1) = 1$ for all $\theta$, whereas for $c < 1$ and some $\theta > c/(1 - c)$, $R(\theta,\delta_c) < 1 < R(\theta,\delta_1)$. Therefore, there is no admissible decision rule in $\Delta$.

The minimax criterion does give rise to a preference. However, in order to guarantee its existence, we need to bound (or rather, compactify) the parameter space: let $M > 0$ be given and assume that $\Theta = [-M,M]$. The minimax risk for $\delta_c$ is given by

$$\sup_{\theta \in \Theta} R(\theta,\delta_c) = c^2 + (1 - c)^2M^2.$$
which is minimal iff \( c = M^2/(1 + M^2) \), i.e. the (unique) minimax decision rule for this problem (or, since we are using decision theory to estimate a parameter in this case, the minimax estimator in \( \Delta \) with respect to \( L_2 \)-loss) is therefore,

\[
\delta^M(Y) = \frac{M^2}{1 + M^2} Y.
\]

Note that if we let \( M \to \infty \), this estimator for \( \theta \) converges to the MLE for said problem.

As demonstrated in the above example, uniform admissibility of a decision rule (c.f. (2.38)) is hard to achieve, but in many such cases a minimax decision rule does exist. One important remark concerning the use the minimax decision principle remains: considering (2.39), we see that the minimax principle chooses the decision rule that minimizes the maximum of the risk \( R(\cdot, \delta) \) over \( \Theta \). As such, the minimax criterion takes into account only the worst-case scenario and prefers decision rules that perform well under those conditions. In practical problems, that means that the minimax principle tends to take a rather pessimistic perspective on decision problems.

### 2.5.2 Bayesian decision theory

Bayesian decision theory presents a more balanced perspective because instead of maximizing the risk function over \( \Theta \), the Bayesian has the prior to integrate over \( \Theta \). Optimization of the resulting integral takes into account more than just the worst case, so that the resulting decision rule is based on a less pessimistic perspective than the minimax decision rule.

**Definition 2.30.** Let the state-space \( \Theta \), states \( P_\theta, (\theta \in \Theta) \), decision space \( \mathcal{A} \) and loss \( L \) be given. In addition, assume that \( \Theta \) is a measurable space with \( \sigma \)-algebra \( \mathcal{G} \) and prior \( \Pi : \mathcal{G} \to \mathbb{R} \). The function

\[
r(\Pi, \delta) = \int_\Theta R(\theta, \delta) d\Pi(\theta),
\]

is called the *Bayesian risk function*. Let \( \delta_1, \delta_2 \in \Delta \) be given. The decision rule \( \delta_1 \) is Bayes-preferred to \( \delta_2 \), if

\[
r(\Pi, \delta_1) < r(\Pi, \delta_2).
\]

If \( \delta^{\Pi} \in \Delta \) minimizes \( \delta \mapsto r(\Pi, \delta) \), i.e.

\[
r(\Pi, \delta^{\Pi}) = \inf_{\delta \in \Delta} r(\Pi, \delta).
\]

then \( \delta^{\Pi} \) is called a *Bayes rule*. The quantity \( r(\Pi, \delta^{\Pi}) \) is called the *Bayes risk*.

**Lemma 2.7.** Let \( Y \in \mathcal{Y} \) denote data in a decision theoretic problem with state space \( \Theta \), decision space \( \mathcal{A} \) and loss \( L : \Theta \times \mathcal{A} \to \mathbb{R} \). For any prior \( \Pi \) and all decision
rules $\delta : \mathcal{Y} \to \mathcal{A}$, 

$$r(\Pi, \delta) \leq \sup_{\theta \in \Theta} R(\theta, \delta),$$

i.e. the Bayesian risk is always upper bounded by the minimax risk.

The proof of this lemma follows from the fact that the minimax risk is an upper bound for the integrand in the Bayesian risk function.

**Example 2.19.** (continuation of example 2.18) Let $\Theta = \mathbb{R}$ and $Y \sim N(\theta_0, 1)$ for some unknown $\theta_0 \in \Theta$. Choose the loss-function $L : \Theta \times \mathcal{A} \to \mathbb{R}$ and the decision space $\Delta$ as in example 2.18. We choose a prior $\Pi = N(0, \tau^2)$ (for some $\tau > 0$) on $\Theta$. Then the Bayesian risk function is given by:

$$r(\Pi, \delta) = \int_{\Theta} R(\theta, \delta) d\Pi(\theta) = \int_{\mathbb{R}} (c^2 + (1-c)^2 \theta^2) d\mathcal{N}(0, \tau^2)(\theta),$$

which is minimal iff $c = \frac{\tau^2}{1 + \tau^2}$. The (unique) Bayes rule for this problem and corresponding Bayes risk are therefore,

$$\delta^\Pi(Y) = \frac{\tau^2}{1 + \tau^2} Y, \quad r(\Pi, \delta^\Pi) = \frac{\tau^2}{1 + \tau^2}.$$

In the Bayesian case, there is no need for a compact parameter space $\Theta$, since we do not maximize but integrate over $\Theta$.

In the above example, we could find the Bayes rule by straightforward optimization of the Bayesian risk function, because the class $\Delta$ was rather restricted. If we extend the class $\Delta$ to contain all non-randomized decision rules, the problem of finding the Bayes rule seems to be far more complicated at first glance. However, as we shall see in theorem 2.1, the following definition turns out to be the solution to this question.

**Definition 2.31.** (The conditional Bayes decision principle) Let the state-space $\Theta$, states $P_\theta$, $(\theta \in \Theta)$, decision space $\mathcal{A}$ and loss $L$ be given. In addition, assume that $\Theta$ is a measurable space with $\sigma$-algebra $\mathcal{G}$ and prior $\Pi : \mathcal{G} \to \mathbb{R}$. We define the decision rule $\delta^* : \mathcal{Y} \to \mathcal{A}$ to be such that for all $y \in \mathcal{Y}$,

$$\int_{\Theta} L(\theta, \delta^*(y)) d\Pi(\theta|Y = y) = \inf_{a \in \mathcal{A}} \int_{\Theta} L(\theta, a) d\Pi(\theta|Y = y), \quad (2.42)$$

i.e. point-wise for every $y$, the decision rule $\delta^*(y)$ minimizes the posterior expected loss.

The above defines the decision rule $\delta^*$ implicitly as a point-wise minimizer, which raises the usual questions concerning existence and uniqueness, of which little can be said in any generality. However, if the existence of $\delta^*$ is established, it is optimal.

**Theorem 2.5.** Let the state-space $\Theta$, states $P_\theta$, $(\theta \in \Theta)$, decision space $\mathcal{A}$ and loss $L$ be given. In addition, assume that $\Theta$ is a measurable space with $\sigma$-algebra $\mathcal{G}$ and
prior \( \Pi : \mathcal{G} \to \mathbb{R} \). Assume that there exists a \( \sigma \)-finite measure \( \mu : \mathcal{B} \to \mathbb{R} \) such that \( P_\theta \ll \mu \) for all \( \theta \in \Theta \). If the decision rule \( \delta^* : \mathcal{Y} \to \mathcal{A} \) is well-defined, then \( \delta^* \) is a Bayes rule.

**Proof.** Denote the class of all decision rules for this problem by \( \Delta \) throughout the proof. We start by rewriting the Bayesian risk function for a decision rule \( \delta : \mathcal{Y} \to \mathcal{A} \):

\[
\begin{align*}
    r(\Pi, \delta) &= \int_\Theta R(\theta, \delta) d\Pi(\theta) = \int_\Theta \int_\mathcal{Y} L(\theta, \delta(y)) dP_\theta(y) d\Pi(\theta) \\
    &= \int_\mathcal{Y} \left( \int_\Theta p_\theta(y) d\Pi(\theta) \right) \int_\Theta L(\theta, \delta(y)) d\Pi(\theta | Y = y) d\mu(y) \\
    &= \int_\mathcal{Y} \left( \int_\Theta p_\theta(y) d\Pi(\theta) \right) \int_\Theta L(\theta, \delta(y)) d\Pi(\theta | Y = y) d\mu(y).
\end{align*}
\]

where we use definitions (2.40) and (2.37), the Radon-Nikodym theorem (see theorem A.7), Fubini’s theorem (see theorem A.6) and the definition of the posterior, c.f. (2.12). Using the prior predictive distribution (2.3), we rewrite the Bayesian risk function further:

\[
\begin{align*}
    r(\Pi, \delta) &= \int_\mathcal{Y} \int_\Theta L(\theta, \delta(y)) d\Pi(\theta | Y = y) dP_\Pi(y). \\
\end{align*}
\]  

(2.43)

By assumption, the conditional Bayes decision rule \( \delta^* \) exists. Since \( \delta^* \) satisfies (2.42) point-wise for all \( y \in \mathcal{Y} \), we have

\[
\int_\Theta L(\theta, \delta^*(y)) d\Pi(\theta | Y = y) = \inf_{\delta \in \Delta} \int_\Theta L(\theta, \delta(y)) d\Pi(\theta | Y = y).
\]

Substituting this in (2.43), we obtain

\[
\begin{align*}
    r(\Pi, \delta^*) &= \int_\mathcal{Y} \inf_{\delta \in \Delta} \int_\Theta L(\theta, \delta(y)) d\Pi(\theta | Y = y) dP_\Pi(y) \\
    &\leq \inf_{\delta \in \Delta} \int_\mathcal{Y} \int_\Theta L(\theta, \delta(y)) d\Pi(\theta | Y = y) dP_\Pi(y) \\
    &= \inf_{\delta \in \Delta} r(\Pi, \delta).
\end{align*}
\]

which proves that \( \delta^* \) is a Bayes rule.

To conclude, it is noted that randomization of the decision is not needed when optimizing with respect to the Bayes risk. The conditional Bayes decision rule is non-randomized and optimal.
2.5.3 Frequentist versus Bayesian classification

Many decision-theoretic questions take the form of a classification problem: under consideration is a population $\Omega$ of objects that each belong to one of a finite number of classes $\mathcal{A} = \{1, 2, \ldots, L\}$. The class $K$ of the object is the unknown quantity of interest. Observing a vector $Y$ of features of the object, the goal is to classify the object, i.e. estimate which class it belongs to. We formalize the problem in decision-theoretic terms: the population is a probability space $(\Omega, \mathcal{F}, P)$; both the feature vector and the class of the object are random variables, $Y : \Omega \to \mathcal{Y}$ and $K : \Omega \to \mathcal{A}$ respectively. The state-space in a classification problem equals the decision space $\mathcal{A}$: the class can be viewed as a “state” in the sense that the distribution $P(Y|K=k)$ of $Y$ given the class $K=k$ depends on $k$. Based on the feature vector $Y$, we decide to classify in class $\delta(Y)$, i.e. the decision rule (or classifier, as it is usually referred to in the context of classification problems) maps features to classes by means of a map $\delta : \mathcal{Y} \to \mathcal{A}$. A classifier $\delta$ can be viewed equivalently as a finite partition of the feature-space $\mathcal{Y}$: for every $k \in \mathcal{A}$, we define

$$\mathcal{Y}_k = \{ y \in \mathcal{Y} : \delta(y) = k \}$$

and note that if $k \neq l$, then $\mathcal{Y}_k \cap \mathcal{Y}_l = \emptyset$ and $\mathcal{Y}_1 \cup \mathcal{Y}_2 \cup \ldots \cup \mathcal{Y}_L = \mathcal{Y}$. The partition of the feature space is such that if $Y = y \in \mathcal{Y}_k$ for certain $k \in \mathcal{A}$, then we classify the object in class $k$.

Depending on the context of the classification problem, a loss-function $L : \mathcal{A} \times \mathcal{A} \to \mathbb{R}$ is defined (see the examples in the introduction to this section, e.g. the example on medical diagnosis). Without context, the loss function in a classification problem can be chosen as follows

$$L(k, l) = 1_{k \neq l},$$

i.e. we incur a loss equal to one for each misclassification. Using the minimax decision principle, we look for a classifier $\delta^M : \mathcal{Y} \to \mathcal{A}$ that minimizes

$$\delta \mapsto \sup_{k \in \mathcal{A}} \int_{\mathcal{Y}} L(k, \delta(y)) \, dP(y|K=k) = \sup_{k \in \mathcal{A}} P(\delta(Y) \neq k \mid K = k),$$

i.e. the minimax decision principle prescribes that we minimize the probability of misclassification uniformly over all classes.

In a Bayesian context, we need a prior on the state-space, which equals $\mathcal{A}$ in classification problems. Note that if known (or estimable), the marginal probability distribution for $K$ is to be used as the prior for the state $k$, in accordance with definition 2.2. In practical problems, frequencies of occurrence for the classes $\{1, \ldots, L\}$ in $\Omega$ are often available or easily estimable; in the absence of information on the marginal distribution of $K$ equal prior weights can be assigned. Here, we assume that the probabilities $P(K=k)$ are known and use them to define the prior density with respect to the counting measure on the (finite) space $\mathcal{A}$:
2.5 Decision theory and classification

\[ \pi(k) = P(K = k). \]

The Bayes rule \( \delta^* : \mathcal{Y} \rightarrow \mathcal{A} \) for this classification problem is defined as the minimizer of

\[ \delta \mapsto \sum_{k \in \mathcal{A}} L(k, \delta(y)) d\Pi(k|y) = \sum_{k=1}^l \Pi(\delta(y) \neq K | Y = y) \]

for every \( y \in \mathcal{Y} \). According to theorem 2.5, the classifier \( \delta^* \) minimizes the Bayes risk, which in this situation is given by:

\[
\begin{align*}
  r(\Pi, \delta) &= \sum_{k \in \mathcal{A}} R(k, \delta) \pi(k) \\
                 &= \sum_{k \in \mathcal{A}} \int_{\mathcal{Y}} L(k, \delta(y)) dP(y|K = k) \pi(k) \\
                 &= \sum_{k \in \mathcal{A}} P(k \neq \delta(y) | K = k) P(K = k) = P(K \neq \delta(Y)).
\end{align*}
\]

Summarizing, the Bayes rule \( \delta^* \) minimizes the overall probability of misclassification, i.e. without referring to the class of the object. (Compare this with the minimax classifier.)

Readers interested in the statistics of classification and its applications are encouraged to read B. Ripley’s “Pattern recognition and neural networks” (1996) [80].

To close the chapter, the following remark is in order: when we started our comparison of frequentist and Bayesian methods, we highlighted the conflict in philosophy. However, now that we have seen some of the differences in more detail by considering estimation, confidence sets, testing and decision theory in both schools, we can be far more specific. Statistical problems can be solved in both schools; whether one chooses for a Bayesian or frequentist solution is usually not determined by deeply felt belief in either philosophy but by much more practical considerations. Perhaps the classification example of this subsection illustrates this point most clearly: if one is concerned about correct classification for objects in the most difficult class, one should opt for the minimax decision rule. If, on the other hand, one wants to minimize the overall misclassification probability (disregarding misclassification per class), one should choose to adopt the conditional Bayes decision rule. In other words, depending on the risk to be minimized (minimax risk and Bayes risk are different!) one arrives at different classifiers.

An argument in favour of Bayesian methods is the control that the statistician can gain over a statistical procedure by choice of a suitable prior. Particularly, a statistical procedure may benefit from a well-chosen form of bias, expressed through the prior. Examples include the subjective bias intended in example 1.8. To give another example of this nature, Bayesian methods are popular in forensic statistics because the freedom to choose a prior leaves room to incorporate background information and common-sense. However, from a more technical point of view, bias may be required for regularization purposes (like a penalty, in frequentist terms, see remark 2.6). Prior bias may even be guided in a data-dependent way, e.g. when we employ empirical Bayesian methods (see section 3.5), to optimize the procedure.
Another reason to use one or the other may be computational advantages or useful theoretical results that exist for one school but have no analog in the other. Philosophical preference should not play a role in the choice for a statistical procedure, practicality should (and usually does).

2.6 Exercises

2.1. CALIBRATION
A physicist prepares for measurement of a physical quantity \( Z \) in his laboratory. To that end, he installs a measurement apparatus that will give him an outcome of the form \( Y = Z + e \) where \( e \) is a measurement error due to the inaccuracy of the apparatus, assumed to be stochastically independent of \( Z \). Note that if the expectation of \( e \) equals zero, long-run sample averages converge to the expectation of \( Z \); if \( \text{Pr} \neq 0 \), on the other hand, averaging does not cancel out the resulting bias. The manufacturer of the apparatus says that \( e \) is normally distributed with known variance \( \sigma^2 > 0 \). The mean \( \theta \) of this normal distribution depends on the way the apparatus is installed and thus requires calibration. The following questions pertain to the calibration procedure.

The physicist decides to conduct the following steps to calibrate his measurement. First, he makes certain that the apparatus receives no input signal, \( Z = 0 \). Then he repeats measurement of \( Y \), generating an i.i.d. sample of size \( n \), which amounts to an i.i.d. sample from the distribution of \( e \) used to estimate the unknown mean \( \theta \). The physicist expects that \( E(e) \) lies close to zero.

a. Explain why, from a subjectivist point of view, the choice \( \theta \sim N(0, \tau^2) \) forms a suitable prior in this situation. Explain the role of the parameter \( \tau^2 > 0 \).

b. With the choice of prior as in part a., calculate the posterior density for \( \theta \).

c. Interpret the influence of \( \tau^2 \) on the posterior, taking into account your answer under part a. (Hint: take limits \( \tau^2 \downarrow 0 \) and \( \tau^2 \uparrow \infty \) in the expression you have found under b.)

d. What is the influence of the sample size \( n \)? Show that the particular choice of the constant \( \tau^2 \) becomes irrelevant in the large-sample limit \( n \to \infty \).

2.2. Let \( X_1, \ldots, X_n \) be an i.i.d. sample from the uniform distribution \( U[0, \theta] \), with unknown parameter \( \theta \in \Theta = (1, \infty) \). As a prior for \( \theta \), choose the Pareto distribution with exponent \( \alpha > 0 \). Calculate the posterior density for \( \theta \) with respect to the Lebesgue measure on \( [0, \infty) \).

2.3. Let \( X_1, \ldots, X_n \) be an i.i.d. sample from the Poisson distribution \( \text{Poisson}(\lambda) \), with unknown parameter \( \lambda > 0 \). As a prior for \( \lambda \), let \( \lambda \sim \Gamma(2, 1) \). Calculate the posterior density for \( \lambda \) with respect to the Lebesgue measure on \( [0, \infty) \).

2.4. Let \( X_1, \ldots, X_n \) be an i.i.d. sample from a binomial distribution \( \text{Bin}(k, \theta) \), with known \( k \geq 1 \) and unknown \( \theta \in \Theta = [0, 1] \). As a prior for \( \theta \), use a beta distribution, \( \theta \sim \beta(2, 2) \). Calculate the posterior density for \( \theta \) with respect to the Lebesgue measure on \( [0, 1] \).
2.5. Let \(X_1, \ldots, X_n\) be an i.i.d. sample from a normal distribution \(N(0, \sigma^2)\), with unknown \(\sigma^2 > 0\). We define the prior for the variance \(\sigma^2\) implicitly, by stating that the inverse \(1/\sigma^2\) is distributed according to a \(\Gamma(\alpha, \beta)\) distribution. Calculate the posterior density for \(\sigma^2\) with respect to the Lebesgue measure on \([0, \infty)\).

2.6. Let \((\mathcal{P}, \mathcal{F}, \Pi)\) be a model with prior for i.i.d. \(X_1, \ldots, X_n\) taking values in a sample space \((\mathcal{X}, \mathcal{B})\). Suppose that the model is dominated by a \(\sigma\)-finite measure \(\mu\) on \((\mathcal{X}, \mathcal{B})\) and that the prior is dominated by a \(\sigma\)-finite measure \(\nu\) on \((\mathcal{P}, \mathcal{G})\). Show that if \(\mu'\) is another \(\sigma\)-finite measure on \((\mathcal{X}, \mathcal{B})\), such that \(\mathcal{P} \ll \mu' \ll \mu\), and \(\nu'\) is another \(\sigma\)-finite measure on \((\mathcal{P}, \mathcal{G})\), such that \(\Pi \ll \nu' \ll \nu\), then the MAP estimator \(\hat{\theta}_2\) does not change with \(\mu'\) (compare with exercise 1.1), but \(\hat{\theta}_2\) does change with \(\nu'\).

2.7. In the model of exercise 2.2, calculate the maximum-likelihood estimator, the posterior mean and the maximum-a-posteriori estimator.

2.8. In the model of exercise 2.3, calculate the maximum-likelihood estimator, the posterior mean and the maximum-a-posteriori estimator.

2.9. In the model of exercise 2.4, calculate the maximum-likelihood estimator, the posterior mean and the maximum-a-posteriori estimator.

2.10. In the model of exercise 2.5, calculate the maximum-likelihood estimator, the posterior mean and the maximum-a-posteriori estimator.

2.11. Consider the following questions in the context of exercise 2.3, after exercise 2.8.
   a. Let \(n \to \infty\) both in the MLE and MAP estimator and conclude that the difference vanishes in the limit, \(P_0\)-almost-surely.
   b. Following remark 2.6, explain the difference between ML and MAP estimators exclusively in terms of the prior.
   c. Consider and discuss the choice of prior \(\lambda \sim \Gamma(2, 1)\) twice, once in a qualitative, subjectivist Bayesian fashion, and once following the frequentist interpretation of the log-prior-density.

2.12. Let \(Y \sim P_0\) denote the data and \(\mathcal{P}\) a model with metric \(d\). Suppose that \(\mathcal{P}\) is endowed with a prior defined on the Borel \(\sigma\)-algebra induced by the metric topology. Assume that \(P_0 \ll P^\Pi\) and that \(\mathcal{P}\) is compact. The following questions pertain to the small-ball estimators defined in definition 2.11 and remark 2.5. We assume that the posterior distribution is such that for all \(\varepsilon > 0\) and all \(P \in \mathcal{P}\), the (topological) boundary of the ball \(B_d(P, \varepsilon)\) receives mass equal to zero: \(\Pi(\partial B_d(P, \varepsilon)|Y) = 0, P_0\)-almost surely.
   a. Show that, for any \(p \in (1/2, 1)\) and large enough \(\varepsilon > 0\), the small-ball estimator \(\hat{P}\) of exists, \(P_0\)-almost-surely.
b. Show that for any two measurable model subsets $A, B \subset \mathcal{P}$,

$$| \Pi(A|Y) - \Pi(B|Y) | \leq \Pi(A \cup B|Y) - \Pi(A \cap B|Y),$$

$\mathcal{P}_0$-almost-surely.

c. Show that for every $\varepsilon > 0$, the map $P \mapsto \Pi(B_d(P,\varepsilon)|Y)$ is continuous, $\mathcal{P}_0$-almost-surely.

d. Show that for every $\varepsilon > 0$, the small-ball estimator of definition 2.11 exists.

e. Let some $p \in (1/2, 1)$ be given. Suppose that $\varepsilon > 0$ denotes some radius for which there exists a ball $B_d(P,\varepsilon) \subset \mathcal{P}$ of posterior probability greater than or equal to $p$. Show that, if both $\hat{P}_1$ and $\hat{P}_2$ are centre points of such balls, then $d(\hat{P}_1, \hat{P}_2) < 2\varepsilon$, $\mathcal{P}_0$-almost-surely.

2.13. Let $Y_n = (X_1, \ldots, X_n)$ be an i.i.d. sample from the normal distribution $N(\mu, \sigma^2)$ for certain $\mu \in \mathbb{R}$, $\sigma^2 > 0$. Show that the sample average is distributed according to the normal distribution,

$$\mathbb{P}_n X \sim N(\mu, \sigma_n^2),$$

with variance $\sigma_n^2 = \sigma^2/n$.

2.14. Let $Y$ be normally distributed with known variance $\sigma^2 > 0$ and unknown location $\theta$. As a prior for $\theta$, choose $\Pi = N(0, \tau^2)$. Let $\alpha \in (0, 1)$ be given. Using the posterior density with respect to the Lebesgue measure, express the level-$\alpha$ HPD-credible set in terms of $Y$, $\sigma^2$, $\tau^2$ and quantiles of the standard normal distribution. Consider the limit $\tau^2 \to \infty$ and compare with level-$\alpha$ confidence intervals centred on the ML estimate for $\theta$.

2.15. Let $Y \sim \text{Bin}(n,p)$ for known $n \geq 1$ and unknown $p \in (0,1)$. As a prior for $p$, choose $\Pi = \text{Beta}(\frac{1}{2}, \frac{1}{2})$. Calculate the posterior distribution for the parameter $p$. Using the Lebesgue measure on $(0,1)$ to define the posterior density, give a level-$\alpha$ (non-HPD!) credible interval for $p$ in terms of $Y$, $n$ and the quantiles of beta-distributions.

2.16. Let $\Theta$ be a subset of $\mathbb{R}$ and let $\Theta \to \mathcal{P} : \theta \mapsto \mathcal{P}_\theta$ describe an identifiable parametrization of the model \( \mathcal{P} \) for an i.i.d. sample $X_1, \ldots, X_n$, and assume that there exists a $\theta_0 \in \Theta$ such that $\mathcal{P}_{\theta_0}$ is the marginal distribution for each of the $X_i$. Let $\theta$ and $\theta'$ with $\theta' > \theta$ from $\Theta$ be given and consider the hypotheses,

$$H_0 : \quad \theta_0 = \theta, \quad H_1 : \theta_0 = \theta',$$

Given a significance level $\alpha \in (0,1)$, write down the Neyman-Pearson test for $H_0$ versus $H_1$ (see lemma 2.4), in each of the following cases,

a. for all $\theta \in [0,1]$, $P_\theta = \text{Bernoulli}(\theta)$;

b. for all $\theta \in (0, \infty)$, $P_\theta = \text{Poisson}(\theta)$;

c. for all $\theta \in [0,1]$, $P_\theta = \text{Bin}(\theta, k)$ for some known integer $k \geq 1$.

2.17. Consider a dominated model $\mathcal{P} = \{ P_\theta : \theta \in \Theta \}$ for data $Y$, where $\Theta \subset \mathbb{R}$ is an interval. For certain $\theta_0 \in \Theta$, consider the simple null-hypothesis and alternative:
2.6 Exercises

\[ H_0 : \, \theta = \theta_0, \quad H_1 : \, \theta \neq \theta_0. \]

Show that if the prior \( \Pi \) is absolutely continuous with respect to the Lebesgue measure on \( \Theta \), then the posterior odds ratio in favour of the hypothesis \( H_0 \) equals zero.

[Remark: conclude that calculation of posterior odds ratios makes sense only if both hypotheses receive non-zero prior mass. Otherwise, the statistical question we ask is rendered invalid ex ante by our beliefs concerning \( \theta \), as expressed through the choice of the prior. (See example 2.3.)]

2.18. Let \( X_1, \ldots, X_n \) be an i.i.d. sample from a binomial distribution \( \text{Bin}(\theta, k) \), for some known integer \( k \geq 1 \) and an unknown parameter \( \theta \in \Theta = [0, 1] \). Let the prior \( \Pi \) for \( \theta \) be a Beta distribution \( B(\alpha, \beta) \), with certain parameters \( \alpha, \beta > 1 \).

a. Calculate the posterior distribution for \( \theta \).

b. Write down the equations that determine the two end-points of the HPD credible interval (based on the density of the posterior relative to Lebesgue measure on \( \Theta \)), for given credible level \( \delta \in (0, 1) \).

Consider the hypotheses,

\[ H_0 : \, \theta \leq \frac{1}{2}, \quad H_1 : \, \theta > \frac{1}{2}. \]

c. Give the prior odds, posterior odds and Bayes factor for the hypotheses \( H_0 \) and \( H_1 \).

2.19. PRISONER’S DILEMMA

Two men have been arrested on the suspicion of burglary and are held in separate cells awaiting interrogation. The prisoners have been told that burglary carries a maximum sentence of \( x \) years. However, if they confess, their prison terms are reduced to \( y \) years (where \( 0 < y < x \)). If one of them confesses and the other does not, the first receives a sentence of \( y \) years while the other is sentenced to \( x \) years.

Guilty of the crime he is accused of, our prisoner contemplates whether to confess to receive a lower sentence, or to deny involvement in the hope of escaping justice altogether. He cannot confess without implicating the other prisoner. If he keeps his mouth shut and so does his partner in crime, they will both walk away free. If he keeps his mouth shut but his partner talks, he gets the maximum sentence. If he talks, he will always receive a sentence of \( y \) years and the other prisoner receives \( y \) or \( x \) years depending on whether he confessed or not himself. To talk or not to talk, that is the question.

There is no data in this problem, so we set \( \theta \) equal to 1 or 0, depending on whether the other prisoner talks or not. Our prisoner can decide to talk \( (t = 1) \) or not \( (t = 0) \). The loss function \( L(\theta, t) \) equals the prison term for our prisoner. In the absence of data, risk and loss are equal.

a. Calculate the minimax risk for both \( t = 0 \) and \( t = 1 \). Argue that the minimax-optimal decision for our prisoner is to confess.

As argued in section 2.5, the minimax decision can be overly pessimistic. In the above, it assumes that the other prisoner will talk and chooses \( t \) accordingly.
The Bayesian perspective balances matters depending on the chance that the other prisoner will confess when interrogated. This chance finds its way into the formalism as a prior for the trustworthiness of the other prisoner. Let $p \in [0, 1]$ be the probability that the other prisoner confesses, i.e. $\Pi(\theta = 1) = p$ and $\Pi(\theta = 0) = 1 - p$.

b. Calculate the Bayes risks for $t = 0$ and $t = 1$ in terms of $x$, $y$ and $p$. Argue that the Bayes decision rule for our prisoner is as follows: if $y/x > p$ then our prisoner does not confess, if $y/x < p$, the prisoner confesses. If $y/x = p$, the Bayes decision criterion does not have a preference.

So, depending on the degree to which our prisoner trusts his associate and the ratio of prison terms, the Bayesian draws his conclusion. The latter is certainly more sophisticated and perhaps more realistic, but it requires that our prisoner quantifies his trust in his partner in the form of a prior $Bernoulli(p)$ distribution.
Chapter 3
Choice of the prior

Bayesian procedures have been the object of much criticism, often focusing on the choice of the prior as an undesirable source of ambiguity. The answer of the subjectivist that the prior represents the “belief” of the statistician or “expert knowledge” pertaining to the measurement elevates this ambiguity to a matter of principle, thus setting the stage for a heated debate between “pure” Bayesians and “pure” frequentists concerning the philosophical merits of either school within statistics. As said, the issue is complicated further by the fact that the Bayesian procedure does not refer to the “true” distribution $P_0$ for the observation (see section 2.1), providing another point of fundamental philosophical disagreement for the fanatically pure to lock horns over. Leaving the philosophical argumentation to others, we shall try to discuss the choice of a prior at a more conventional, practical level.

In this chapter, we look at the choice of the prior from various points of view: in section 3.1, we consider the priors that emphasize the subjectivist’s prior “belief”. In section 3.2 we construct priors with the express purpose not to emphasize any part of the model, as advocated by objectivist Bayesians. Because it is often desirable (and always computationally advantageous) to have closed-form expressions for posterior distributions, so-called conjugacy of families of distributions over the model is considered in section 3.3. Hierarchical prior construction and Bayesian modelling are the subject of section 3.4 and the practice of choosing priors by frequentist means (commonly known as empirical Bayes) forms the subject of section 3.5. Special attention goes to the Dirichlet distributions of section 3.6 because they describe distributions on spaces of probability measures (rather than their parametrizing spaces). As will become clear in the course of the chapter, the choice of a “good” prior is highly dependent on the model under consideration, as well as on the purpose of the analysis.

Since the Bayesian school has taken up an interest in non-parametric statistics only relatively recently, most (if not all) of the material presented in the first sections of this chapter applies only to parametric models. To find a suitable prior for a non-parametric model can be surprisingly complicated. Not only does the formulation involve topological aspects that do not play a role in parametric models, but also the properties of the posterior may be surprisingly different from those encountered
Choice of the prior

3.1 Subjective priors

As was explained in chapters 1 and 2, all statistical procedures require the statistician to make certain choices, e.g. for model and method of inference. The subjectivist chooses the model as a collection of stochastic explanations of the data that he finds “reasonable”, based on criteria no different from those frequentists and objectivist Bayesians would use.

3.1.1 Motivation for the subjectivist approach

Bayesians then proceed to choose a prior, in such a manner that the support of this prior is not essentially smaller than the model itself. But even when the support of the prior is fixed, there is a large collection of possible priors left to be considered, each leading to a different posterior distribution. The objectivist Bayesian will choose from those possibilities a prior that is “homogeneous” (in a suitable sense), in the hope of achieving unbiased inference. The subjectivist, however, chooses his prior such as to emphasize parts of the model that he believes in stronger than others, thereby introducing a bias in his inferential procedure explicitly. Such a prior is called a subjective prior, or informative prior. The reason for this approach is best explained by examples like 1.8 which demonstrate that intuitive statistical reasoning is not free of bias either.

Subjectivity finds its mathematical expression when high prior “belief” is translated into “relatively large” amounts of assigned prior mass to certain regions of the model. However, there is no clear rule directing the exact fashion in which prior mass is to be distributed. From a mathematical perspective this is a rather serious shortcoming, because it leaves us without a precise definition of the subjectivist approach. Often the subjectivist will have a reasonably precise idea about his “beliefs” at the roughest level (e.g. concerning partitions of the model into a few subsets) but none at more detailed levels. When the parameter space $\Theta$ is unbounded this lack of detail becomes acute, given that the tail of the prior is hard to fix by subjective reasoning, yet highly influential for the inferential conclusions based on it. In practice, a subjectivist will often choose his prior without mathematical precision. He considers the problem, interprets the parameters in his model and chooses a prior to reflect all the (background) information at his disposition, ultimately filling in remaining details in an ad-hoc manner. It is worthwhile to mention that studies have been conducted focused on the ability of people to make a realistic guess at a probability distribution: they have shown that without specific training or practice, people
3.1 Subjective priors

Subjective priors tend to be overconfident in their assessment, assigning too much mass to possibilities they deem most likely and too little to others [1]. A tentative conclusion might be, that people tend to formulate their “beliefs” on a deterministic basis and deviate from that point of view only slightly (or, too little) when asked to give a realistic probabilistic perspective. (For more concerning the intricacies of choosing subjective prior distributions, see Berger (1985) [8].)

Remark 3.1. For this reason, it is imperative that a subjectivist prior is always reported alongside inferential conclusions based upon it! Reporting methods is important in any statistical setting, but if chosen methods lead to express bias, explanation is even more important. Indeed, not only the prior but also the reasoning leading to its choice should be reported, because in a subjectivist setting, the motivation for the choice of a certain prior (and not any other) is part of the analysis rather than an external consideration.

3.1.2 Methods for the construction of subjective priors

If the model \( \Theta \) is one-dimensional and the parameter \( \theta \) has a clear interpretation, it is often not exceedingly difficult to find a reasonable prior \( \Pi \) expressing the subjectivist’s “belief” concerning the value of \( \theta \).

Example 3.1. If one measures the speed of light in vacuo \( c \) (a physical constant, approximately equal to 299792458 m/s), the experiment will be subject to random perturbations outside the control of the experimenter. For example, imperfection of the vacuum in the experimental equipment, small errors in timing devices, electronic noise and countless other factors may influence the resulting measured speed \( Y \). We model the perturbations collectively as a normally distributed error \( e \sim N(0, \sigma^2) \) where \( \sigma \) is known as a characteristic of the experimental setup. The measured speed is modelled as \( Y = c + e \), i.e. the model \( \mathcal{P} = \{N(c, \sigma^2) : c > 0\} \) is used to infer on \( c \). Based on experiments in the past (most famous is the Michelson-Morley experiment (1887)), the experimenter knows that \( c \) has a value close to \( 3 \cdot 10^8 \) m/s, so he chooses his prior to reflect this: a normal distribution located at 300000000 m/s with a standard deviation of (say) 1000000 m/s will do. The latter choice is arbitrary, just like the choice for a normal location model over other families.

The situation changes when the parameter has a higher dimension, \( \Theta \subset \mathbb{R}^d \): first of all, interpretability of each of the \( d \) components of \( \theta = (\theta_1, \theta_2, \ldots, \theta_d) \) can be far from straightforward, so that concepts like prior “belief” or “expert knowledge” become inadequate guidelines for the choice of a prior. Additionally, the choice for a prior in higher-dimensional models also involves choices concerning the dependence structure between parameters!

Remark 3.2. Often, subjectivist inference employs exceedingly simple, parametric models for the sake of interpretability of the parameter (and to be able to choose a prior accordingly). Most frequentists would object to such choices for their obvious
lack of realism, since they view the data as being generated by a “true, underlying
distribution”, usually assumed to be an element of the model. However, the sub-
jectivist philosophy does not involve the ambition to be strictly realistic and calls
for interpretability instead; to the subjectivist, inference is a personal rather than a
universal matter. As such, the preference for simple parametric models is a matter
of subjective interpretation rather than an assumption concerning reality or realistic
distributions for the data.

When confronted with the question which subjective prior to use on a higher-
dimensional model, it is often of help to define the prior in several steps based on
a choice for the dependence structure between various components of the parameter.
Suppose that the subjectivist can formulate a reasonable distribution for the first
component \( \theta_1 \), if he has some definite values for all other components \( \theta_2, \ldots, \theta_d \).
Then this distribution is \( \Pi_{\theta_1|\theta_2, \ldots, \theta_d} \), the subjectivist prior distribution of \( \theta_1 \), conditional
on \( \theta_2, \ldots, \theta_d \). Next suppose that a reasonable subjective prior for the second
component may be found, conditional on \( \theta_3, \ldots, \theta_d \) but independent of \( \theta_1 \). This
amounts to specification of the conditional distribution \( \Pi_{\theta_3|\theta_2, \ldots, \theta_d} \). If we continue
like this, eventually defining the marginal prior for the last component \( \theta_d \), we have
found a prior for the full parameter \( \theta \), because for all \( A_1, \ldots, A_d \in \mathcal{G} \),

\[
\Pi(\theta_1 \in A_1, \ldots, \theta_d \in A_d) = \Pi(\theta_1 \in A_1|\theta_2 \in A_2, \ldots, \theta_d \in A_d) \Pi(\theta_2 \in A_2|\theta_3 \in A_3, \ldots, \theta_d \in A_d)
\]

\[
\times \ldots \times \Pi(\theta_{d-1} \in A_{d-1}|\theta_d \in A_d) \Pi(\theta_d \in A_d).
\]

Because prior beliefs may be more easily expressed when imagining a situation
where other parameters have fixed values, one eventually succeeds in defining the
prior for the high-dimensional model.

Example 3.2. Suppose that we measure pairs \( (W_i, L_i) \), \( 1 \leq i \leq n \), where \( W_i \) is the
weight and \( L_i \) is the length of the \( i \)-th draw from an i.i.d. sample of monkeys from a
certain population. As our model for \( (W, L) \), we choose model distributions that are
products of Gamma distributions with shape parameter \( k = 3 \): \( (W, L) \sim \Gamma(w/3, 3) \times \Gamma(l/3, 3) \), so that \( (W, L) \) given \( (w, l) \) has expectation \( (w, l) \). To choose a prior for the
parameter \( (w, l) \), we note that a relatively tall monkey will also be relatively heavy.
We express this through the specification of the prior: we assume that weight \( w \) and
length \( l \) approximately follow the relationship \( w = K l^n \), for some known \( K > 0 \) and
a known exponent \( \alpha \). In that case, given the length \( l \), we specify (for some choice
\( \lambda > 0 \)),

\[
w|l \sim \Gamma(\lambda^{-1} K l^n, \lambda),
\]

so that the conditional prior expectation for \( w|l \) is \( K l^n \). For \( l \), we choose a marginal
prior,

\[
l \sim \Gamma(\lambda^{-1} \ell, \lambda),
\]

where \( \ell \) is an approximate mean length for a monkey from the population. The prior
variances of \( l \) and \( w|l \) are equal to \( \ell^2 / \lambda \) and \( K^2 l^2 \alpha / \lambda \) respectively, i.e. \( \lambda \) has the
interpretation of being inversely proportional to uncertainty expressed in the prior
(higher values of \( \lambda \) bias the prior (and hence also the posterior) more to the prior
expectation \( (\ell, K l^n) \)).
The construction indicated here is reminiscent of that of a so-called \textit{hyperprior}, which is discussed in section 3.3. The difference is that components of $\theta$ all occur in the definition of model distributions $P_\theta$, whereas hyperparameters do not. Note that it is important to choose a parametrization of the model in which the independence between $\theta_i$ and $(\theta_1, \ldots, \theta_{i-1})$, given $(\theta_{i+1}, \ldots, \theta_d)$, is plausible for all $i \geq 1$.

In certain situations, the subjectivist has more factual information at his disposal when defining the prior for his analysis. In particular, if a probability distribution on the model reflecting the subjectivist’s “beliefs” can be found by other statistical means, it can be used as a prior. Suppose the statistician is planning to measure a quantity $Y$ and infer on a model $\mathcal{P}$; suppose also that this experiment repeats or extends an earlier analysis. From the earlier analysis, the statistician may have obtained a posterior distribution on $\mathcal{P}$. For the new experiment, this posterior may serve as a prior.

\textit{Example 3.3.} Let $\Theta \to \mathcal{P} : \theta \to P_\theta$ be a parametrized model for i.i.d. data $X_1, X_2, \ldots, X_n$ with prior measure $\Pi_1 : \mathcal{G} \to [0, 1]$. Let the model be dominated (see definition 1.3), so that the posterior $\Pi_1(\cdot | X_1, \ldots, X_n)$ satisfies (2.13). Suppose that this experiment has been conducted, with the sample realised as $(X_1, X_2, \ldots, X_n) = (x_1, x_2, \ldots, x_n)$. Next, consider a new, independent experiment in which a quantity $X_{n+1}$ is measured (with the same model). As a prior $\Pi_2$ for the new experiment, we use the (realised) posterior of the earlier experiment, i.e. for all $G \in \mathcal{G}$,

$$\Pi_2(G) = \Pi_1(G | X_1 = x_1, \ldots, X_n = x_n).$$

The posterior for the second experiment then satisfies:

$$d\Pi_2(\theta | X_{n+1}) = \frac{p_\theta(X_{n+1}) d\Pi_1(\theta | X_1 = x_1, \ldots, X_n = x_n)}{\int_\Theta p_\theta(X_{n+1}) d\Pi_1(\theta | X_1 = x_1, \ldots, X_n = x_n)} = \frac{\int_\Theta p_\theta(X_{n+1}) \prod_{i=1}^n p_\theta(x_i) d\Pi_1(\theta)}{\prod_{j=1}^n p_\theta(x_j) d\Pi_1(\theta)}. \quad (3.1)$$

The latter form is comparable to the posterior that would have been obtained if we had conducted a single experiment with an i.i.d. sample $X_1, X_2, \ldots, X_{n+1}$ of size $n+1$ and prior $\Pi_1$. In that case, the posterior would have been of the form:

$$\Pi(\cdot | X_1, \ldots, X_{n+1}) = \frac{\prod_{i=1}^{n+1} p_\theta(X_i) d\Pi_1(\theta)}{\int_\Theta \prod_{j=1}^{n+1} p_\theta(X_j) d\Pi_1(\theta)}, \quad (3.2)$$

\textit{i.e.} the only difference is the fact that the posterior $\Pi_1(\cdot | X_1 = x_1, \ldots, X_n = x_n)$ is realised. As such, we may interpret independent consecutive experiments as a sin-
Choice of the prior

Clearly, there are other ways to obtain a distribution on the model that can be used as an informative prior. One example is the distribution that is obtained when a previously obtained frequentist estimator $\hat{\theta}$ for $\theta$ is subject to a procedure called the bootstrap. Although the bootstrap gives rise to a distribution that is interpreted (in the frequentist sense) as the distribution of the estimator $\hat{\theta}$ rather than $\theta$ itself, a subjectivist may reason that the estimator provides him with the “expert knowledge” on $\theta$ that he needs to define a prior on $\Theta$. (For more on bootstrap methods, see Efron and Tibshirani (1993) [33].)

3.2 Non-informative priors

Objectivist Bayesians agree with frequentists that the “beliefs” of the statistician analyzing a given measurement should play a minimal role in the methodology. Obviously, the model choice already introduces a bias, but rather than embrace this necessity and expand upon it like subjectivists, they seek to keep the remainder of the procedure unbiased. In particular, they aim to use priors that do not introduce additional information (in the form of prior “belief”) in the procedure. Subjectivists introduce their “belief” by concentrating prior mass in certain regions of the model; correspondingly, objectivists prefer priors that are “homogeneous” in an appropriate sense.

3.2.1 Uniform priors

At first glance, one may be inclined to argue that a prior is objective (or non-informative) if it is uniform over the parameter space: if we are inferring on parameter $\theta \in [-1, 1]$ and we do not want to favour any part of the model over any other, we would choose a prior of the form, $(A \in \mathcal{B})$,

$$\Pi(A) = \frac{1}{2} \mu(A),$$  \hspace{1cm} (3.3)

where $\mu$ denotes the Lebesgue measure on $[-1, 1]$. Attempts to minimize the amount of subjectivity introduced by the prior therefore focus on uniformity (argumentation that departs from the Shannon entropy in discrete probability spaces reaches the same conclusion (see, for example, Ghosh and Ramamoorthi (2003) [44], p. 47)).

The original references on Bayesian methods (e.g. Bayes (1763) [4], Laplace (1774) [62]) use uniform priors as well. But there are several problems with this approach: first of all, one must wonder how to extend such reasoning when $\theta \in \mathbb{R}$ (or any other unbounded subset of $\mathbb{R}$). In that case, $\mu(\Theta) = \infty$ and we can not normalize $\Pi$ to be a probability measure! Any attempt to extend $\Pi$ to such unbounded models as a
probability measure would eventually lead to inhomogeneity, \textit{i.e.} go at the expense of the unbiasedness of the procedure.

The compromise some objectivists are willing to make, is to relinquish the interpretation that subjectivists give to the prior: they do not express any prior “degree of belief” in $A \in \mathcal{G}$ through the subjectivist statement that the (prior) probability of finding $\vartheta \in A$ equals $\Pi(A)$. Although they maintain the Bayesian interpretation of the posterior, they view the prior as a mathematical definition rather than a philosophical concept. Then, the following definition can be made without further reservations.

**Definition 3.1.** Given a model $(\Theta, \mathcal{G})$, a prior measure $\Pi : \mathcal{G} \to \mathbb{R}$ such that $\Pi(\Theta) = \infty$ is called an improper prior.

Note that the normalization factor $\frac{1}{2}$ in (3.3) cancels in the expression for the posterior, \textit{c.f.} (2.6): any finite multiple of a (finite) prior is equivalent to the original prior as far as the posterior is concerned. However, this argument does not extend to the improper case: integrability problems or other infinities may ruin the procedure, even to the point where the posterior measure becomes infinite or ill-defined. So not just the philosophical foundation of the Bayesian approach is lost, mathematical integrity of the procedure can no longer be guaranteed either! When confronted with an improper prior, the entire procedure must be checked for potential problems. In particular, one must verify that the posterior is a well-defined probability measure.

**Remark 3.3.** Throughout these notes, whenever we refer to a prior measure, it is implied that this measure is a probability measure unless stated otherwise.

But even if one is willing to accept that objectivity of the prior requires that we restrict attention to models on which “uniform” probability measures exist (\textit{e.g.} with $\Theta$ a bounded subset of $\mathbb{R}^d$), a more fundamental problem exists: the very notion of uniformity is dependent on the parametrization of the model! To see this we look at a model that can be parametrized in two ways and we consider the way in which uniformity as seen in one parametrization manifests itself in the other parametrization. Suppose that we have a $d$-dimensional parametric model $\mathcal{P}$ with two different parametrizations, on $\Theta_1 \subset \mathbb{R}^d$ and $\Theta_2 \subset \mathbb{R}^d$ respectively,

$$\phi_1 : \Theta_1 \to \mathcal{P}, \quad \phi_2 : \Theta_2 \to \mathcal{P}$$

both of which are bijective. Assume that $\mathcal{P}$ has a topology and is endowed with the corresponding Borel $\sigma$-algebra $\mathcal{G}$; let $\phi_1$ and $\phi_2$ be continuous and assume that their inverses $\phi_1^{-1}$ and $\phi_2^{-1}$ are continuous as well. Assuming that $\Theta_1$ is bounded, we consider the uniform prior $\Pi_1$ on $\Theta_1$, \textit{i.e.} the normalized Lebesgue measure on $\Theta_1$, \textit{i.e.} for all $A \in \mathcal{B}_1$,

$$\Pi_1(A) = \mu(\Theta_1)^{-1}\mu(A),$$

This induces a prior $\Pi'_1$ on $\mathcal{P}$: for all $B \in \mathcal{G}$,

$$\Pi'_1(B) = (\Pi_1 \circ \phi_1^{-1})(B).$$
In turn, this induces a prior $\Pi''_1$ on $\Theta_2$: for all $C \in \mathcal{B}_2$,

$$
\Pi''_1(C) = (\Pi'_1 \circ (\phi_2^{-1})^{-1})(C) = (\Pi'_1 \circ \phi_2)(C) = (\Pi'_1 \circ (\phi_1^{-1} \circ \phi_2))(C).
$$

Even though $\Pi_1$ is uniform, generically $\Pi''_1$ is not, because, effectively, we are mapping (a subset of) $\mathbb{R}^d$ to $\mathbb{R}^d$ by $\phi_2^{-1} \circ \phi_1 : \Theta_1 \to \Theta_2$. (Such re-coordinatizations are used extensively in differential geometry, where a manifold can be parametrized in various ways by sets of maps called charts.)

**Example 3.4.** Consider the model $\mathcal{P}$ of all normal distributions centred on the origin with unknown variance between 0 and 1. We may parametrize this model in many different ways, but we consider only the following two:

$$
\phi_1 : (0, 1) \to \mathcal{P} : \tau \mapsto N(0, \tau), \quad \phi_2 : (0, 1) \to \mathcal{P} : \sigma \mapsto N(0, \sigma^2).
$$

(3.6)

Although used more commonly than $\phi_1$, parametrization $\phi_2$ is not special in any sense: both parametrizations describe exactly the same model. Now, suppose that we choose to endow the first parametrization with a uniform prior $\Pi'_1$, equal to the Lebesgue measure $\mu$ on $(0, 1)$. By (3.5), this induces a prior on $\mathcal{P}$. Let us now see what this prior looks like if we consider $\mathcal{P}$ parametrized by $\sigma$: for any constant $C \in (0, 1)$ the point $N(0, C)$ in $\mathcal{P}$ is the image of $\tau = C$ and $\sigma = \sqrt{\tau}$, so the relation between $\tau$ and corresponding $\sigma$ is given by

$$
\tau(\sigma) = (\phi_2^{-1} \circ \phi_1)(\sigma) = \sigma^2.
$$

Since $\Pi_1$ equals the Lebesgue measure, we find that the density of $\Pi''_1$ with respect to the Lebesgue measure equals:

$$
\pi''_1(\sigma) = \pi_1(\tau(\sigma)) \frac{d\tau}{d\sigma}(\sigma) = 2\sigma.
$$

This density is non-constant and we see that $\Pi''_1$ is non-uniform. In a subjectivist sense, the prior $\Pi''_1$ places higher prior “belief” on values of $\sigma$ close to 1 than on values close to 0.

From the above argument and example 3.4, we see that uniformity of the prior is entirely dependent on the parametrization: what we call “uniform” in one parametrization, may be highly non-uniform in another. Consequently, what is deemed “objective” in one parametrization may turn out to be highly subjective in another.

What matters is the model $\mathcal{P}$, not its parametrization in terms of one parameter or another! The parametrization is a mere choice made by the statistician analyzing the problem. Therefore, any statistical concept that depends on the parametrization is flawed from the outset. Through $\mathcal{P}$ and only through $\mathcal{P}$ do the parameters $\sigma$ and $\tau$ have any bearing on (the law of) the observation in example 3.4. If we could define what is meant by uniformity on the model $\mathcal{P}$ itself, instead of on its parametrizing spaces, one would obtain a viable way to formalize objectivity. But spaces of probability measures do not have an intrinsic notion of uniformity (like translation-
3.2 Non-informative priors

invariance of Lebesgue measure on \( \mathbb{R}^d \), or more generally, left-invariance of the Haar measure on locally compact topological groups).

### 3.2.2 Jeffreys prior and reference priors

Once it is clear that uniformity on any parametrizing space does not have intrinsic meaning in the model \( \mathcal{P} \), the very definition of objectivity in terms of uniformity of the prior is void. A subjectivist can use any parametrization to formulate his prejudice (note that the subjectivist uses relative prior weights rather than deviations from uniformity to express his prior “belief”), but an objectivist has to define his notion of “objectivity” regardless of the parametrization used. Therefore, the emphasis is shifted: instead of looking for uniform priors, we look for priors that are well-defined on \( \mathcal{P} \) and declare them objective. For differentiable parametric models, a construction from Riemannian geometry can be used to define a parameterisation-independent prior (see Jeffreys (1946), (1961) \([50, 51]\) if we interpret the Fisher information as a Riemannian metric on the model (as first proposed by Rao (1945) \([78]\) and extended by Efron (1975) \([32]\); for an overview, see Amari (1990) \([2]\)) and use the square-root of its determinant as a density with respect to the Lebesgue measure.

**Definition 3.2.** Let \( \Theta \subset \mathbb{R}^d \) be open and let \( \mathcal{P} \) be a dominated model with identifiable, differentiable parametrization \( \Theta \to \mathcal{P} \). Assume that for every \( \theta \in \Theta \), the score-function \( \dot{\ell}_\theta \) is square-integrable with respect to \( P_\theta \). Then Jeffreys prior \( \Pi \) has the square root of the determinant of the Fisher information \( I_\theta = P_\theta \dot{\ell}_\theta \dot{\ell}_\theta^T \) as its density with respect to the Lebesgue measure on \( \Theta \):

\[
d\Pi(\theta) = \sqrt{\det(I_\theta)} \, d\theta. \tag{3.7}
\]

Although the expression for Jeffreys prior has the appearance of being parametrization-dependent, the form (3.7) of this prior is the same in any parametrization (a property referred to sometimes as (coordinate-)covariance). In other words, no matter which parametrization we use to calculate \( \Pi \) in (c.f. (3.7)), the induced measure \( \Pi' \) on \( \mathcal{P} \) is always the same one. As such, Jeffreys prior is a measure defined on \( \mathcal{P} \) rather than a parametrization-dependent measure.

**Example 3.5.** We calculate the density of Jeffreys prior in the normal model of example 3.4. The score-function with respect to the parameter \( \sigma \) in parametrization \( \phi_2 \) of \( \mathcal{P} \) is given by:

\[
\dot{\ell}_\sigma(x) = \frac{1}{\sigma} \left( \frac{x^2}{\sigma^2} - 1 \right).
\]

The Fisher information (which is a 1 \times 1-matrix in this case), is then given by:

\[
I_\sigma = P_\sigma \dot{\ell}_\sigma \dot{\ell}_\sigma = \frac{1}{\sigma^2} P_\sigma \left( \frac{x^2}{\sigma^2} - 1 \right)^2 = \frac{2}{\sigma^2}.
\]
Therefore, the density for Jeffries prior $\Pi$ takes the form
\[
d\Pi(\sigma) = \frac{\sqrt{2}}{\sigma} \, d\sigma,
\]
for all $\sigma \in \Theta_2 = (0, 1)$. A similar calculation using the parametrization $\phi_1$ shows that, in terms of the parameter $\tau$, Jeffries prior takes the form:
\[
d\Pi(\tau) = \frac{1}{\sqrt{2\tau}} \, d\tau,
\]
for all $\tau \in \Theta_1 = (0, 1)$. That both densities give rise to the same measure on $\mathcal{P}$ is the assertion of the following lemma.

**Lemma 3.1.** (Parameterization-independence of Jeffreys prior)
Consider the situation of (3.4) and assume that the parametrizations $\phi_1$ and $\phi_2$ satisfy the conditions of definition 3.2. In addition, we require that the map $\phi_1^{-1} \circ \phi_2 : \Theta_2 \to \Theta_1$ is differentiable. Then the densities (3.7), calculated in coordinates $\phi_1$ and $\phi_2$ induce the same measure on $\mathcal{P}$, Jeffreys prior.

**Proof.** Since the Fisher information can be written as:
\[
I_{\theta_1} = \mathbb{P}_{\theta_1}(\ell_{\theta_1} \ell_{\theta_1}^T),
\]
and the score $\ell_{\theta_1}(X)$ is defined as the derivative of $\theta_1 \mapsto \log \mathbb{P}_{\theta_1}(X)$ with respect to $\theta_1$, a change of parametrization $\theta_1(\theta_2) = (\phi_1^{-1} \circ \phi_2)(\theta_2)$ induces a transformation of the form
\[
I_{\theta_2} = S_{1,2}(\theta_2) I_{\theta_1(\theta_2)} S_{1,2}(\theta_2)^T,
\]
on the Fisher information matrix, where $S_{1,2}(\theta_2)$ is the total derivative matrix of $\theta_2 \mapsto \theta_1(\theta_2)$ in the point $\theta_2$ of the model. Therefore,
\[
\sqrt{\det I_{\theta_2}} \, d\theta_2 = \sqrt{\det(S_{1,2}(\theta_2) I_{\theta_1(\theta_2)} S_{1,2}(\theta_2)^T)} \, d\theta_2 = \sqrt{\det(S_{1,2}(\theta_2))^2 \, \det(I_{\theta_1(\theta_2)})} \, d\theta_2
\]
\[
= \sqrt{\det(I_{\theta_1(\theta_2)})} \left| \det(S_{1,2}(\theta_2)) \right| \, d\theta_2 = \sqrt{\det(I_{\theta_1})} \, d\theta_1
\]
\]
i.e. the form of the density is such that reparametrization leads exactly to the Jacobian for the transformation of $d\theta_2$ to $d\theta_1$.

Ultimately, the above construction derives from the fact that the Fisher information $I_{\theta}$ (or in fact, any other positive-definite symmetric matrix-valued function on the model, e.g. the Hessian of a twice-differentiable, convex function) can be viewed as a Riemann metric on the “manifold” $\mathcal{P}$. The construction of a measure with Lebesgue density (3.7) is then a standard construction in differential geometry.

**Example 3.6.** To continue with the normal model of examples 3.4 and 3.5, we note that $\sigma(\tau) = \sqrt{\tau}$, so that $d\sigma / d\tau(\tau) = 1/2\sqrt{\tau}$. As a result,
\[
\sqrt{\text{det} I_\theta} \, d\theta_2 = \frac{\sqrt{2}}{\sigma} d\sigma = \frac{\sqrt{2}}{\sigma(t)} \frac{1}{\sqrt{2\sqrt{\tau}}} d\tau = \frac{1}{\sqrt{2\tau}} d\tau = \sqrt{\text{det}(I_\theta)} \, d\theta_1,
\]

which verifies the assertion of lemma 3.1 explicitly.

Other constructions and criteria for the construction of non-informative priors exist: currently very popular is the use of so-called reference priors, as introduced in Lindley (1956) [72] and rediscovered in Bernardo (1979) [12] (see also Berger and Bernardo (1992) [9]). By defining principle, a reference prior is required to maximize the Kullback-Leibler divergence between prior and posterior. To motivate this condition, we have to look at information theory, from which the Kullback-Leibler divergence has emerged as one (popular but by no means unique) way to quantify the notion of the “amount of information” contained in a probability distribution. Sometimes called the Shannon entropy, the Kullback-Leibler divergence of a distribution \( P \) with respect to the counting measure in discrete probability spaces,

\[
S(P) = \sum_{\omega \in \Omega} p(\omega) \log(p(\omega)),
\]

can be presented as such convincingly (see Boltzmann (1895, 1898) [22], Shannon (1948) [85]). For lack of a default dominating measure, the argument does not extend formally to continuous probability spaces but is generalized nevertheless. A reference prior \( \Pi \) on a dominated, parametrized model \( \Theta \rightarrow P : \theta \mapsto P_\theta \) for an observation \( Y \) is to be chosen such that the Lindley entropy,

\[
S_L = \int \int \log\left( \frac{\pi(\theta|Y = y)}{\pi(\theta)} \right) d\Pi(\theta|Y = y) dP^\Pi(y),
\]

is maximized. Note that this definition does not depend on the specific parametrization, since the defining property is parametrization independent. Usually, the derivation of a reference prior [12] is performed in the limit where the posterior becomes asymptotically normal, in accordance with the Bernstein-von Mises theorem. Jeffreys prior emerges as a special case of a reference prior.

For an overview of various objective methods of constructing priors, the reader is referred to Kass and Wasserman (1995) [53]. When using non-informative priors, however, the following general warning should be heeded.

\textit{Remark 3.4.} In many models, non-informative priors, including Jeffreys prior and reference priors, are improper.

### 3.3 Conjugate families

In this section, we consider a type of prior choice that is motivated primarily by mathematical convenience, rather than philosophy or statistical utility. Recall that if we model the data with normal distributions of known variance but unknown location \( \theta \) and we supply \( \theta \) with a normal prior, then the posterior for \( \theta \) is again a
normal distribution. Since the calculation of the posterior is tractable, any choice for
the parameters of the normal prior can immediately be updated to values for location
and variance of the normal posterior upon observation of $Y = y$. Not only does this
signify ease of manipulation in calculations with the posterior, it also reduces the
computational burden dramatically since numerical integration or simulation from
the posterior is no longer necessary.

### 3.3.1 Basic definitions and some examples

The subject of this section revolves around the following definition.

**Definition 3.3.** Let $(\mathcal{P}, \mathcal{A})$ be a measurable model for an observation $Y \in \mathcal{Y}$. Let $M$ denote a collection of probability distributions on $(\mathcal{P}, \mathcal{A})$. The set $M$ is called a *conjugate family* for the model $\mathcal{P}$, if the posterior based on a prior from $M$ again lies in $M$:

$$\Pi \in M \Rightarrow \Pi(\cdot | Y = y) \in M,$$

(3.8)

for all almost all $y \in \mathcal{Y}$.

(Like before, the phrase “almost all” in the above definition refers to the prior predictive distribution for Bayesians, and to the true $P_0$ for frequentists.) Such structure was first proposed by Raiffa and Schlaifer (1961) [77]. Their method for the prior choice is usually classified as objectivist because it does not rely on subjectivist notions and is motivated without reference to outside factors.

**Remark 3.5.** Often in the literature, a prior is referred to as a “conjugate prior” if the posterior is of the same form. This is somewhat misleading, since it is the family $M$ that is closed under conditioning on the data $Y$, a property that depends on the model and on $M$ itself, but not on the particular $\Pi \in M$.

**Example 3.7.** Consider an experiment in which we observe $n$ independent Bernoulli trials and consider the total number of successes, $Y \sim \text{Bin}(n, p)$ with unknown parameter $p \in [0, 1]$, $P_p(Y = k) = \binom{n}{k} p^k (1 - p)^{n-k}$.

For the parameter $p$ we choose a prior $p \sim \text{Beta}(\alpha, \beta)$ from the Beta-family, for some $\alpha, \beta > 0$,

$$d\Pi(p) = B(\alpha, \beta) p^{\alpha-1} (1 - p)^{\beta-1} dp,$$

where $B(\alpha, \beta) = \Gamma(\alpha + \beta)/\Gamma(\alpha) \Gamma(\beta)$ normalizes $\Pi$. Then the posterior density with respect to the Lebesgue measure on $[0, 1]$ is proportional to:

$$d\Pi(p|Y) \propto p^Y (1 - p)^{n-Y} p^{\alpha-1} (1 - p)^{\beta-1} dp = p^{\alpha+Y-1} (1 - p)^{\beta+n-Y-1} dp,$$

We conclude that the posterior again lies in the Beta-family, with parameters equal to a data-amended version of those of the prior, as follows:
\[ \Pi(\cdot | Y) = \text{Beta}(\alpha + Y, \beta + n - Y). \]

So the family of Beta-distributions is a conjugate family for the binomial model. Depending on the available amount of prior information on \( \theta \), the prior’s parameters may be chosen on subjective grounds (see figure 2.1 for graphs of the densities of Beta-distributions for various parameter values). However, in the absence thereof, the parameters \( \alpha, \beta \) suffer from the same ambiguity that plagues the parameter \( \tau^2 \) featuring in the example with which we opened this section.

Example 3.7 indicates a strategy to find conjugate families for a given parametrized, dominated model \( \mathcal{P} = \{P_\theta : \theta \in \Theta\} \). We view densities \( y \mapsto p_\theta(y) \) as functions of the outcome \( Y = y \) foremost, but they are functions of the parameter \( \theta \) as well and their dependence \( \theta \mapsto p_\theta(y) \) determines which prior densities \( \theta \mapsto \pi(\theta) \) preserve their functional form when multiplied by the likelihood \( p_\theta(Y) \) to yield the posterior density.

### 3.3.2 Exponential families

Although we shall encounter an example of a conjugate family for a non-parametric model in section 3.6, conjugate families are, by and large, part of parametric statistics. Many of these families are so-called exponential families, for which conjugate families of priors can be found readily.

**Definition 3.4.** A dominated collection of probability measures \( \mathcal{P} = \{P_\theta : \theta \in \Theta\} \) is called a \( k \)-parameter exponential family, if there exists a \( k \geq 1 \) such that for all \( \theta \in \Theta \),

\[
p_\theta(x) = \exp\left( \sum_{i=1}^{k} \eta_i(\theta) T_i(x) - B(\theta) \right) h(x),
\]

(3.9)

where \( h \) and \( T_i, i = 1, \ldots, k \), are statistics and \( B, \eta_i, i = 1, \ldots, k \) are real-valued functions on \( \Theta \).

Any exponential family can be parametrized such that the exponent in (3.9) is linear in the parameter: by the mapping \( \Theta \rightarrow H : \eta_i = \eta_i(\theta) \) (a bijection if the original parametrization is identifiable), taking \( \Theta \) into \( H = \eta(\Theta) \) and \( B \) into \( A(\eta) = B(\theta(\eta)) \), any exponential family can be rewritten in its so-called canonical form.

**Definition 3.5.** An exponential family \( \mathcal{P} = \{P_\eta : \eta \in H\} \), \( H \subset \mathbb{R}^k \) is said to be in its canonical representation, if

\[
p_\eta(x) = \exp\left( \sum_{i=1}^{k} \eta_i T_i(x) - A(\eta) \right) h(x).
\]

(3.10)

In addition, \( \mathcal{P} \) is said to be of full rank if the interior of \( H \subset \mathbb{R}^k \) is non-void, i.e. \( \hat{H} \neq \emptyset \).
Although parametric, exponential families are both versatile modelling tools and mathematically tractable; many common models, like the Bernoulli-, normal-, binomial-, Gamma-, Poisson-models, etcetera, can be rewritten in the form (3.9). To give an example of a type of parameter that cannot be accommodated in an exponential family, consider models in which the support of model distributions is parameter-dependent, like the family of all uniform distributions on \( \mathbb{R} \), or the parameter that describes the domain offset in the Pareto-model. Their statistical practicality stems primarily from the fact that for an exponential family of full rank, the statistics \( T_i, i = 1, \ldots, k \) are sufficient and complete, enabling the use of the Lehmann-Scheffé theorem for minimal-variance unbiased estimation (see, for instance, Lehmann and Casella (1998) [64]). Their versatility can be understood in many ways, e.g. by the Pitman-Koopman-Darmois theorem (see, Jeffreys (1961) [51]), which says that a family of distributions whose support does not depend on the parameter, is exponential, if and only if in the models describing its i.i.d. samples, there exist sufficient statistics whose dimension remains bounded asymptotically (i.e. as we let the sample size diverge to infinity).

Example 3.8. The model of all normal distributions \( \mathcal{P} = \{ N(\mu, \sigma^2) : \theta \in \mathbb{R}, \sigma^2 > 0 \} \) on \( \mathbb{R} \) forms an exponential family. To see this, write \( \theta = (\mu, \sigma^2) \in \Theta = \mathbb{R} \times (0, \infty) \) and rewrite the usual parametrization in the form (3.9), as follows,

\[
p_{\mu,\sigma^2}(x) = (2\pi)^{-1/2} \sigma^{-1} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) = \exp\left(-\frac{1}{2\theta_2} x^2 + \frac{\theta_1}{\theta_2} x - \frac{\theta_1^2}{2\theta_2} - \frac{1}{2} \log(2\pi) - \frac{1}{2} \log \sigma^2\right)
\]

and, comparing with (3.9), we read off,

\[
\begin{align*}
\eta_1(\theta) &= \frac{\theta_1}{\theta_2}, & \eta_2(\theta) &= -\frac{1}{2\theta_2}, & B(\theta) &= \frac{\theta_1^2}{2\theta_2} + \frac{1}{2} \log \theta_2, \\
T_1(x) &= x, & T_2(x) &= x^2, & h(x) &= (2\pi)^{-1/2}.
\end{align*}
\]

The map \( \eta : \Theta \rightarrow H : \theta \mapsto (\eta_1, \eta_2)(\theta) \) takes the original parameter into the canonical parameter \( \eta \in H = \mathbb{R} \times (-\infty, 0) \). Note that the inverse of \( \eta \) takes the form,

\[
(\theta_1, \theta_2)(\eta) = \left(-\frac{\eta_1}{2\eta_2}, -\frac{1}{2\eta_2}\right),
\]

from which we deduce that,

\[
A(\eta) = B(\theta(\eta)) = -\frac{\eta_1^2}{4\eta_2} + \frac{1}{2} \log\left(-\frac{1}{2\eta_2}\right),
\]

for the new normalization. Expressed in these new parameters \( \eta \), the density takes the form (3.10). Note that \( H = \mathbb{R} \times (-\infty, 0) \) has non-empty interior, so the normal model is an exponential family of full rank. In case we had started with the model
3.3 Conjugate families

\( P = \{ N(\theta, 0) : \theta > 0 \} \), for example, the analysis would have been largely analogous; however, the latter \( P \) is not of full rank.

Presently our interest lies with the following theorem which says that if a model \( P \) constitutes an exponential family, there exists a conjugate family of priors for \( P \).

**Theorem 3.1.** Let \( P \) be a model that can be written as an exponential family, c.f. definition 3.4. Then there exists a parametrization of \( P \) of the form (3.10) and the family of distributions \( \Pi_{\mu, \lambda} \), defined by Lebesgue probability densities

\[
\pi_{\mu, \lambda}(\eta) = K(\mu, \lambda) \exp\left( \sum_{i=1}^{k} \eta_i \mu_i - \lambda A(\eta) \right),
\]

(3.11)

(where \( \mu \in \mathbb{R}^k \) and \( \lambda \in \mathbb{R} \) are such that \( 0 < K(\mu, \lambda) < \infty \)), is a conjugate family for \( P \).

**Proof.** Proof It follows from the argument preceding definition 3.5 that \( P \) can be parametrized as in (3.10). Choosing a prior on \( H \) of the form (3.11), we find that the posterior again takes the form (3.11),

\[
\pi(\eta | X) \propto \exp\left( \sum_{i=1}^{k} \eta_i (\mu_i + T(X)) - (\lambda + 1) A(\eta) \right)
\]

(the factor \( h(X) \) arises both in numerator and denominator of (2.6) and is \( \eta \)-independent, so that it cancels). The data-amended versions of the parameters \( \mu \) and \( \lambda \) that emerge from the posterior are therefore given by:

\[
(\mu + T(X), \lambda + 1),
\]

and we conclude that the distributions \( \Pi_{\mu, \lambda} \) form a conjugate family for \( P \).

From a frequentist perspective, it is worth noting the import of the factorization theorem, which says that the parameter-dependent factor in the likelihood is a function of the data only through the sufficient statistic. Since the posterior is a function of the likelihood, in which data-dependent factors that do not depend on the parameter can be cancelled between numerator and denominator, the posterior is a function of the data \( Y \) only through the sufficient statistic \( T(Y) \). Specifying to the case of exponential families, we note the following conclusion regarding \( L_2 \)-optimality.

**Lemma 3.2.** If \( P \) is an exponential family of full rank, \( T \) is not just sufficient but also complete for \( P \), and any point-estimator \( \hat{\theta} \) based on the posterior (e.g. the posterior mean, see definition 2.7) that is unbiased and quadratically integrable (for all \( \theta \in \Theta \)), is optimal in the sense that, for all \( \theta \in \Theta \),

\[
P_{\theta}(\hat{\theta} - \theta)^2 \leq P_{\theta}(\hat{\eta} - \theta)^2,
\]

for any other unbiased estimator \( \hat{\eta} \) for \( \theta \).

We omit the proof because it is a direct consequence of the famous Lehmann-Scheffé theorem (see, e.g., Lehmann and Casella (1998) [64]).
3.4 Hierarchical priors

Consider again the problem of estimating the mean of a single, normally distributed observation $Y$ with known variance. The model consists of all normal distributions $P_\theta = N(\theta, \sigma^2)$, where $\theta \in \mathbb{R}$ is unknown and $\sigma^2 > 0$ is known. Imposing a normal prior on the parameter $\theta$, $\Pi = N(0, \tau^2)$, for some choice of $\tau^2 > 0$, we easily calculate the posterior distribution,

$$\Pi(\theta \in A|Y) = N\left(\frac{\tau^2}{\sigma^2 + \tau^2} Y, \frac{\sigma^2 \tau^2}{\sigma^2 + \tau^2}\right)(A),$$

for every $A \in \mathcal{B}$. The posterior mean, a point-estimator for $\theta$, is then given by,

$$\hat{\theta}(Y) = \frac{\tau^2}{\sigma^2 + \tau^2} Y.$$

As long as expert knowledge is available in some sufficiently strong form, the subjectivist choice for a certain value of $\tau^2$ is well-motivated. However in situations where no prior belief or information on the parameter $\theta$ is available, or if the parameter itself does not have a clear interpretation, the subjectivist has no answer. Yet a choice for $\tau^2$ is required! One may express ignorance about $\tau^2$ either by choosing a prior on objectivist grounds, or by considering more and more homogeneous (but still normal) priors by means of the limit $\tau \to \infty$

Remark 3.6. From a statistical perspective, however, there exists a better answer to the question regarding $\tau^2$: if $\tau$ is not known, why not estimate its value from the data!

In this section and the next, we consider this answer from the Bayesian and from the frequentist’s angle respectively, giving rise to procedures known as hierarchical Bayesian modelling and empirical Bayesian estimation.

3.4.1 Hyperparameters and hyperpriors

Next, we turn to the Bayesian answer to remark 3.5 which said that parameters of the prior (e.g. $\tau^2$) are to be estimated themselves. Recall that the Bayesian views a parameter to be estimated as just another random variable in the probability model. In case we want to estimate the parameter for a family of priors, then that parameter is to be included in the probability space from the start. Going back to the example with which we started this section, this means that we still use normal distributions $P_\theta = N(\theta, \sigma^2)$ to model the uncertainty in the data $Y$, supply $\theta \in \mathbb{R}$ with a prior $\Pi_1 = N(0, \tau^2)$ and then proceed to choose a another prior $\Pi_2$ for $\tau^2 \in (0, \infty)$:

$$Y|\theta, \tau^2 = Y|\theta \sim P_\theta = N(\theta, \sigma^2), \quad \theta|\tau^2 \sim \Pi_1 = N(0, \tau^2), \quad \tau^2 \sim \Pi_2,$$
Note that the parameter $\tau^2$ has no direct bearing on the model distributions: conditional on $\theta$, $Y$ is independent of $\tau^2$. In a sense, the hierarchical Bayesian approach to prior choice combines subjective and objective philosophies: whereas the subjectivist will make a definite, informed choice for $\tau^2$ and the objectivist will keep himself as uncommitted as possible by striving for uniformity, the choice for a hierarchical prior expresses uncertainty about the value of $\tau^2$ in the form of a probability distribution $\Pi_2$. As such, the hierarchical Bayesian approach allows for intermediate prior choices: if $\Pi_2$ is chosen highly concentrated around one point in the model, resembling a degenerate measure, the procedure will be close to subjective; if $\Pi_2$ is spread widely and is far from degenerate, the procedure will be less biased and closer to objective. Besides interpolating between objective and subjective prior choices, the flexibility gained through introduction of $\Pi_2$ offers a much wider freedom of modelling. In particular, we may add several levels of modelled parameter uncertainty to build up a hierarchy of priors for parameters of priors. Such structures are used to express detailed subjectivist beliefs, much in the way graphical models are used to build intricate dependency structures for observed data. The origins of the hierarchical approach go back, at least, to Lindley and Smith (1972) [73].

**Definition 3.6.** Let the data $Y$ be random in $(\mathcal{F}, \mathcal{B})$. A hierarchical Bayesian model for $Y$ consists of a collection of probability measures $\mathcal{P} = \{P_0 : \theta \in \Theta_0\}$, with $(\Theta_0, \mathcal{B}_0)$ measurable and endowed with a prior $\Pi : \mathcal{B}_0 \rightarrow [0, 1]$ built up in the following way: for some $k \geq 1$, we introduce measurable spaces $(\Theta_i, \mathcal{F}_i)$, $i = 1, 2, \ldots, k$ and conditional priors

$$\mathcal{F}_i \times \Theta_{i+1} \rightarrow [0, 1] : (G, \theta_{i+1}) \mapsto \Pi_i(G|\theta_{i+1}),$$

for $i = 1, \ldots, k - 1$ and a marginal $\Pi_k : \mathcal{F}_k \rightarrow [0, 1]$ on $\Theta_k$. The prior for the original parameter $\theta$ is then defined by,

$$\Pi(\theta \in G) = \int_{\Theta_1 \times \ldots \times \Theta_k} \Pi_0(\theta \in G|\theta_1) d\Pi(\theta_1|\theta_2) \ldots d\Pi(\theta_{k-1}|\theta_k) d\Pi_0(\theta_k), \quad (3.12)$$

for all $G \in \mathcal{B}_0$. The parameters $\theta_1, \ldots, \theta_k$ and the priors $\Pi_1, \ldots, \Pi_2$ are called hyperparameters and their hyperpriors.

Definition 3.6 is very close to the general Bayesian model that incorporates all parameters $(\theta, \theta_1, \ldots, \theta_k)$ as modelling parameters. What distinguishes hierarchical modelling from the general situation is the dependence structure imposed on the parameters. The parameter $\theta$ is distinct from the hyperparameters by the fact that conditional on $\theta$, the data $Y$ is independent of all hyperparameters $\theta_1, \ldots, \theta_k$. This distinction is repeated at higher levels in the hierarchy, i.e. levels are separate from one another through the conditional independence of $\theta_i|\theta_{i+1}$ from $\theta_{i+2}, \ldots, \theta_k$.

**Remark 3.7.** The hierarchy indicated in definition 3.6 inherently loses interpretability as we ascend in level. One may be able to give a viable interpretation to the parameter $\theta$ and to the hyperparameter $\theta_1$, but higher-level parameters $\theta_2, \theta_3, \ldots$ become harder and harder to understand heuristically. Since the interpretation of the
hierarchy requires a subjective motivation of the hyperpriors, interpretability of each level is imperative, or left as a non-informative choice. In practice, Bayesian hierarchical models are rarely more than two levels deep \((k = 2)\) and the last hyperprior \(\Pi_k\) is often chosen by objective criteria.

### 3.4.2 Hierarchical prior construction in an example

This subsection considers a more-or-less practical example of a hierarchical prior in some detail.

**Example 3.9.** We observe the number \(Y\) of surviving offspring from a bird’s litter and aim to estimate the number of eggs the bird has laid: the bird lays \(N \geq 0\) eggs, distributed according to a Poisson distribution with parameter \(\lambda > 0\). For the particular species of bird in question, the Poisson rate \(\lambda\) is not known exactly: the uncertainty in \(\lambda\) can be modelled in many ways; here we choose to model it by a Gamma-distribution \(\Gamma(\alpha, \beta)\), where \(\alpha\) and \(\beta\) are chosen to reflect our imprecise knowledge of \(\lambda\) as well as possible. Each of the eggs then comes out, producing a viable chick with known probability \(p \in [0, 1]\), independently. Hence, the total number \(Y\) of surviving chicks from the litter is distributed according to a binomial distribution, conditional on \(N\),

\[
Y | N \sim \text{Bin}(N, p), \quad N | \lambda \sim \text{Poisson}(\lambda), \quad \lambda \sim \Gamma(\alpha, \beta).
\]

The posterior distribution is now obtained as follows: conditional on \(N = n\), the probability of finding \(Y = k\) is binomial,

\[
P(Y = k | N = n) = \binom{n}{k} p^k (1 - p)^{n - k},
\]

so Bayes’s rule tells us that the posterior is given by:

\[
P(N = n | Y = k) = \frac{P(N = n)}{P(Y = k)} \binom{n}{k} p^k (1 - p)^{n - k}.
\]

Since \(\sum_{n \geq 0} P(N = n | Y = k) = 1\) for every \(k\), the marginal \(P(Y = k)\) (viz. the denominator or normalization factor for the posterior given \(Y = k\)) can be read off once we have the expression for the numerator. We therefore concentrate on the marginal for \(N = n\), \((n \geq 0)\):

\[
P(N = n) = \int_{\mathbb{R}} P(N = n | \lambda) p_{\alpha, \beta}(\lambda) d\lambda = \frac{1}{\Gamma(\alpha) \beta^\alpha} \int_0^\infty e^{-\lambda} \frac{\lambda^n}{n!} e^{-\lambda/\beta} d\lambda.
\]

The integral is solved using the normalization constant of the \(\Gamma((\alpha + n), (\beta/\beta + 1))\)-distribution:
3.5 Empirical prior choice

\[ \int_0^{\infty} e^{-\lambda} \frac{\beta}{\pi} \lambda^{\alpha+n-1} d\lambda = \Gamma(\alpha+n) \left( \frac{\beta}{\beta+1} \right)^{\alpha+n}. \]

Substituting and using the identity \( \Gamma(\alpha+1) = \alpha \Gamma(\alpha) \), we find:

\[ P(N = n) = \frac{\Gamma(\alpha+n)}{\Gamma(\alpha)} \frac{1}{n!} \frac{\beta}{\beta+1} \left( \frac{\beta}{\beta+1} \right)^{\alpha+n} \frac{1}{(\beta+1)^n} \prod_{l=1}^{n} (\alpha+l-1) \]

(3.13)

Although not in keeping with the subjective argumentation we insist on in the introduction to this example, for simplicity we consider \( \alpha = \beta = 1 \) and find that in that case,

\[ P(N = n) = (1/2)^{n+1}. \]

The posterior for \( N = n \) given \( Y = k \) then takes the form:

\[ P(N = n|Y = k) = \frac{1}{2^n} \binom{n}{k} p^k (1-p)^{n-k} / \sum_{m=0}^{\infty} \frac{1}{2^m} \binom{m}{k} p^k (1-p)^{m-k}. \]

The eventual form of the posterior illustrates that the hierarchy contributes only to the construction of the prior: in case we choose \( \alpha = \beta = 1 \), the posterior we find from the hierarchical approach does not differ from the posterior that we would have found if we had started from the model that incorporates a geometric prior for \( N \),

\[ Y|N \sim \text{Bin}(N, p), \quad N \sim \text{Geo}(1/2). \]

Indeed, even if we leave \( \alpha \) and \( \beta \) free, the marginal distribution for \( N \) we found in (3.13) is none other than the prior (3.12) for this problem.

The hierarchical approach to prior construction allows for greater freedom and a more solid foundation to motivate the choice for certain prior over other possibilities. This point is all the more significant in light of remark 3.1: the motivation of a subjectivist choice for the prior is part of the statistical analysis rather than an external aspect of the procedure. Hierarchical Bayesian modelling helps to refine and justify motivations for subjectivist priors.

### 3.5 Empirical prior choice

More unexpected is the frequentist perspective on remark 3.5: if \( \tau^2 \) is an unknown, point-estimate it first and then perform the Bayesian analysis with this point-estimate as a “plug-in” for the unknown \( \tau^2 \). Critical notes can be placed with the philosophical foundations for this practice, since it appears to combine the methods of two contradictory schools of statistics. Be that as it may, the method is used routinely based on its practicality: eventually, the justification comes from the subjectivist who does not reject frequentist methods to obtain expert knowledge on his parameters, as required in his own paradigm.
Remark 3.8. Good statistical practice dictates that one may not “peek” at the data to decide which statistical method to use for the analysis of the same data. The rationale behind this dictum is that pre-knowledge of the data could bias the analysis. If we take this point strictly, the choice for a prior (read, the point-estimate for $\tau^2$) should not be made on the basis of the same data $Y$ that is to be used later to derive the posterior for $\theta$. If one has two independent realisations of the data, one can be used to choose the prior, (here, by a point-estimate for $\tau^2$) and the other to condition on, in the posterior.

Yet the above “rule” cannot be taken too strictly. Any statistician (and common sense) will tell you that it is crucial for the statistical analysis that one first obtains a certain feeling for the statistical problem by inspection of the data, before making decisions on how to analyse it (to see this point driven to the extreme, read, e.g. Tukey (1977) [89]). Ideally, one would make those decisions based on a sample of the data that is independent of the data used in the analysis proper. This precaution is often omitted, however: for example, it is common practice to use “plug-in” parameters based on the sample $Y$ whenever the need arises, possibly leading to a bias in the subsequent analysis of the same data $Y$ (unless the “plug-in” estimator is independent of all other estimators used, of course).

There are many different ways in which the idea of a prior chosen by frequentist methods is applied, all of which go under the name empirical Bayes. Following Berger [8], we note two types of statistical questions that are especially well suited for application. When we analyse data pertaining to an individual from a larger population and it is reasonable to assume that the prior can be inferred from the population, then one may estimate parameters like $\tau^2$ above from population data and use the estimates in the prior for the individual.

A more sophisticated form of applying empirical Bayesian methods is the use of “plug-in” hyperparameters, estimated by maximum-likelihood applied to the prior predictive distribution (see definition 2.4). Recall that the marginal distribution of the data in the subjectivist Bayesian formulation (c.f. section 2.1) predicts how the data is distributed. This prediction may be reversed to decide which value for the hyperparameter leads to the best explanation of the observed data, where our notion of “best” is based on the likelihood principle.

Denote the data by $Y$ and assume that it takes its values in a measurable space $(\mathcal{Y}, \mathcal{B})$. Denote the model by $\mathcal{P} = \{P_\theta : \theta \in \Theta_0\}$. Consider a family of priors parametrized by a hyperparameter $\eta \in H$, $\{\Pi_\eta : \eta \in H\}$. For every $\eta$, the prior predictive distribution $P_\eta$ is given by:

$$P_\eta(A) = \int_\Theta P_\theta(A) d\Pi_\eta(\theta),$$

for all $A \in \mathcal{B}$, i.e. we obtain a new model for the observation $Y$, given by $\mathcal{P}' = \{P_\eta : \eta \in H\}$, contained in the convex hull of the original model co($\mathcal{P}$) (under some mild conditions, see lemma ??). Note that this new model is parametrized by the hyperparameter; hence if we close our eyes to the rest of the problem and we follow the maximum-likelihood procedure for estimation of $\eta$ in this new model, we find
the value of the hyperparameter that best explains the observation \( Y \). Assuming that the model \( \mathcal{P} \) is dominated, with densities \( \{ p_\eta : \eta \in \mathcal{H} \} \), the maximum-likelihood estimate is found as the point \( \hat{\eta}(Y) \in \mathcal{H} \) such that

\[
p_\eta(Y) = \sup_{\eta \in \mathcal{H}} p_\eta(Y).
\]

under the assumptions of existence and uniqueness, by the usual methods for maximum-likelihood estimation.

**Definition 3.7.** The estimator \( \hat{\eta}(Y) \) is called the **ML-II estimator**, provided it exists and is unique.

**Remark 3.9.** There is one caveat that applies to the ML-II approach: in case the data \( Y \) consists of an i.i.d.-distributed sample, the prior predictive distribution describes the sample as exchangeable, but not i.i.d. Hence, comparison of prior predictive distributions with the data suffer from the objection raised in remark 2.1. The frequentist who assumes that the true, underlying distribution \( P_{n0} \) of the sample is i.i.d., has to keep in mind that the ML-II model is misspecified.

### 3.5.1 Model selection with empirical methods

A situation where empirical Bayes is often used, is in model selection: suppose that there are several models \( \mathcal{P}_1, \mathcal{P}_2, \ldots \) with priors \( \Pi_1, \Pi_2, \ldots \), each of which may serve as a reasonable explanation of the data, depending on an unknown parameter \( K \in \{1, 2, \ldots\} \). The choice to use model-prior pair \( k \) in the determination of the posterior can only be made after observation (or estimation) of \( K \). If \( K \) is estimated by frequentist methods, the resulting procedure belongs to the realm of the empirical Bayes methods.

**Example 3.10.** Consider the situation where we are provided with a specimen from a population that is divided into an unknown number of classes. Assume that all we know about the classes is that they occur with equal probabilities in the population. The particular class of our specimen remains unobserved. We perform a real-valued measurement \( Y \) on the specimen, which is normally distributed with known variance \( \sigma^2 \) and an unknown mean \( \mu_k \) that depends on the class \( k \). Then \( Y \) is distributed according to a discrete mixture of normal distributions of the form,

\[
Y \sim P_{K; \mu_1, \ldots, \mu_K} = \sum_{k=1}^{K} P_{Y|K=k} P(K = k) = \frac{1}{K} \sum_{k=1}^{K} N(\mu_k, 1),
\]

where \( \mu = (\mu_1, \ldots, \mu_K) \in \mathbb{R}^K \) are unknown. For every \( K \geq 1 \), we have a model of the form,

\[
\mathcal{P}_K = \{ P_{K; \mu_1, \ldots, \mu_K} : (\mu_1, \ldots, \mu_K) \in \mathbb{R}^K \}.
\]
Each of these models can be endowed with a prior $\Pi_K$ on $\mathbb{R}^K$, for example, by declaring $\mu_1, \ldots, \mu_K$ independent and marginally distributed standard normal:

$$\mu \sim \Pi_K = N(0, I_K).$$

At this point, a Bayesian would choose a hyperprior $\Pi_2$ for the discrete hyperparameter $K \geq 1$ and proceed to calculate the posterior using all models $\mathcal{P}_K$, weighed by the prior masses $\Pi_2(K = k)$ for all $k \geq 1$. Alternatively, the Bayesian can use Bayes factors to make a decision as to which value of $K$ to use, reducing the analysis to a selected, or estimated value for $K$.

Here, we concentrate on the frequentist approach. The frequentist also aims to select one of the models $\mathcal{P}_K$: in the empirical Bayes approach, we “point-estimate” which model-prior combination we shall be using to analyse the data, from the choices $(\mathcal{P}_K, \Pi_K), K \geq 1$. In such a case, inspection of the data may reveal which number of classes is most appropriate, if one observes clearly separated peaks in the observations, in accordance with the second point made in remark 3.8. Otherwise, frequentist methods exist to estimate $K$, for instance from a larger population of specimens. After we have an estimate $\hat{K}$ for $K$, we are in a position to calculate the posterior for $\mu$ based on $(\mathcal{P}_{\hat{K}}, \Pi_{\hat{K}})$.

There are two remarks to be made with regard to the estimation of $K$ from a larger population of specimens: first of all, maximization of the likelihood will always lead to a number of classes in the order of the samplesize, simply because the largest number of classes offers the most freedom and hence always provides the best fit to the data. A similar phenomenon arises in regression, where it is called overfitting, if we allow regression polynomials of arbitrary degree: the MLE will fit the data perfectly by choosing a polynomial of degree in the order of the samplesize. Therefore in such questions of model selection, penalized likelihood criteria are employed which favour low-dimensional models over high-dimensional ones, i.e. smaller choices for $K$ over larger ones. Note that it is not clear, neither intuitively nor mathematically, how the penalty should depend on $K$, nor which proportionality between penalty and likelihood is appropriate. Well-known standard choices come in the form of the so-called AIC and BIC criteria for model selection [84]: the AIC criterion argues for maximization of the likelihood and subsequent subtraction of twice the dimension of the $k$’th parameter space, motivated from information theory and large sample sizes. The BIC criterion weighs the penalty by the logarithm of the sample size, motivated from the large sample limit for the posterior.

The Bayesian faces the same problem when he chooses a prior for $K$: if he assigns too much prior weight to the higher-dimensional models, his estimators (or, equivalently, the bulk of the resulting posterior’s mass) will get the chance to “run off” to infinity with growing samplesize, indicating inconsistency from over-fitting. Indeed, the correspondence between the frequentist’s necessity for a penalty in maximum-likelihood methods on the one hand, and the Bayesian’s need for a prior expressing sufficient bias for the lower-dimensional model choices on the other, is explained in remark 2.6.
On another sidenote: it is crucial in the example above that all classes are represented in equal proportions. Otherwise identifiability and testability problems arise and persist even after we decide to exclude from the model the vectors $\mu$ which have $\mu_i = \mu_j$ for some $i \neq j$. If one imagines the situation where the number of observations is of the same order as the number of classes, this should come as no surprise.

### 3.6 Dirichlet priors

The construction of priors on non-parametric models is far from trivial. Broadly, there are two mathematical reasons for this: whereas the usual norm topology on $\mathbb{R}^k$ is unique (in the sense that all other norm topologies are equivalent, see [74]), infinite-dimensional vector spaces support many different norm topologies and various other topologies besides. Similarly, whereas on $\mathbb{R}^k$ the (unique shift-invariant) Lebesgue measure provides a solid foundation for the definition of models in terms of densities, no such default uniform dominating measure exists in infinite-dimensional spaces.

Nevertheless examples of probability measures on infinite-dimensional spaces exist. Some of the constructions and properties of the measures they result in, are discussed in detail in Ghosh and Ramamoorthi (2003) [44]. In this section, we look at a class of priors first proposed by Ferguson (1973) [35], which have become known as Dirichlet process priors.

#### 3.6.1 Dirichlet distributions

Let $\mathcal{X} = \{1, 2, \ldots, k\}$ (with its powerset $2^{\mathcal{X}}$ as a $\sigma$-algebra) and consider the collection $M(\mathcal{X})$ of all probability measures on $\mathcal{X}$. Every $P \in M(\mathcal{X})$ has a density $p : \mathcal{X} \to [0, 1]$ (with respect to the counting measure on $\mathcal{X}$) and we denote $p_i = p(i) = P(\{i\})$, so that for every $A \in 2^{\mathcal{X}}$,

$$P(A) = \sum_{i \in A} p_i.$$  

Therefore, the space $M(\mathcal{X})$ can be parametrized as follows,

$$M(\mathcal{X}) = \left\{ P : 2^{\mathcal{X}} \to [0, 1] : \sum_{i=1}^k p_i = 1, p_i \geq 0, (1 \leq i \leq k) \right\},$$

and is in bijective correspondence with the simplex in $\mathbb{R}^k$. For reasons to be discussed shortly, we consider the following family of distributions on $M(\mathcal{X})$. 


Definition 3.8. (Finite-dimensional Dirichlet distribution)

Let $\alpha = (\alpha_1, \ldots, \alpha_k)$ with $\alpha_i > 0$ for all $1 \leq i \leq k$. A stochastic vector $p = (p_1, \ldots, p_k)$ is said to have Dirichlet distribution $D\alpha$ with parameter $\alpha$, if the density $\pi$ for $p$ satisfies:

$$
\pi(p) = \frac{\Gamma\left(\sum_{i=1}^{k} \alpha_i\right)}{\Gamma(\alpha_1) \cdots \Gamma(\alpha_k)} p_1^{\alpha_1-1} p_2^{\alpha_2-1} \cdots p_{k-1}^{\alpha_{k-1}-1} \left(1 - \sum_{i=1}^{k-1} p_i\right)^{\alpha_k-1}
$$

If $\alpha_i = 0$ for some $i$, $1 \leq i \leq k$, then we set $D\alpha(p_i = 0) = 1$ marginally and we treat the remaining components of $p$ as $(k-1)$-dimensional.

As an example, consider the case where $k = 2$ (so that $p_2 = 1 - p_1$): in that case, the density of the Dirichlet distribution takes the form:

$$
\pi(p_1, p_2) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1) \Gamma(\alpha_2)} p_1^{\alpha_1-1} (1 - p_1)^{\alpha_2-1},
$$

i.e. $p_1$ has a Beta distribution $B(\alpha_1, \alpha_2)$. (Examples of graphs of Beta densities with $\alpha_1 = k + 1$, $\alpha_2 = n - k + 1$ for various integer values of $k$ are depicted in figure 2.1). We also note the following two well-known facts on the Dirichlet distribution (proofs can be found in [44]).

**Lemma 3.3.** (Gamma-representation of $D\alpha$)

If $Z_1, \ldots, Z_k$ are independent and each marginally distributed according to a $\Gamma$-distribution with parameter $\alpha$, i.e.

$$
Z_i \sim \Gamma(\alpha_i),
$$

for all $1 \leq i \leq k$, then the normalized vector

$$
\left(\frac{Z_1}{S}, \ldots, \frac{Z_k}{S}\right) \sim D\alpha,
$$

(3.14)

with $S = \sum_{i=1}^{k} Z_i$.

Lemma 3.3 shows that we may think of a $D\alpha$-distributed vector as being composed of $k$ independent, $\Gamma$-distributed components, normalized to form a probability distribution, through division by $S$ in (3.14). This division should be viewed as an $L_1$-projection from the positive cone in $\mathbb{R}^k$ onto the $k-1$-dimensional simplex. The following property can also be viewed as a statement on the effect of a projection on a distribution, this time from the simplex in $\mathbb{R}^k$ to lower-dimensional simplices. It is this property (related to a property called infinite divisibility of the Dirichlet distribution) that motivates the choice for the Dirichlet distribution made by definition 3.8.

**Lemma 3.4.** Let $\mathcal{X}$ be a finite pointset. If the density $p : \mathcal{X} \to [0, 1]$ of a distribution $P$ is itself distributed according to a Dirichlet distribution with parameter $\alpha$, $p \sim D\alpha$, then for any partition $\{A_1, \ldots, A_m\}$ of $\mathcal{X}$, the vector of probabilities $(P(A_1), P(A_2), \ldots, P(A_m))$ has a Dirichlet distribution again.
\[ (P(A_1), P(A_2), \ldots, P(A_m)) \sim D_{\alpha'}, \]

where the parameter \( \alpha' \) is given by:

\[ (\alpha'_1, \ldots, \alpha'_m) = \left( \sum_{l \in A_1} \alpha_l, \ldots, \sum_{l \in A_m} \alpha_l \right). \quad (3.15) \]

The identification (3.15) in lemma 3.4 suggests that we adopt a slightly different perspective on the definition of the Dirichlet distribution: we view \( \alpha' \) as a finite measure on \( \mathcal{X} \), so that \( P \sim D_\alpha \) if and only if, for every partition \( (A_1, \ldots, A_m) \),

\[ (P(A_1), \ldots, P(A_m)) \sim D(\alpha(A_1), \ldots, \alpha(A_m)). \quad (3.16) \]

Property (3.16) serves as the point of departure of the generalization to the non-parametric model, because it does not depend on the finite nature of \( \mathcal{X} \).

**Definition 3.9.** Let \( \mathcal{X} \) be a finite pointset; denote the collection of all probability measures on \( \mathcal{X} \) by \( M(\mathcal{X}) \). The Dirichlet family \( D(\mathcal{X}) \) is defined to be the collection of all Dirichlet distributions on \( M(\mathcal{X}) \), i.e. \( D(\mathcal{X}) \) consists of all \( D_\alpha \) with \( \alpha \) a finite measure on \( \mathcal{X} \).

The following property of the Dirichlet distribution describes two independent Dirichlet-distributed quantities in convex combination, which form a new Dirichlet-distributed quantity if mixed by means of an (independent) Beta-distributed parameter.

**Lemma 3.5.** Let \( \mathcal{X} \) be a finite pointset and let \( \alpha_1, \alpha_2 \) be two measures on \( (\mathcal{X}, 2^{\mathcal{X}}) \). Let \( (P_1, P_2) \) be independent and marginally distributed as

\[ P_1 \sim D_{\alpha_1}, \quad P_2 \sim D_{\alpha_2}. \]

Furthermore, let \( \lambda \) be independent of \( P_1, P_2 \) and marginally distributed according to \( \lambda \sim B(\alpha_1(\mathcal{X}), \alpha_2(\mathcal{X})) \). Then the convex combination \( \lambda P_1 + (1 - \lambda) P_2 \) again has a Dirichlet distribution with base measure \( \alpha_1 + \alpha_2 \):

\[ \lambda P_1 + (1 - \lambda) P_2 \sim D_{\alpha_1 + \alpha_2}. \]

Many other properties of the Dirichlet distribution could be considered here, most notably the so-called tail-free property and neutrality to the right (see [44]). We do not provide details because both are rather technical and we do not use them in following chapters, but the reader should be aware of their existence because some authors use them extensively.

A most important property of the family of Dirichlet distributions is its conjugacy for the full non-parametric model.

**Theorem 3.2.** Let \( \mathcal{X} \) be a finite pointset; let \( X_1, \ldots, X_n \) denote an i.i.d. sample of observations taking values in \( \mathcal{X} \). The Dirichlet family \( D(\mathcal{X}) \) is a conjugate family: if the prior equals \( D_\alpha \), the posterior equals \( D_{\alpha + nP_n} \).
Proof. Since $\mathcal{X}$ is finite ($\#(\mathcal{X}) = k$), $M(\mathcal{X})$ is dominated (by the counting measure), so the posterior can be written as in (2.13). The likelihood takes the form:

$$P \mapsto n \prod_{i=1}^{n} p(X_i) = k \prod_{l=1}^{k} p_l^{n_l},$$

where $n_l = \#\{X_i = l : 1 \leq i \leq n\}$. Multiplying by the prior density for $\Pi = D_\alpha$, we find that the posterior density is proportional to,

$$\pi(p_1, \ldots, p_k | X_1, \ldots, X_n) \propto \pi(p_1, \ldots, p_k) n \prod_{i=1}^{n} p_{X_i} \propto k \prod_{l=1}^{k} p_l^{n_l} \alpha_{k-1} \prod_{l=1}^{k} p_l^{n_l-1} \left(1 - \sum_{l=1}^{k} p_l\right)^{\alpha_k},$$

which is again a Dirichlet density, but with changed base measure $\alpha$. Since the posterior is a probability distribution, we know that the normalization factor follows suit. Noting that we may view $n_l$ as the density of the measure $nP_n$ since

$$n_l = \sum_{i=1}^{n} \{X_i = l\} = nP_n \{X = l\},$$

we complete the argument.

### 3.6.2 The Dirichlet process

Next we consider the Dirichlet process prior, a probability measure on the full non-parametric model for a measurable space $(\mathcal{X}, \mathcal{B})$. For the sake of simplicity, we assume that $\mathcal{X} = \mathbb{R}$ and $\mathcal{B}$ is the Borel $\sigma$-algebra on $\mathbb{R}$. We denote the collection of all probability measures on $(\mathbb{R}, \mathcal{B})$ by $M(\mathbb{R}, \mathcal{B})$. We consider the collection of random quantities $\{P(A) : A \in \mathcal{B}\}$ and impose two straightforward conditions on its finite-dimensional marginals. The Kolmogorov existence theorem (see theorem A.8) then guarantees existence of a stochastic process with finitely additive sample path $P : \mathcal{B} \rightarrow [0, 1]$. Said straightforward conditions are satisfied if we choose the finite-dimensional marginal distributions to be (finite-dimensional) Dirichlet distributions (3.16). Also by this choice, $\sigma$-additivity of $P$ can be guaranteed. The resulting process on the space of all probability measures on $(\mathcal{X}, \mathcal{B})$ is called the called the Dirichlet process and the associated probability measure $\Pi$ is called the Dirichlet process prior.

**Theorem 3.3.** (Existence of the Dirichlet process)

Given a finite measure $\alpha$ on $(\mathbb{R}, \mathcal{B})$, there exists a probability measure $D_\alpha$ on $M(\mathbb{R}, \mathcal{B})$ (called the Dirichlet process prior with parameter $\alpha$) such that for $P \sim D_\alpha$ and every $\mathcal{B}$-measurable partition $(B_1, \ldots, B_k)$ of $\mathbb{R}$,
3.6 Dirichlet priors

\((P(B_1),\ldots,P(B_k)) \sim D(\alpha(B_1),\ldots,\alpha(B_k))\).  \hspace{1cm} (3.17)

**Proof.** Proof Let \(k \geq 1\) and \(A_1,\ldots,A_k \in \mathcal{B}\) be given. Through the indicators \(1_{A_i}\) for these sets, we define \(2^k\) new sets

\[1_{A_{v_1}\ldots v_k} = \prod_{i=1}^k 1_{A_i}^{v_i}(1-1_{A_i})^{1-v_i},\]

where \(v_1,\ldots,v_k \in \{0,1\}\). Then the collection \(\{B_{v_1\ldots v_k} : v_i \in \{0,1\}, 1 \leq i \leq k\}\) forms a partition of \(\mathbb{R}\). For the \(P\)-probabilities corresponding to this partition, we assume finite-dimensional marginals

\((P(B_{v_1}\ldots v_k) : v_i \in \{0,1\}, 1 \leq i \leq k) \sim \Pi_{B_{v_1}\ldots v_k : v_i \in \{0,1\}, 1 \leq i \leq k}\).

The distribution of the vector \((P(A_1),\ldots,P(A_k))\) then follows from the definition:

\[P(A_i) = \sum_{\{v_i=1\}} P(B_{v_1\ldots v_k}),\]

for all \(1 \leq i \leq k\). This defines marginal distributions for all finite subsets of \(\mathcal{B}\), as needed in theorem A.8. To define the underlying probability space \((\Omega, \mathcal{F}, \Pi)\) we now impose two conditions.

(F1) With \(\Pi\)-probability one, the empty set has \(P\)-measure zero:

\[\Pi(P(\emptyset) = 0) = 1.\]

(F2) Let \(k, k' \geq 1\) be given. If \((B_1,\ldots,B_k)\) is a partition and \((B'_1,\ldots,B'_{k'})\) a refinement thereof, with

\[B_1 = \bigcup_{i=1}^{r_1} B'_i, \ldots, B_k = \bigcup_{i=r_{k-1}+1}^{k'} B'_i,\]

(for certain \(r_1 < \ldots < r_{k-1}\)), then we have the following equality in distribution:

\[\mathcal{L} \left( \sum_{i=1}^{r_1} P(B'_i), \ldots, \sum_{i=r_{k-1}+1}^{k'} P(B'_i) \right) = \mathcal{L} \left( P(B_1),\ldots,P(B_k) \right).\]

Condition (F1) ensures that if \((A_1,\ldots,A_k)\) is itself a partition of \(\mathbb{R}\), the above construction does not lead to a contradiction. Condition (F2) ensures finite additivity of \(P\) with prior probability one, \(i.e.\) for any \(A,B,C \in \mathcal{B}\) such that \(A \cap B = \emptyset\) and \(A \cup B = C\),

\[\Pi(P(A) + P(B) = P(C)) = 1.\]  \hspace{1cm} (3.18)

Ferguson (1973,1974) [35, 36] has shown that conditions (F1) and (F2) imply that Kolmogorov’s consistency conditions (K1) and (K2) (see section A.4) are satisfied. As we have seen in the first part of this section, if we impose the Dirichlet distribution:
and \( \alpha \) is a measure on \( \mathcal{B} \), condition (F2) is satisfied. Combining all of this, we conclude that there exists a probability space \((\Omega, \mathcal{F}, \Pi)\) on which the stochastic process \( \{ P(A) : A \in \mathcal{B} \} \) can be represented with finite dimensional marginals c.f. (3.19). Lemma 3.6 shows that \( \Pi(P \in \mathcal{M}(\mathbb{R}, \mathcal{B})) = 1 \), completing the proof.

The last line in the above proof may require some further explanation: \( P \) is merely the sample-path of our stochastic process. The notation \( P(A) \) suggests that \( P \) is a probability measure, but all we have shown up to that point, is that (F1) and (F2) imply that \( P \) is a finitely additive set-function such that:

\[
\Pi(P(B) \in [0, 1]) = 1,
\]

with \( \Pi \)-probability equal to one. What remains to be demonstrated is \( \Pi \)-almost-sure \( \sigma \)-additivity of \( P \).

**Lemma 3.6.** If \( \Pi \) is a Dirichlet process prior \( D_\alpha \) on \( \mathcal{M}(\mathcal{X}, \mathcal{B}) \),

\[
\Pi(P \text{ is } \sigma\text{-additive}) = 1.
\]

**Proof.** Proof Let \((A_n)_{n \geq 1}\) be a sequence in \( \mathcal{B} \) that decreases to \( \varnothing \). Since \( \alpha \) is \( \sigma \)-additive, \( \alpha(A_n) \to \alpha(\varnothing) = 0 \). Therefore, there exists a subsequence \((A_{n_j})_{j \geq 1}\) such that \( \sum_j \alpha(A_{n_j}) < \infty \). For fixed \( \varepsilon > 0 \), using Markov’s inequality first,

\[
\sum_{j \geq 1} \Pi(P(A_{n_j}) > \varepsilon) \leq \sum_{j \geq 1} \frac{1}{\varepsilon} \int P(A_{n_j}) d\Pi(P) = \frac{1}{\varepsilon} \sum_{j \geq 1} \frac{\alpha(A_{n_j})}{\alpha(\mathbb{R})} < \infty,
\]

according to lemma 3.7. From the Borel-Cantelli lemma (see lemma A.2), we see that

\[
\Pi(\limsup_{j \to \infty} \{ P(A_{n_j}) > \varepsilon \}) = \Pi(\bigcap_{j \geq 1} \bigcup_{j \geq j} \{ P(A_{n_j}) > \varepsilon \}) = 0,
\]

which shows that \( \lim_j P(A_{n_j}) = 0 \), \( \Pi \)-almost-surely. Since, by \( \Pi \)-almost-sure finite additivity of \( P \),

\[
\Pi(P(A_n) \geq P(A_{n+1}) \geq \ldots) = 1,
\]

we conclude that \( \lim_n P(A_n) = 0 \), \( \Pi \)-almost-surely. By the continuity theorem for measures (see theorem A.1 and the proof in [57], theorem 3.2), \( P \) is \( \sigma \)-additive \( \Pi \)-almost-surely.

The proof of lemma 3.6 makes use of the following lemma, which establishes the basic properties of the Dirichlet process prior.

**Lemma 3.7.** Let \( \alpha \) be a finite measure on \((\mathbb{R}, \mathcal{B})\) and let \( \{ P(A) : A \in \mathcal{B} \} \) be the associated Dirichlet process with distribution \( D_\alpha \). Let \( B \in \mathcal{B} \) be given.

(i) If \( \alpha(B) = 0 \), then \( P(B) = 0 \), \( \Pi \)-a.s.

(ii) If \( \alpha(B) > 0 \), then \( P(B) > 0 \), \( \Pi \)-a.s.
The expectation of $P$ under $D_\alpha$ is given by

$$\int P(B) dD_\alpha(P) = \frac{\alpha(B)}{\alpha(\mathbb{R})}.$$ 

**Proof.** Proof Let $B \in \mathcal{B}$ be given. Consider the partition $(B_1, B_2)$ of $\mathbb{R}$, where $B_1 = B, B_2 = \mathbb{R} \setminus B$. According to (3.17),

$$\left( P(B_1), P(B_2) \right) \sim D_{\left( \alpha(B), \alpha(\mathbb{R}) - \alpha(B) \right)},$$

so that $P(B) \sim B(\alpha(B), \alpha(\mathbb{R}) - \alpha(B))$. Stated properties then follow from the properties of the Beta-distribution.

This concludes the proof for the existence of Dirichlet processes and the associated priors. One may then wonder what is the nature of the prior we have constructed. As it turns out, the Dirichlet process prior has some remarkable properties.

**Lemma 3.8. (Support of the Dirichlet process prior)**

Consider $M(\mathbb{R}, \mathcal{B})$, endowed with the topology of weak convergence. Let $\alpha$ be a finite measure on $(\mathbb{R}, \mathcal{B})$. The support of $D_\alpha$ is given by

$$M_\alpha(\mathbb{R}, \mathcal{B}) = \{ P \in M(\mathbb{R}, \mathcal{B}) : \supp(P) \subset \supp(\alpha) \}.$$ 

In fact, we can be more precise, as shown in the following lemma.

**Lemma 3.9.** Let $\alpha$ be a finite measure on $(\mathbb{R}, \mathcal{B})$ and let $\{ P(A) : A \in \mathcal{B} \}$ be the associated Dirichlet process with distribution $D_\alpha$. Let $Q \in M(\mathbb{R}, \mathcal{B})$ be such that $Q \ll \alpha$. Then, for any $m \geq 1$ and $A_1, \ldots, A_m \in \mathcal{B}$ and $\varepsilon > 0$,

$$D_\alpha \{ P \in M(\mathbb{R}, \mathcal{B}) : |P(A_i) - Q(A_i)| < \varepsilon, 1 \leq i \leq m \} > 0.$$ 

**Proof.** Proof The proof of this lemma can be found in [44], theorem 3.2.4.

So if we endow $M(\mathbb{R}, \mathcal{B})$ with the (slightly stronger) topology of pointwise convergence (see definition A.19), the support of $D_\alpha$ remains large, consisting of all $P \in M(\mathbb{R}, \mathcal{B})$ that are dominated by $\alpha$.

The following property reveals a most remarkable characterization of Dirichlet process priors: the subset $D(\mathbb{R}, \mathcal{B})$ of all finite convex combinations of Dirac measures (see example A.3) receives prior mass equal to one.

**Lemma 3.10.** Let $\alpha$ be a finite measure on $(\mathbb{R}, \mathcal{B})$ and let $\{ P(A) : A \in \mathcal{B} \}$ be the associated Dirichlet process with distribution $D_\alpha$. Then,

$$D_\alpha \{ P \in D(\mathbb{R}, \mathcal{B}) \} = 1.$$ 

**Proof.** Proof The proof of this lemma can be found in [44], theorem 3.2.3.

The above phenomenon leads to problems with support or convergence in stronger topologies (like total variation or Hellinger topologies) and with regard to the
Kullback-Leibler criteria that govern asymptotic concentration of posterior mass. Generalizing this statement somewhat, we may infer from the above that the Dirichlet process prior is not suited to (direct) estimation of densities. Although clearly dense enough in \( M(\mathbb{R}, \mathcal{B}) \) in the topology of weak convergence, the set \( D(\mathbb{R}, \mathcal{B}) \) may be rather sparse in stronger topologies! (Notwithstanding the fact that mixture models with a Dirichlet process prior for the mixing distribution can be (minimax) optimal for the estimation of mixture densities [42].)

**Lemma 3.11.** Let \( \alpha \) be a finite measure on \((\mathbb{R}, \mathcal{B})\) and let \( \{P(A) : A \in \mathcal{B}\} \) be the associated Dirichlet process with distribution \( D_\alpha \). Let \( g : \mathbb{R} \to \mathbb{R} \) be non-negative and Borel-measurable. Then,
\[
\int_{\mathbb{R}} g(x) \, d\alpha(x) < \infty \iff \int_{\mathbb{R}} g(x) \, dP(x) < \infty, \quad (D_\alpha \text{ a.s.}).
\]

**Proof.** Proof Add proof!

Perhaps the most important result of this section is the fact that the family of Dirichlet process priors on \( M(\mathbb{R}, \mathcal{B}) \) is a conjugate family for the full, non-parametric model on \((\mathbb{R}, \mathcal{B})\), as stated in the following theorem.

**Theorem 3.4.** Let \( X_1, X_2, \ldots \) be an i.i.d. sample of observations in \( \mathbb{R} \). Let \( \alpha \) be a finite measure on \((\mathbb{R}, \mathcal{B})\) with associated Dirichlet process prior \( \Pi = D_\alpha \). For any measurable \( C \subset M(\mathbb{R}, \mathcal{B}) \),
\[
\Pi \left( P \in C \mid X_1, \ldots, X_n \right) = D_{\alpha + nP_n}(C),
\]
i.e. the posterior is again a Dirichlet process distribution, with base measure \( \alpha + nP_n \).

**Proof.** Proof The proof is a direct consequence of theorem 3.2 and the fact that equality of two measures on a generating ring implies equality on the whole \( \sigma \)-algebra. (Cylindersets generate the relevant \( \sigma \)-algebra and for cylindersets, theorem 3.2 asserts equality.)

**Example 3.11.** Let \( X_1, X_2, \ldots \) be an i.i.d. sample of observations in \( \mathbb{R} \). Let \( \alpha \) be a finite measure on \((\mathbb{R}, \mathcal{B})\) with associated Dirichlet process prior \( \Pi = D_\alpha \). Let \( B \in \mathcal{B} \) be given. The expectation of \( P(B) \) under the prior distribution equals,
\[
\int P(B) \, dD_\alpha(P) = \frac{\alpha(B)}{\alpha(\mathbb{R})}, \quad (3.20)
\]
the measure of \( B \) under \( \alpha \) normalized to be a probability measure (which we denote by \( P_\alpha(B) \)). The posterior mean (see definition 2.7), is then given by:
\[
\int P(B) \, d\Pi \bigg( P \mid X_1, \ldots, X_n \bigg) = \int P(B) \, dD_{\alpha + nP_n}(P) = \frac{(\alpha + nP_n)(B)}{(\alpha + nP_n)(\mathbb{R})} = \frac{\alpha(\mathbb{R})}{\alpha(\mathbb{R}) + n} P_\alpha(B) + \frac{n}{\alpha(\mathbb{R}) + n} P_n(B),
\]
3.7 Exercises

3.7.1 Exercises 97

$P_0^n$-almost-surely. Defining $\lambda_n = \alpha(R)/(\alpha(R) + n)$, we see that the posterior mean $\hat{P}_n$ can be viewed as a convex combination of the prior mean distribution and the empirical distributions,

$$\hat{P}_n = \lambda_n P_\alpha + (1 - \lambda_n) P_n,$$

$P_0^n$-almost-surely. As a result, we see that

$$\|\hat{P}_n - P_n\|_{TV} = \lambda_n \|P_\alpha - P_n\| \leq \lambda_n,$$

$P_0^n$-almost-surely. Since $\lambda_n \to 0$ as $n \to \infty$, the difference between the sequence of posterior means $(\hat{P}_n)_{n \geq 1}$ and the sequence of empirical measures $(P_n)_{n \geq 1}$ converges to zero in total variation as we let the samplesize grow to infinity. Generalizing likelihood methods to non-dominated models, Dvoretzky, Kiefer and Wolfowitz (1956) [31] have shown that the empirical distribution $P_n$ can be viewed as the non-parametric maximum-likelihood estimator (usually abbreviated NPMLE). This establishes (an almost-sure form of) consistency for the posterior mean, in the sense that it has the same point of convergence as the NPMLE.

Remark 3.10. The above example provides the subjectivist with a guideline for the choice of the base measure $\alpha$. More particularly, equality (3.20) says that the prior predictive distribution equals the (normalized) base measure $\alpha$. In view of the fact that subjectivists should choose the prior to reflect their prior “beliefs”, $\alpha$ should therefore be chosen such that it assigns relatively high mass to sets $B \in \mathcal{B}$ that are believed to be probable.

3.7 Exercises

3.1. A PROPER JEFFREYS PRIOR

Let $X$ be a random variable, distributed $\text{Bin}(n; p)$ for known $n$ and unknown $p \in (0, 1)$. Calculate Jeffreys prior for this model, identify a standard family of probability distributions that this prior would belong to, if it were normalized as a probability distribution.

3.2. JEFFREYS AND UNIFORM PRIORS

Let $\mathcal{P}$ be a model parametrized according to some mapping $\Theta \to \mathcal{P} : \theta \mapsto P_\theta$. Assuming differentiability of this map, Jeffreys prior $\Pi$ takes the form (3.7). In other parametrizations, the form of this expression remains the same, but the actual dependence on the parameter changes. This makes it possible that there exists another parametrization of $\mathcal{P}$ such that Jeffreys prior is equal to the uniform prior. We shall explore this possibility below.

For each of the following models in their ‘standard’ parametrizations $\theta \mapsto P_\theta$, find a parameter $\eta \in H$, $\eta = \eta(\theta)$, such that the Fisher information $I_\eta$, expressed in terms of $\eta$, is constant.

a. Find $\eta$ for $\mathcal{P}$ the model of all Poission distributions.
b. In the cases $\alpha = 1, 2, 3$, find $\eta$ for the model $\mathcal{P}$ consisting of all $\Gamma(\alpha, \theta)$-distributions, with $\theta \in (0, \infty)$.

c. Find $\eta$ for the model $\mathcal{P}$ of all $\text{Bin}(n; \theta)$ distributions, where $n$ is known and $\theta \in (0, 1)$.

Note that if the Fisher information $I_\eta$ is constant, Jeffries prior is uniform. Therefore, if a parametrization like above exists and $H$ is unbounded, Jeffries prior is improper (in all parametrizations).

3.3. **Optimality of Unbiased Bayesian Point Estimators**

Let $\mathcal{P}$ be a dominated, parametric model, parametrized identifiably by $\Theta \rightarrow \mathcal{P} : \theta \mapsto P_{\theta}$, for some $\Theta \subset \mathbb{R}^k$. Assume that $(X_1, \ldots, X_n) \in \mathcal{X}^n$ form an i.i.d. sample from a distribution $P_0 = P_{\theta_0} \in \mathcal{P}$, for some $\theta_0 \in \Theta$. Let $\Pi$ be a prior on $\Theta$ and denote the posterior by $\Pi(X_1, \ldots, X_n)$. Assume that $T : \mathcal{X}^n \rightarrow \mathbb{R}^m$ is a sufficient statistic for the model $\mathcal{P}$.

a. Use the factorization theorem to show that the posterior depends on the data only through the sufficient statistic $T(X_1, \ldots, X_n)$.

b. Let $\hat{\theta}_n : \mathcal{X}^n \rightarrow \Theta$ denote a point-estimator derived from the posterior. Use a. above to argue that there exists a function $\tilde{\theta}_n : \mathbb{R}^m \rightarrow \Theta$, such that,

$$
\hat{\theta}_n(X_1, \ldots, X_n) = \tilde{\theta}_n(T(X_1, \ldots, X_n)).
$$

Bayesian point-estimators share this property with other point-estimators that are derived from the likelihood function, like the maximum-likelihood estimator and penalized versions thereof. Next, assume that $T$ is complete, that $P_0^\theta(\hat{\theta}_n)^2 < \infty$ and that $\hat{\theta}_n$ is unbiased, i.e. $P_0^\theta \hat{\theta}_n = \theta_0$.

c. Apply the Lehmann-Scheffé theorem to prove that, for any other unbiased estimator $\hat{\theta}_n' : \mathcal{X}^n \rightarrow \Theta$,

$$
P_0^\theta(\hat{\theta}_n' - \theta_0)^2 \leq P_0^\theta(\hat{\theta}_n - \theta_0)^2.
$$

The message of this exercise is, that Bayesian point-estimators that happen to be unbiased and quadratically integrable, are automatically $L_2$-optimal in the class of all unbiased estimators for $\theta$. They share this remarkable property with maximum-likelihood estimators.

3.4. **Conjugate Model-prior Pairs**

In this exercise, conjugate model-prior pairs $(\mathcal{P}, \Pi)$ are provided. In each case, we denote the parameter we wish to estimate by $\theta$ and assume that other parameters have known values. Let $X$ denote a single observation.

In each case, derive the posterior distribution to prove conjugacy and identify the $X$-dependent transformation of parameters that takes prior into posterior.

a. $X|\theta \sim N(\theta, \sigma^2)$ and $\theta \sim N(\mu, \tau^2)$.

b. $X|\theta \sim \text{Poisson}(\theta)$ and $\theta \sim \Gamma(\alpha, \beta)$.

c. $X|\theta \sim \Gamma(\rho, \theta)$ and $\theta \sim \Gamma(\alpha, \beta)$. 
d. \( X|\theta \sim \text{Bin}(n; \theta) \) and \( \theta \sim \beta(\alpha, \beta) \).
e. \( X|\theta \sim N(\mu, \theta^{-1}) \) and \( \theta \sim \Gamma(\alpha, \beta) \).
f. \( X|\theta_1, \ldots, \theta_k \sim M(n; \theta_1, \ldots, \theta_k) \) and \( \theta \sim D_\alpha \), where \( M \) denotes the multinomial distribution for \( n \) observations drawn from \( k \) classes with probabilities \( \theta_1, \ldots, \theta_k \) and \( D_\alpha \) is a Dirichlet distribution on the simplex in \( \mathbb{R}^k \) (see definition 3.8).

3.5. In this exercise, we generalize the setup of example 3.9 to multinomial rather than binomial context. Let \( k \geq 1 \) be known. Consider an observed random variable \( Y \) and an unobserved \( N = 1, 2, \ldots \), such that, conditionally on \( N \), \( Y \) is distributed multinomially over \( k \) classes, while \( N \) has a Poisson distribution with hyperparameter \( \lambda > 0 \),

\[
Y|N \sim M_k(N; p_1, p_2, \ldots, p_k), \quad N \sim \text{Poisson}(\lambda).
\]

Determine the prior predictive distribution of \( Y \), as a function of the hyperparameter \( \lambda \).

3.6. Let \( X_1, \ldots, X_n \) form an i.i.d. sample from a Poisson distribution \( \text{Poisson}(\theta) \) with unknown \( \theta > 0 \). As a family of possible priors for the Bayesian analysis of this data, consider exponential distributions \( \theta \sim \Pi_\lambda = \text{Exp}(\lambda) \), where \( \lambda > 0 \) is a hyperparameter.

a. Calculate the prior predictive distribution for \( X \).
b. Give the ML-II estimate \( \hat{\lambda} \) for \( \lambda \).
c. With the estimated hyperparameter, give the posterior distribution \( \theta|X_1, \ldots, X_n \).
d. Calculate the posterior mean. Compare its data-dependence to that of the posterior mean we would have obtained if we had not made an empirical choice for the hyperparameter, but a fixed choice.

3.7. Let \( X_1, \ldots, X_n \) form an i.i.d. sample from a binomial distribution \( \text{Bin}(N; p) \), for known \( N \) and unknown \( p \in [0, 1] \). For the parameter \( p \) we take a prior \( p \sim \beta(\alpha, \beta) \) with hyperparameters \( \alpha, \beta > 0 \).

a. Show that the family of \( \beta \)-distributions is conjugate for binomial data.
b. Using (standard expressions for) the expectation and variance of \( \beta \)-distributions, give the posterior mean and variance in terms of the original \( \alpha \) and \( \beta \) chosen for the prior and the data.
c. Calculate the prior predictive distribution and discuss the steps one would perform in the ML-II procedure to estimate \( p \).
Given an infinite \textit{i.i.d.} sample $X_1, X_2, \ldots$ drawn from $P_0$ and a model $\mathcal{P}$, an estimation procedure prescribes a sequence of estimates $\hat{P}_n \in \mathcal{P}$, each calculated using only the first $n$ observations. More generally, any statistical procedure can be indexed by the size $n$ of the sample used to calculate it, leading to sequences of (parameter) estimates, tests, confidence regions, \textit{etcetera}. Properties of such sequences reflect the behaviour of the estimation procedure with growing sample-size. An intuitively reasonable requirement of any estimation procedure is a property known as consistency: the sequence $\hat{P}_n$ approaches the true distribution $P_0$ to within arbitrary precision if the sample on which the estimation is based is made large enough. Similarly, samples of arbitrarily large size should enable one to test with power arbitrarily close to one and define arbitrarily small confidence regions. Further analysis of a consistent sequence $\hat{P}_n$ concerns the (suitably rescaled) distribution of the estimator-sequence around its point of convergence. The mathematical formulation of these concepts is based on so-called limit theorems, which describe the behaviour of an estimation procedure in the limit that the number of measurements goes to infinity.

The study of the asymptotic regime of an estimation procedure is interesting for two reasons. First of all, asymptotic results provide approximations to exact values; finite-sample calculations often become intractable, even in relatively simple (parametric) situations. However, the analysis of the large-sample limit is often still possible when finite-sample are hard to carry out exactly. The answer obtained in the large-sample limit may then be used as an approximation to the finite-sample answer (asymptotic confidence intervals are a good example). Secondly, if we have several possible estimation procedures available for a certain problem, asymptotic behaviour provides us with the means to compare their performance for large samples. Of course, the first performance criterion is consistency. To choose between two consistent procedures, one may consider rate of convergence and properties of the limit distribution characterising the degree of concentration (like asymptotic variance or asymptotic risk).

In this chapter, we consider the asymptotic behaviour of the Bayesian procedure in cases where the model is parametric and depends on the parameter in a smooth fashion. Certainly the most useful reference for this subject is Le Cam and Yang
Asymptotics and the Bernstein-von Mises theorem

and a version of the Bernstein-von Mises theorem can also be found in Le Cam (1986) [69]. A more readable version of the argument can be found in chapter 10 of van der Vaart (1998) [90].

4.1 Efficiency in smooth parametric models

In this section we consider estimation in smooth, parametric models and formulate a theorem that characterizes efficiency, a notion of optimality in the class of all so-called regular estimators. The aim of this lecture is to prepare for the Bernstein-von Mises theorem, which asserts that posterior distributions in smooth parametric models tend to follow efficient estimators and lead to efficient inferential conclusions.

Recall from chapter 2 that at the conceptual level, the Bayesian posterior plays a role that is analogous to that of the frequentist sampling distribution: it is a distribution on the model or on its parameter space, supposedly informative at the inferential level. In the following, we shall not be too strict in Bayesian, subjectivist orthodoxy and interpret the posterior as a frequentist device, in a role very close conceptually to that of the sampling distribution of an estimator used above.

From that perspective it is natural to wonder whether credible sets and confidence sets have anything to do with each other. Since they are conceptually so close, could it be that they are close also mathematically, at least, when explained as frequentist devices? In this section we discuss efficiency of (point-)estimation culminating in the so-called convolution theorem, which provides a notion of asymptotic optimality at the inferential level (for the class of all regular estimators). In the next lecture, we switch to the Bayesian leg of the story and show that a correspondence between confidence sets and credible sets does exist asymptotically in smooth, parametric models.

The so-called Bernstein-von Mises theorem (see theorem 4.4 below [71]) not only demonstrates asymptotic equivalence of credible sets and confidence sets, it also shows that the relevant sets are optimal in the sense that they are associated with so-called efficient estimators. Essential to the development of the optimality theory are two concepts: differentiability of the model and regularity of the estimator. Combined, these two properties lead to a notion of optimality comparable to estimators that achieve optimality within the family of unbiased estimators in the Cramér-Rao sense.

4.1.1 Optimality in smooth, parametric estimation problems

The concept of efficiency has its origin in Fisher’s 1920’s claim of asymptotic optimality of the maximum-likelihood estimator in differentiable parametric models. Here, optimality of the ML estimate means that they are consistent, achieve opti-
mal $n^{-1/2}$ rate of convergence and possessed a asymptotic sampling distribution of minimal variance. In 1930’s and 40’s, Fisher’s ideas on optimality in differentiable models were sharpened and elaborated upon. To illustrate, consider the following classical result from $M$-estimation (which can be found as theorem 5.23 in [90]).

**Theorem 4.1.** Let $\Theta$ be open in $\mathbb{R}^k$ and assume that $\mathcal{P}$ is characterized by densities $p_\theta : \mathcal{X} \to \mathbb{R}$ such that $\theta \mapsto \log p_\theta (x)$ is differentiable at $\theta_0$ for all $x \in \mathcal{X}$, with derivative $\ell_\theta(x)$. Assume that there exists a function $\ell : \mathcal{X} \to \mathbb{R}$ such that $P_0 |\ell|^2 < \infty$ and

$$|\log p_{\theta_1}(x) - \log p_{\theta_2}(x)| \leq \ell(x) \|\theta_1 - \theta_2\|,$$

for all $\theta_1, \theta_2$ in an open neighbourhood of $\theta_0$. Furthermore, assume that $\theta \mapsto P_0 \log p_\theta$ has a second-order Taylor expansion around $\theta_0$ of the form,

$$P_{\theta_0} \log p_{\theta} = P_{\theta_0} \log p_{\theta_0} + \frac{1}{2} (\theta - \theta_0)^T I_{\theta_0} (\theta - \theta_0) + o(\|\theta - \theta_0\|^2),$$

with non-singular $I_{\theta_0}$. If $(\hat{\theta}_n)$ is a sequence satisfying,

$$\mathbb{P}_n \log \hat{p}_{\theta_0} \geq \sup_{\theta \in \Theta} \mathbb{P}_n \log p_{\theta_0} - o_p(n^{-1}),$$

such that $\hat{\theta}_n \overset{\mathbb{P}}{\to} \theta_0$, then the estimator sequence is asymptotically linear,

$$n^{1/2}(\hat{\theta}_n - \theta_0) = n^{-1/2} \sum_{i=1}^n I_{\theta_0}^{-1/2} \ell_{\theta_0}(X_i) + o_P(1).$$

In particular, $n^{1/2}(\hat{\theta}_n - \theta_0) \overset{\mathbb{P}}{\to} N(0, I_{\theta_0}^{-1}).$

The last assertion of theorem 4.1 says that the (near-)maximum-likelihood estimators $(\hat{\theta}_n)$ are asymptotically consistent, converge at rate $n^{-1/2}$ and have the inverse Fisher information $I_{\theta_0}^{-1}$ as the covariance matrix for their (normal) limit distribution. At this stage of the discussion, we do not have an argument to show that this asymptotic behaviour is in any sense optimal. Nevertheless, let us take the opportunity to illustrate briefly how asymptotic behaviour translates into inference on $\theta$ by considering associated asymptotic confidence sets.

An asymptotic confidence set is an approximate confidence set that is derived not from exact sampling distributions, but from approximations implied by limit distributions, e.g. from $n^{1/2}(\hat{\theta}_n - \theta_0) \overset{\mathbb{P}}{\to} N(0, I_{\theta_0}^{-1})$ in the above example. To demonstrate, first suppose that the model is one-dimensional and satisfies the conditions of theorem 4.1. Denoting quantiles of the standard normal distribution by $\xi_{1/2}$, we see from the last assertion of the theorem that:

$$P_{\theta_0} \left( - \xi_{1/2} I_{\theta_0}^{-1/2} \leq n^{1/2}(\hat{\theta}_n - \theta_0) \leq \xi_{1/2} I_{\theta_0}^{-1/2} \right) \to 1 - 2\alpha.$$

If the Fisher information were known, this would give rise immediately to a confidence interval: the above display implies that,
has coverage probability $1 - 2\alpha$. Since the Fisher information is not known exactly, we substitute an estimator for it, for example the sample variance $S_n^2$, to arrive at a studentized version of the above, which has the same asymptotic coverage and can therefore be used as an asymptotic confidence interval. But we could also have chosen to “plug in” the estimator $\hat{\theta}_n$ for $\theta_0$ in the expression for the Fisher information to arrive at an estimate $I_{\hat{\theta}_n}$. To generalize to higher-dimensional $\Theta \subset \mathbb{R}^k$, recall that if $Z$ has a $k$-dimensional multivariate normal distribution $N_k(0, \Sigma)$, then $Z^T \Sigma^{-1} Z$ possesses a $\chi^2$-distribution with $k$ degrees of freedom. Denoting quantiles of the $\chi^2$-distribution with $k$ degrees of freedom by $\chi^2_{k, \alpha}$, we find that ellipsoids of the form,

$$C_{\alpha}(X_1, \ldots, X_n) = \{ \theta \in \Theta : n(\theta - \hat{\theta}_n)^T I_{\hat{\theta}_n} (\theta - \hat{\theta}_n) \leq \chi^2_{k, \alpha} \},$$

(4.1)

have coverage probabilities converging to $1 - \alpha$ and are therefore asymptotic confidence sets.

### 4.1.2 Regularity and efficiency

Theorem 4.1 requires a rather large number of smoothness properties of the model: log-densities are required to be differentiable and Lipschitz and the Kullback-Leibler divergence must display a second-order expansion with non-singular second derivative matrix. These sufficient conditions are there to guarantee that the ML estimator displays a property known as regularity and the conditions listed are usually referred to as “regularity conditions”. The prominence of regularity in the context of optimality questions was not fully appreciated until J. Hodges discovered an estimator that displayed a property now known as superefficiency in 1951.

**Example 4.1.** Suppose that we estimate a parameter $\theta \in \Theta = \mathbb{R}$ with an estimator sequence $(T_n)$, satisfying limiting behaviour described by $n^{1/2}(T_n - \theta) \overset{\Theta}{\rightarrow} L_\theta$ for some laws $L_\theta$, for all $\theta \in \Theta$. In addition, we define a so-called shrinkage estimator $S_n$, by $S_n = T_n$ as long as $|T_n| \geq n^{-1/4}$ and $S_n = 0$ otherwise. The name shrinkage estimator arises because any realization of $T_n$ that is close enough to 0 is shrunk to 0 fully. One shows quite easily that $S_n$ has the same asymptotic behaviour as $T_n$ as long as $\theta \neq 0$, i.e. $n^{1/2}(S_n - \theta) \overset{\Theta}{\rightarrow} L_\theta$ if $\theta \neq 0$. By contrast, if $\theta = 0$, $e_n(S_n - 0) \overset{\Theta}{\rightarrow} 0$ for any rate sequence $e_n$. In other words, the asymptotic quality of $S_n$ is as good as that of $T_n$, or strictly better if $\theta = 0$! (NB: Superefficiency does come at a price, paid in terms of the behaviour of risk functions in neighbourhoods of the point of shrinkage. Furthermore, in one dimensional parametric models, superefficiency can be achieved on a subset of Lebesgue measure no greater than zero. In models of dimension 3 or higher, this restriction does not apply, as demonstrated by the James-Stein phenomenon.)
So at certain points in the parameter space, Hodges’ shrinkage estimators and other superefficient estimators outperform the MLE and other estimators like it asymptotically, while doing equally well for all other points. Superefficiency indicated that Fisher’s 1920’s claim was false without further refinement and that a comprehensive understanding of optimality in differentiable estimation problems remained elusive.

To resolve the issue and arrive at a sound theory of asymptotic optimality of estimation in differentiable models, we have to introduce two concepts. The first is a concise notion of smoothness that describes local behaviour of likelihood products directly in terms of score functions. The “local” aspect of the definition stems from the $n$-dependent re-coordinatization in terms of the local parameter $h = n^{1/2}(\theta - \theta_0)$. (In the following we assume that the sample is i.i.d., although usually the definition is extended to more general models for the data.)

**Definition 4.1.** (Local asymptotic normality, [67])

Let $\Theta \subset \mathbb{R}^k$ be open, parametrizing a model $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ that is dominated by a $\sigma$-finite measure with densities $p_\theta$. The model is said to be locally asymptotically normal (LAN) at $\theta_0$ if, for any converging sequence $h_n \to h$:

$$\log \prod_{i=1}^n \frac{p_{\theta_0 + n^{-1/2}h_n}(X_i)}{p_{\theta_0}} = h^T \Gamma_{n,\theta_0} - \frac{1}{2} h^T I_{\theta_0} h + o_p(1), \quad (4.2)$$

for random vectors $\Gamma_{n,\theta_0}$ such that $\Gamma_{n,\theta_0} \overset{\mathcal{L}}{\Rightarrow} N_k(0, I_{\theta_0})$.

For example, if the data is distributed i.i.d., differentiability of the log-density $\theta \mapsto \log p_\theta(x)$ at $\theta_0$ for every $x$ (with score $\ell_{\theta_0}(x) = (d/d\theta) \log p_\theta(x)$) implies that the model is LAN at $\theta_0$ with,

$$\Gamma_{n,\theta_0} = n^{-1/2} \sum_{i=1}^n \ell_{\theta_0}(X_i).$$

But local asymptotic normality can be achieved under weaker conditions; best known is the following property, best described as Hadamard differentiability of square-roots of model densities relative to the $L_2(P_{\theta})$ norm.

**Definition 4.2.** Let $\Theta \subset \mathbb{R}^k$ be open. A model $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ that is dominated by a $\sigma$-finite measure $\mu$ with densities $p_\theta$ is said to be differentiable in quadratic mean (DQM) at $\theta_0$ if, there exists a score function $\ell_{\theta_0} \in L_2(P_{\theta_0})$ such that:

$$\int \left( P_{\theta_0 + h}^{1/2} - P_{\theta_0}^{1/2} - \frac{1}{2} h^T \ell_{\theta_0} P_{\theta_0}^{1/2} \right)^2 d\mu = o(||h||^2),$$

as $h \to 0$.

Theorem 7.2 in [90] shows that a model that is DQM at $\theta_0$ is LAN at $\theta_0$. However, in many situations, it is quite straightforward to demonstrate the LAN property directly.

The second concept is a property that characterizes the class of estimators over which optimality is achieved, in particular excluding Hodges’ shrinkage estimators.
(and all other examples of superefficiency, as becomes clear below). To prepare the
definition heuristically, note that, given Hodges’ counterexample, it is not enough
to have estimators with pointwise convergence to limit laws; we must restrict the
behaviour of estimators over \((n^{-1/2})\)-neighbourhoods rather than allow the type of
wild variations that make superefficiency possible.

**Definition 4.3.** Let \(\Theta \subset \mathbb{R}^k\) be open. An estimator sequence \((T_n)\) for the parameter
\(\theta\) is said to be regular at \(\theta\) if, for all \(h \in \mathbb{R}^k\),

\[
n^{1/2}\left(T_n - (\theta + n^{-1/2}h)\right) \overset{L}{\rightarrow} L_\theta, \text{ (under } P_{\theta + n^{-1/2}h}),
\]

i.e. with a limit law independent of \(h\).

So regularity describes the property that convergence of the estimator to a limit law
is insensitive to perturbation of the parameter of \(n\)-dependent size \(n^{-1/2} h\). The two properties covered above come together through the following theorem (see theo-
rems 7.10, 8.3 and 8.4 in [90]), which formulate the foundation for the convolution
theorem that follows.

**Theorem 4.2.** Let \(\Theta \subset \mathbb{R}^k\) be open; let \(\mathcal{P} = \{P_\theta : \theta \in \Theta\}\) be LAN at \(\theta_0\) with non-singular Fisher information \(I_{\theta_0}\). Let \((T_n)\) be regular estimators in the “localized models” \(\{P_{\theta_0 + n^{-1/2}h} : h \in \mathbb{R}^k\}\). Then there exists a (randomized) statistic \(T\) in the
normal location model \(\{N_k(h, I_{\theta_0}^{-1}) : h \in \mathbb{R}^k\}\) such that \(T \sim L_{\theta_0}\) for all \(h \in \mathbb{R}^k\).

Theorem 4.2 provides every regular estimator sequence with a limit in the form of a
statistic in a very simple model in which the only parameter is the location of a
normal distribution: the (weak) limit distribution that describes the local asympto-
tics of the sequence \((T_n)\) under \(P_{\theta_0 + n^{-1/2}h}\) equals the distribution of \(T\) under \(\theta,\) for all
\(h \in \mathbb{R}^k\). Moreover, regularity of the sequence \((T_n)\) implies that under \(N_k(h, I_{\theta_0}^{-1})\), the
distribution of \(T\) relative to \(h\) is independent of \(h\), an invariance usually known as
equivariance-in-law. The class of equivariant-in-law estimators for location in the
model \(\{N_k(h, I_{\theta_0}^{-1}) : h \in \mathbb{R}^k\}\) is fully known: for any equivariant-in-law estimator \(T\)
for \(h\), there exists a probability distribution \(M\) such that \(T \sim N_k(h, I_{\theta_0}^{-1}) \ast M\). The
most straightforward example is \(T = X,\) for which \(M = \delta_0\). This argument gives rise
to the following central result in the theory of efficiency.

**Theorem 4.3. (Convolution theorem (146))**

Let \(\Theta \subset \mathbb{R}^k\) be open and let \(\{P_\theta : \theta \in \Theta\}\) be LAN at \(\theta_0\) with non-singular Fisher
information \(I_{\theta_0}\). Let \((T_n)\) be a regular estimator sequence with limit distribution \(L_{\theta_0}\);
Then there exists a probability distribution \(M_{\theta_0}\) such that,

\[
L_{\theta_0} = N_k(0, I_{\theta_0}^{-1}) \ast M_{\theta_0},
\]

In particular, if \(L_{\theta_0}\) has a covariance matrix \(\Sigma_{\theta_0}\), then \(\Sigma_{\theta_0} \geq I_{\theta_0}^{-1}\).

The occurrence of the inverse Fisher information is no coincidence: the estima-
tors \(T\) are unbiased so they satisfy the Cramér-Rao bound in the limiting model
4.1 Efficiency in smooth parametric models

\{N_k(h, I_{\theta_0}^{-1}) : h \in \mathbb{R}^k\}. Convolution of \(N_k(0, I_{\theta_0}^{-1})\) with any distribution \(M\) raises its variance unless \(M\) is degenerate: the last assertion of the convolution theorem says that, within the class of regular estimates, asymptotic variance is lower-bounded by the inverse Fisher information. A regular estimator that is optimal in this sense, is called best-regular. Anderson’s lemma broadens the notion of optimality, in the sense that best-regular estimators outperform other regular estimators with respect to a large family of loss functions.

**Definition 4.4.** A loss-function is any \(\ell : \mathbb{R}^k \rightarrow [0, \infty)\); a subconvex loss-function is a loss function such that the level sets \(\{x \in \mathbb{R}^k : \ell(x) \leq c\}\) are closed, convex and symmetric around the origin.

Examples of subconvex loss-functions are many and include, for example, the common choices \(\ell(x) = \|x\|^p, p \geq 1\).

**Lemma 4.1.** (Anderson’s lemma)
For any \(k \geq 1\), any subconvex loss function \(\ell'' : \mathbb{R}^k \rightarrow [0, \infty)\), any probability distribution \(M\) on \(\mathbb{R}^k\) and any \(k\)-dimensional covariance matrix \(\Sigma\),

\[
\int \ell dN_k(0, \Sigma) \leq \int \ell d(N_k(0, \Sigma) * M).
\]

(A proof of Anderson’s lemma can be found, for instance, in [49].) Finally, we mention the following equivalence, which characterizes efficiency concisely in terms of a weakly converging sequence.

**Lemma 4.2.** In a LAN model, estimators \((T_n)\) for \(\theta\) are best-regular if and only if the \((T_n)\) are asymptotically linear, i.e. for all \(\theta\) in the model,

\[
n^{1/2}(T_n - \theta) = \frac{1}{\sqrt{n}} \sum_{i=1}^n I_{\theta}^{-1}(X_i) + o_P(1). \tag{4.3}
\]

The random sequence of differences on the r.h.s. of (4.3) is denoted by \(\Delta_n, \theta_0\) below.

Coming back to theorem 4.1, we see that under stated conditions, a consistent sequence of MLE’s \((\hat{\theta}_n)\) is best-regular, finally giving substance to Fisher’s 1920’s claim. Referring to the discussion on confidence sets with which we opened this lecture, we now know that in a LAN model, confidence sets of the form (4.1) based on best-regular estimators \((\hat{\theta}_n)\) satisfy a similar notion of optimality: according to the convolution theorem, the asymptotic sampling distributions of best-regular estimator sequences are all the same and sharpest among asymptotic sampling distributions for regular estimators. The question remains if we can somehow identify confidence sets and credible intervals; in the next chapter, that identification is made asymptotically.
4.2 Le Cam’s Bernstein-von Mises theorem

To address the question of efficiency in smooth parametric models from a Bayesian perspective, we turn to the Bernstein-von Mises theorem. In the literature many different versions of the theorem exist, varying both in (stringency of) conditions and (strength or) form of the assertion. We following Le Cam and Yang (1990) [71] (For later reference, define a parametric prior to be thick at $\theta_0$, if it has a Lebesgue density that is continuous and strictly positive at $\theta_0$.)

The (proof of the) Bernstein-Von-Mises theorem depends crucially on local asymptotic normality of the model at $\theta_0$, as required through differentiability in quadratic mean. A quick sketch of the proof can be given as follows. Suppose that the local parameter $H = \sqrt{n}(\theta - \theta_0)$ has a Lebesgue-density given by:

$$\pi_n(h|X_1,X_2,\ldots,X_n) = \frac{\prod_{i=1}^{n} p_{\theta_0+h/\sqrt{n}}(X_i) \pi(\theta_0+h/\sqrt{n})}{\int \prod_{i=1}^{n} p_{\theta_0+h'/\sqrt{n}}(X_i) \pi(\theta_0+h'/\sqrt{n}) dh'},$$

$P_{\theta_0}^n$-almost-surely. Continuity of $\pi$ at $\theta_0$ implies that (up to an $n$-dependent proportionality constant), $\pi(\theta_0 + h/\sqrt{n})$ converges to the constant $\pi(\theta_0)$, which is strictly positive by assumption. This makes it plausible that upon substitution of the likelihood expansion (5.1), the posterior density converges to:

$$\frac{\prod_{i=1}^{n} p_{\theta_0+h/\sqrt{n}}(X_i)}{\int \prod_{i=1}^{n} p_{\theta_0+h'/\sqrt{n}}(X_i) dh'} \approx \frac{e^{h^T \Delta_n \phi_n - \frac{1}{2} h^T I_{\theta_0} h}}{\int e^{h'^T \Delta_n \phi_n - \frac{1}{2} h'^T I_{\theta_0} h'} dh'} dN(h,I_{\theta_0}^{-1})(\Delta) \rightarrow dN(h',I_{\theta_0}^{-1})(\Delta) dh'$$

(in a suitable sense with respect to $P_{\theta_0}$). Here $\Delta$ is an observation in the normal limit model $\{N(h,I_{\theta_0}^{-1}) : h \in \mathbb{R}^k\}$. The l.h.s. of the last display equals $dN(\Delta,I_{\theta_0}^{-1})(h)$ and is the posterior based on a sample consisting only of $\Delta$ and the (improper) Lebesgue prior for the limit model.

**Theorem 4.4. (Bernstein-Von Mises, Le Cam and Yang (1990) [71])**

Assume that $\Theta \subset \mathbb{R}^k$ is open and that the model $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ is identifiable and dominated. Suppose $X_1,X_2,\ldots$ forms an i.i.d. sample from $P_{\theta_0}$, for some $\theta_0 \in \Theta.$ Assume that the model is locally asymptotically normal at $\theta_0$ with non-singular Fisher information $I_{\theta_0}$. Furthermore, suppose that, the prior $\Pi_\Theta$ is thick at $\theta_0$ and that for every $\varepsilon > 0$, there exists a test sequence $(\phi_n)$ such that,

$$P_{\theta_0}^n \phi_n \rightarrow 0, \quad \sup_{\|\theta - \theta_0\| > \varepsilon} P_{\theta}^n (1 - \phi_n) \rightarrow 0.$$

Then the posterior distributions converge in total variation,

$$\sup_B \left| \Pi(\theta \in B \mid X_1,\ldots,X_n) - N_{\theta_0,(nI_{\theta_0})^{-1}}(B) \right| \rightarrow 0,$$
in $P_{\theta_0}$-probability, where $(\hat{\theta}_n)$ denotes any best-regular estimator sequence.

Since the total-variational distance $\|N(\mu, \Sigma) - N(\nu, \Sigma)\|$ is bounded by a multiple of $\|\mu - \nu\|$, we find that the assertion of the Bernstein-Von-Mises theorem can also be formulated with $\sqrt{n}(\hat{\theta}_n - \theta_0)$ replacing $\Delta_n \theta_0$. Using the invariance of total-variation under rescaling and shifts, this leads to the conclusion that:

$$\left\| \Pi_{\theta|X_1, \ldots, X_n} - N(\tilde{\theta}_n, n^{-1}I_{\theta_0}) \right\| \xrightarrow{P} 0,$$

for any best-regular estimator-sequence $\tilde{\theta}_n$. In particular, according to theorem 4.1 and the lemma 4.3, the maximum-likelihood estimator is best-regular under smoothness conditions on the (log-)likelihood. This serves to motivate the often-heard statement that “Bayesian statistics coincides with the maximum-likelihood estimator asymptotically”. In figure 4.2, Bernstein-von Mises-type of convergence of the posterior is demonstrated with a graphical/numerical example. Also displayed in

---

Fig. 4.1 Convergence of the posterior density. The samples used for calculation of the posterior distributions consist of $n$ observations; the model consists of all normal distributions with mean between $-1$ and $2$ and variance $1$ and has a polynomial prior, shown in the first ($n = 0$) graph. For all sample sizes, the maximum a posteriori and maximum likelihood estimators are indicated by a vertical line and a dashed vertical line respectively. (From Kleijn (2003))
figure 4.2 are the so-called MAP estimator (the location of maximal posterior density, a popular point-estimator derived from the posterior) and the ML estimator. It is noted that, here, the MLE is efficient so it forms a possible centring sequence for the limiting sequence of normal distributions in the assertion of the Bernstein-Von Mises theorem. Furthermore, it is noted that the posterior concentrates more and more sharply, reflecting the \( n^{-1} \)-proportionality of the variance of its limiting sequence of normals. It is perhaps a bit surprising in figure 4.2 to see limiting normality obtain already at such relatively low values of the sample size \( n \). It cannot be excluded that, in this case, that is a manifestation of the normality of the underlying model, but onset of normality of the posterior appears to happen at unexpectedly low values of \( n \) also in other smooth, parametric models. It suggests that asymptotic conclusions based on the Bernstein-Von Mises limit accrue validity fairly rapidly, for \( n \) in the order of several hundred to several thousand i.i.d. replications of the observation.

The uniformity in the assertion of the Bernstein-Von Mises theorem over model subsets \( B \) implies that it holds also for model subsets that are random. In particular, given some \( 0 < \alpha < 1 \), it is noted that the smallest sets \( C_\alpha(X_1, \ldots, X_n) \) such that,

\[
N_{\hat{\theta}_n}(\theta_0)^{-1}(C_\alpha(X_1, \ldots, X_n)) \geq 1 - \alpha,
\]

are ellipsoids of the form (4.1). Since posterior coverage of \( C_\alpha \) converges to the l.h.s. in the above display, in accordance with the Bernstein-Von Mises limit, we see that the \( C_\alpha \) are asymptotic credible sets of posterior coverage \( 1 - \alpha \). Conversely, any sequence \((C_n(X_1, \ldots, X_n))\) of (data-dependent) credible sets of coverage \( 1 - \alpha \), is also a sequence of sets that have asymptotic confidence level \( 1 - \alpha \) (where we use that \( \hat{\theta}_n \) is best-regular). This gives rise to an identification in smooth, parametric models between inference based on frequentist best-regular point-estimators and inference based on Bayesian posteriors. In a practical sense, it eliminates the need to estimate \( \theta \) and the Fisher information \( I_\theta \) at \( \theta \) to arrive at asymptotic confidence sets, if we have an approximation of the posterior distribution of high enough quality (e.g. from MCMC simulation), if we know that the Bernstein-Von Mises theorem holds. In high dimensional parametric models, maximization of the likelihood may be much more costly computationally than generation of a suitable MCMC approximation. As a consequence, the Bernstein-Von Mises theorem has an immediate practical implication of some significance.

Before we continue with the proof of the Bernstein-Von Mises theorem, let is briefly reflect on its conditions: local asymptotic normality and non-singularity of the associated Fisher information are minimal smoothness conditions. They also arise in theorem 4.1 and form the backdrop for any discussion of efficiency. More significant is the required existence of a “consistent” test sequence: what is required is that, asymptotically, we can distinguish \( R_\theta \) from any complement of a \( \theta \)-neighbourhood around \( \theta_0 \) uniformly. One should compare this condition with that of consistency of near-maximizers of the likelihood in theorem 4.1. Apparently, if such a global (rather than \( n^{-1/2} \)-sized local) consistency guarantee can not be given, likelihood-based methods like ML or Bayesian estimation cannot be trusted to give
rise to asymptotic normality (in their respective forms). In the next section, we shall divide the Bernstein-Von Mises theorem in two parts, with a requirement of local $n^{-1/2}$-sized consistency for the posterior in between. In a separate lemma, we show that a score-test can fill in the gap between local and global consistency.

### 4.2.1 Proof of the Bernstein-von Mises theorem

We prove the assertion of the Bernstein-Von Mises theorem using a smoothness property that is slightly stronger than necessary, because we shall need a similar formulation in the semiparametric case.

**Definition 4.5.** We say that a parametric model $\mathcal{P}$ is stochastically LAN at $\theta_0$, if the LAN property of definition 4.1 is satisfied for every random sequence $(h_n)$ that is bounded in probability, i.e. for all $h_n = O_P(1)$:

$$
\log \prod_{i=1}^{n} \frac{p_{\theta_0}^n + n^{-1/2}h_n}{p_{\theta_0}} (X_i) - h_n^T \Gamma_n,\theta_0 - \frac{1}{2} h_n^T I_{\theta_0} h_n = o_{P_0}(1), \quad (4.4)
$$

for random vectors $\Gamma_n,\theta_0$ such that $\Gamma_n,\theta_0 \rightarrow N_k(0, I_{\theta_0})$.

**Theorem 4.5.** Let the sample $X_1, X_2, \ldots$ be distributed i.i.d. $\cdot P_0$. Let $\Theta \subset \mathbb{R}^k$ be open, let $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ be stochastically LAN at $\theta_0$ with non-singular Fisher information $I_{\theta_0}$ and let the prior $\Pi$ on $\Theta$ be thick. Furthermore, assume that for every sequence of balls $(K_n) \subset \mathbb{R}^d$ with radii $M_n \rightarrow \infty$, we have:

$$
\Pi_n \left( h \in K_n \mid X_1, \ldots, X_n \right) \xrightarrow{P_0} 1. \quad (4.5)
$$

Then the sequence of posteriors converges to a sequence of normal distributions in total variation:

$$
\sup_B \left| \Pi_n \left( h \in B \mid X_1, \ldots, X_n \right) - N_{\Delta_n,\theta_0}^{-1}(B) \right| \xrightarrow{P_0} 0. \quad (4.6)
$$

**Proof.** The proof is split into two parts: in the first part, we prove the assertion conditional on a compact neighbourhood $K$ of 0 in $\Theta$, while in the second part we use this to prove (5.4). Throughout the proof we denote the posterior for $h$ given $X_1, X_2, \ldots, X_n$ by $\Pi_n$ and the normal distribution $N_{\Delta_n,\theta_0}^{-1}(B)$ by $\Phi_n$ (for the definition of $\Delta_n,\theta_0$, see lemma 4.2). For $K \subset \mathbb{R}^k$, conditional versions are denoted $\Pi^K_n$ and $\Phi^K_n$ respectively (assuming that $\Pi_n(K) > 0$ and $\Phi_n(K) > 0$, of course).

Let $K \subset \Theta$ be a ball centered on 0. For every open neighbourhood $U \subset \Theta$ of $\theta_0$, $\theta_0 + n^{-1/2} K \subset U$ for large enough $n$. Since $\theta_0$ is an internal point of $\Theta$, we can define, for large enough $n$, the random functions $f_n : K \times K \rightarrow \mathbb{R}$ by:

$$
f_n(g, h) = \left( 1 - \frac{\phi_n(h) s_n(g)}{\phi_n(g) s_n(h)} \frac{\pi_n(g)}{\pi_n(h)} \right)^+, \nonumber
$$
where $\phi_n : K \to \mathbb{R}$ is the Lebesgue density of the (randomly located) distribution $N_{\Delta_n, \theta_0} \mathcal{N}_1$, $\pi_n : K \to \mathbb{R}$ is the Lebesgue density of the prior for the centred and rescaled parameter $h$ and $s_n : K \to \mathbb{R}$ equals the likelihood product:

$$s_n(h) = \prod_{i=1}^{n} \frac{p_{h_i + \sqrt{n} h_i}}{p_{h_i}}(X_i).$$

Since the model is stochastically LAN by assumption, we have for every random sequence $(h_n) \subset K$: For any two sequences $(h_n)$, $(g_n) \subset K$, $\pi_n(g_n)/\pi_n(h_n) \to 1$ as $n \to \infty$. Combining this with the above display we see that: as $n \to \infty$. Since $x \mapsto (1 - e^x)_+$ is continuous on $\mathbb{R}$, we conclude that for every pair of random sequences $(g_n, h_n) \subset K \times K$:

$$f_n(g_n, h_n) \xrightarrow{p_0} 0, \quad (n \to \infty).$$

For fixed, large enough $n$, $P_0^n$-almost-sure continuity of $(g, h) \mapsto \log s_n(g)/s_n(h)$ on $K \times K$ is guaranteed by the stochastic LAN-condition. Each of the locations $\Delta_n, \theta_0$ for $\Phi_0$ is is tight, so $(g, h) \mapsto \phi_n(g)/\phi_n(h)$ is continuous on all of $K \times K$ $P_0^n$-almost-surely. Continuity (in a neighbourhood of $\theta_0$) and positivity of the prior density guarantee that this holds for $(g, h) \mapsto \pi_n(g)/\pi_n(h)$ as well. We conclude that for large enough $n$, the random functions $f_n$ are continuous on $K \times K$, $P_0^n$-almost-surely. Application of lemma 4.4 then leads to the conclusion that,

$$\sup_{g, h \in K} f_n(g, h) \xrightarrow{p_0} 0, \quad (n \to \infty). \quad (4.7)$$

Since $K$ contains a neighbourhood of 0, $\Phi_n(K) > 0$ is guaranteed. Let $\Xi_n$ denote the event that $\Pi_n(K) > 0$. Let $\eta > 0$ be given and based on that, define the events:

$$\Omega_n = \{ \omega : \sup_{g, h \in K} f_n(g, h) \leq \eta \}.$$ 

Consider the expression (recall that the total-variation norm is bounded by 2):

$$P_0^n \| \Pi_n^K - \Phi_n^K \|_1 \Xi_n \leq P_0^n \| \Pi_n^K - \Phi_n^K \|_1 \Omega_n \cap \Xi_n + 2P_0^n(\Xi_n \setminus \Omega_n). \quad (4.8)$$

As a result of (4.7) the latter term is $o(1)$ as $n \to \infty$. The remaining term on the r.h.s. can be calculated as follows: Note that for all $g, h \in K$ we have $\phi_n^K(h)/\phi_n^K(g) = \phi_n(h)/\phi_n(g)$ since, on $K$, $\phi_n^K$ differs from $\phi_n$ only by a normalisation factor. We use Jensen’s inequality (with respect to the $\Phi_n^K$-expectation) for the (convex) function $x \mapsto (1 - x)_+$ to derive:

Combination with (4.8) shows that for all compact $K \subset \mathbb{R}^d$ containing a neighbourhood of 0,

$$P_0^n \| \Pi_n^K - \Phi_n^K \|_1 \Xi_n \to 0.$$
Now let \((K_m)\) be a sequence of balls centred at 0 with radii \(M_m \to \infty\). For each \(m \geq 1\), the above display holds, so if we choose a sequence of balls \((K_n)\) that traverses the sequence \(K_m\) slowly enough, convergence to zero can still be guaranteed. Moreover, the corresponding events \(\Xi_n = \{ \omega : \Pi_n(K_n) > 0 \}\) satisfy \(P_0^\epsilon(\Xi_n) \to 1\) as a result of (5.3). We conclude that there exists a sequence of radii \((M_n)\) such that \(M_n \to \infty\) and

\[
P_0^\epsilon \| \Pi_n^{K_n} - \Phi_n^{K_n} \| \to 0,
\]

where it is understood that the conditional probabilities on the l.h.s. are well-defined on sets of probability growing to one. Combining (5.3) and lemma 5.10, we then use lemma 5.9 to conclude that:

\[
P_0^\epsilon \| \Pi_n - \Phi_n \| \to 0,
\]

which implies (5.4).

Aside from a slightly stronger smoothness property in the form of the stochastic LAN condition, theorem 4.5 appears to require more than theorem 4.4, in the sense that it requires posterior consistency at rate \(n^{-1/2}\) rather than the (fixed) tests for consistency. The following lemma shows that, assuming smoothness, the latter condition is enough to satisfy the former. Its proof is based on the construction of a score test that fills in the “gap” left between the fixed-alternative tests and the growing alternative \(\| \theta - \theta_0 \| \geq n^{-1/2} M_n\). However, the proof is long and detailed and it does not have a semiparametric analog. For that reason the proof is given only in the form of a reference.

**Lemma 4.3.** Assume that \(\Theta \subset \mathbb{R}^k\) is open and that the model \(\mathcal{P} = \{P_\theta : \theta \in \Theta\}\) is identifiable and dominated. Assume that the model is locally asymptotically normal at \(\theta_0\) with non-singular Fisher information \(I_{\theta_0}\) and that the prior is thick at \(\theta_0\). Furthermore, suppose that there exists a test sequence \((\phi_n)\) such that,

\[
P_{\theta_0}^\epsilon \phi_n \to 0, \quad \sup_{\|\theta - \theta_0\| > \epsilon} P_\theta^\epsilon(1 - \phi_n) \to 0.
\]

Then the posterior converges at rate \(n^{-1/2}\), i.e. for every sequence \(M_n \to \infty\),

\[
\Pi_n(\| \theta - \theta_0 \| \geq n^{-1/2} M_n \mid X_1, \ldots, X_n) \xrightarrow{\text{i.i.d.}} 0.
\]

**Proof.** Proof This lemma is a well-specified version of theorem 2.2 in [58], which incorporates theorem 2.3 therein, also found as lemma 10.3 in [90].

### 4.2.2 Three subsidiary lemmas

The proof of theorem 4.5 also makes use of the following three lemmas which are of a more general character then lemma 4.3.
Lemma 4.4. Let \((f_n)\) be a sequence of random functions \(K \to \mathbb{R}\), where \(K\) is compact. Assume that for large enough \(n \geq 1\), \(f_n\) is continuous \(P_0\)-almost-surely. Then the following are equivalent:

(i) Uniform convergence in probability:
\[
\sup_{h \in K} |f_n(h)| \xrightarrow{P_0} 0, \quad (n \to \infty),
\]

(ii) For any random sequence \((h_n) \subset K\):
\[
f_n(h_n) \xrightarrow{P_0} 0, \quad (n \to \infty),
\]

Proof. Proof ((ii)⇒(i), by contradiction.) Assume that there exist \(\delta, \varepsilon > 0\) such that:
\[
\limsup_{n \to \infty} P_0\left( \sup_{h \in K} |f_n(h)| > \delta \right) = \varepsilon > 0.
\]

Since the functions \(f_n\) are continuous \(P_0\)-almost-surely, there exists (with \(P_0\)-probability one) a sequence \((\tilde{h}_n)\) such that for every \(n \geq 1\), \(\tilde{h}_n \in K\) and
\[
|f_n(\tilde{h}_n)| = \sup_{h \in K} |f_n(h)|.
\]

Consequently, for this particular random sequence in \(K\), we have:
\[
\limsup_{n \to \infty} P_0\left( |f_n(\tilde{h}_n)| > \delta \right) = \varepsilon > 0.
\]

which contradicts (ii). (i)⇒(ii.) Given a random sequence \((h_n) \subset K\), and for every \(\delta > 0\),
\[
P_0\left( \sup_{h \in K} |f_n(h)| > \delta \right) \geq P_0\left( |f_n(h_n)| > \delta \right).
\]

Given (i), the l.h.s. converges to zero and hence so does the r.h.s..

The next lemma shows that given two sequences of probability measures, a sequence of balls that grows fast enough can be used conditionally to calculate the difference in total-variational distance, even when the sequences consist of random measures.

Lemma 4.5. Let \((\Pi_n)\) and \((\Phi_n)\) be two sequences of random probability measures on \(\mathbb{R}^k\). Let \((K_n)\) be a sequence of subsets of \(\mathbb{R}^k\) such that
\[
\Pi_n(\mathbb{R}^k \setminus K_n) \xrightarrow{P_0} 0, \quad \Phi_n(\mathbb{R}^k \setminus K_n) \xrightarrow{P_0} 0. \quad (4.10)
\]

Then
\[
\|\Pi_n - \Phi_n\| - \|\Pi_n^{K_n} - \Phi_n^{K_n}\| \xrightarrow{P_0} 0. \quad (4.11)
\]

Proof. Proof Let \(K\), a measurable subset of \(\mathbb{R}^k\) and \(n \geq 1\) be given and assume that \(\Pi_n(K) > 0\) and \(\Phi_n(K) > 0\). Then for any measurable \(B \subset \mathbb{R}^k\) we have:
\[
|\Pi_n(B) - \Pi_n^K(B)| = \left|\Pi_n(B) - \frac{\Pi_n(B \cap K)}{\Pi_n(K)}\right|
\]
\[
= \left|\Pi_n(B \cap (\mathbb{R}^k \setminus K)) + (1 - \Pi_n(K)^{-1})\Pi_n(B \cap K)\right|
\]
\[
\leq \Pi_n(B \cap (\mathbb{R}^k \setminus K)) + \Pi_n(\mathbb{R}^k \setminus K)\Pi_n^K(B) \leq 2\Pi_n(\mathbb{R}^k \setminus K).
\]
and hence also:
\[
\left|\left(\Pi_n(B) - \Pi_n^K(B)\right) - \left(\Phi_n(B) - \Phi_n^K(B)\right)\right| \leq 2\left(\Pi_n(\mathbb{R}^k \setminus K) + \Phi_n(\mathbb{R}^k \setminus K)\right). \tag{4.12}
\]

As a result of the triangle inequality, we then find that the difference in total-variation distances between \(\Pi_n\) and \(\Phi_n\) on the one hand and \(\Pi_n^K\) and \(\Phi_n^K\) on the other is bounded above by the expression on the right in the above display (which is independent of \(B\)).

Define \(A_n, B_n\) to be the events that \(\Pi_n(K_n) > 0\), \(\Phi_n(K_n) > 0\) respectively. On \(\mathcal{F}_n = A_n \cap B_n\), \(\Pi_n^K\) and \(\Phi_n^K\) are well-defined probability measures. Assumption (5.37) guarantees that \(P_n^0(\mathcal{F}_n)\) converges to 1. Restricting attention to the event \(\mathcal{F}_n\) in the above upon substitution of the sequence \(\{K_n\}\) and using (5.37) for the limit of (5.39) we find (5.38), where it is understood that the conditional probabilities on the l.h.s. are well-defined with probability growing to 1.

To apply the above lemma in the concluding steps of the proof of theorem 4.5, rate conditions for both posterior and limiting normal sequences are needed. The rate condition (5.3) for the posterior is assumed and the following lemma demonstrates that its analog for the sequence of normals is satisfied when the sequence of centre points \(\Delta_n, \delta_0\) is uniformly tight.

**Lemma 4.6.** Let \(K_n\) be a sequence of balls centred on the origin with radii \(M_n \to \infty\). Let \((\Phi_n)\) be a sequence of normal distributions (with fixed covariance matrix \(V\)) located respectively at the (random) points \((\Delta_n) \subset \mathbb{R}^k\). If the sequence \(\Delta_n\) is uniformly tight, then:

\[
\Phi_n(\mathbb{R}^k \setminus K_n) = N_{\Delta_n, V}(\mathbb{R}^k \setminus K_n) \xrightarrow{P} 0.
\]

**Proof.** Proof Let \(\delta > 0\) be given. Uniform tightness of the sequence \((\Delta_n)\) implies the existence of a constant \(L > 0\) such that:

\[
\sup_{n \geq 1} P_n^0(\|\Delta_n\| \geq L) \leq \delta.
\]

For all \(n \geq 1\), call \(A_n = \{\|\Delta_n\| \geq L\}\). Let \(\mu \in \mathbb{R}^k\) be given. Since \(N(\mu, V)\) is tight, for every given \(\varepsilon > 0\), there exists a constant \(L'\) such that \(N_{\mu, V}(B(\mu, L')) \geq 1 - \varepsilon\) (where \(B(\mu, L')\) defines a ball of radius \(L'\) around the point \(\mu\)). Assuming that \(\mu \leq L, B(\mu, L') \subset B(0, L + L')\) so that with \(M = L + L', N_{\mu, V}(B(0, M)) \geq 1 - \varepsilon\) for all \(\mu\) such that \(\|\mu\| \leq L\). Choose \(N \geq 1\) such that \(M_n \geq M\) for all \(n \geq N\). Let \(n \geq N\) be given. Then:
4.3 Exercises

4.1. Assume that $n^{1/2}(\hat{\theta}_n - \theta_0) \sim N(0, I_{\theta_0}^{-1})$. Show that the ellipsoids (4.1) are of minimal Lebesgue measure among all subsets of coverage $1 - \alpha$.

4.2. Consider Hodges’ estimators $S_n$ of example 4.1. Show that, for any rate sequence $(\varepsilon_n)$, $\varepsilon_n \downarrow 0$, $\varepsilon_n(S_n - 0) \to 0$.

4.3. Let $\Theta = (0, \infty)$ and let $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ be the model of Poisson distributions $P_\theta$ with means $\theta$. Let the data be an i.i.d. sample from $P_{\theta_0}$ for some $\theta_0 \in \Theta$. Show that this model is LAN for all $\theta$.

4.4. Let $\Theta = \mathbb{R}$ and let $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ be the model of normal distributions $N(\theta, 1)$ of unit variance with means $\theta$. Let the data be an i.i.d. sample from $P_{\theta_0}$ for some $\theta_0 \in \Theta$. Show that this model is LAN for all $\theta$.

4.5. Let $f$ be a Lebesgue density on $\mathbb{R}$ that is symmetric around the origin. Define the model $\mathcal{P} = \{P_{\mu, \sigma} : \mu \in \mathbb{R}, \sigma \in (0, \infty)\}$ by densities $f_{\mu, \sigma}(x) = \sigma^{-1}f((x - \mu)/\sigma)$. Show that the Fisher information matrix is diagonal.

4.6. Let $P$ and $Q$ be probability measures on a measurable space $(\mathcal{X}, \mathcal{B})$,

a. Show that there exists a $\sigma$-finite measure $\mu$ such that $P, Q \ll \mu$.

b. Using Radon-Nikodym derivatives $p = dP/d\mu$ and $q = dQ/d\mu$, prove that,

$$\sup_{B \in \mathcal{B}} |P(B) - Q(B)| = \int |p - q| \, d\mu.$$ 

c. Show that, for any sequence $(Q_n)$ of probability measures on $(\mathcal{X}, \mathcal{B})$, there exists a probability measure $P$ that dominates all $Q_n$, $(n \geq 1)$.

d. Use the completeness of $L_1(\mathcal{X}, \mathcal{B}, \mu)$ to show that the metric space $M(\mathcal{X}, \mathcal{B})$ of all probability measures on $(\mathcal{X}, \mathcal{B})$ is complete in the topology of total variation.

4.7. Let $\Theta = (0, \infty)$ and $\mathcal{P} = \{N(0, \theta^2) : \theta \in \Theta\}$. Let $\Pi$ be a thick prior on $\Theta$. Show that this model satisfies the conditions of the Bernstein-von Mises theorem 4.4. Find
the problematic range of parameter values in this model. *(Hint: calculate the Fisher information, find a problematic limit for it and describe the effect on the limiting sequence of normal distributions for parameter values close to the problematic limit.)*

4.8. Approximation in measure from within by compact subsets has a deep background in analysis. Central is the notion of a Radon measure. Given a Hausdorff topological space \( \Theta \), a **Radon measure** \( \Pi \) is a Borel measure that is **locally finite** (meaning that any \( \theta \in \Theta \) has a neighbourhood \( U \) such that \( \Pi(U) < \infty \)) and **inner regular** (meaning that for any measurable subset \( S \subset \Theta \) and any \( \varepsilon > 0 \), there exists a compact \( K \subset S \) such that \( \mu(S \setminus K) < \varepsilon \)). Show that any probability measure on a Polish space is Radon. *(NB: This statement can be generalized to continuous images of Polish spaces, known as Suslin spaces.)*

4.9. Prove the following: for \( \theta \in \Theta = \mathbb{R} \), let \( F_\theta(x) = (1 - e^{-(x-\theta)}) \lor 0 \) be the standard exponential distribution function located at \( \theta \). Assume that \( X_1, X_2, \ldots \) form an i.i.d. sample from \( F_{\theta_0} \), for some \( \theta_0 \). Let \( \Pi \) be a thick prior on \( \Theta \). Then the associated posterior distribution satisfies, with \( h = n(\theta - \theta_0) \),

\[
\sup_A \left| \Pi_n \left( h \in A \mid X_1, \ldots, X_n \right) - \text{Exp}_{n(\hat{\theta}_n - \theta_0)}^- (A) \right| \xrightarrow{\theta_0 \to 0} 0,
\]

where \( \hat{\theta}_n = X_{(1)} \) is the maximum likelihood estimate for \( \theta_0 \) and \( \text{Exp}_a^- \) denotes the standard negative exponential distribution located at \( a \). *(NB: This is an example of an irregular estimation problem: clearly the model does not depend on \( \theta \) in a differentiable way. Inspection of the assertion shows that the rate of convergence is \( n^{-1} \) rather than \( n^{-1/2} \), the rate of convergence in regular situations. In addition, the limiting shape of the posterior is not normal but exponential.)*
Chapter 5
Model misspecification

We prove that the posterior distribution of a parameter in misspecified LAN parametric models can be approximated by a random normal distribution. We derive from this that Bayesian credible sets are not valid confidence sets if the model is misspecified. We obtain the result under conditions that are comparable to those in the well-specified situation: uniform testability against fixed alternatives and sufficient prior mass in neighbourhoods of the point of convergence. The rate of convergence is considered in detail, with special attention for the existence and construction of suitable test sequences. We also give a lemma to exclude testable model subsets which implies a misspecified version of Schwartz’ consistency theorem, establishing weak convergence of the posterior to a measure degenerate at the point at minimal Kullback-Leibler divergence with respect to the true distribution.

The Bernstein-Von Mises theorem asserts that the posterior distribution of a parameter in a smooth finite-dimensional model is approximately a normal distribution if the number of observations tends to infinity. Apart from having considerable philosophical interest, this theorem is the basis for the justification of Bayesian credible sets as valid confidence sets in the frequentist sense: (central) sets of posterior probability $1 - \alpha$ cover the parameter at confidence level $1 - \alpha$. In this paper we study the posterior distribution in the situation that the observations are sampled from a “true distribution” that does not belong to the statistical model, i.e. the model is misspecified. Although consistency of the posterior distribution and the asymptotic normality of the Bayes estimator (the posterior mean) in this case have been considered in the literature, by Berk (1966,1970) [2, 10] and Bunke and Milhaud (1998) [?], the behaviour of the full posterior distribution appears to have been neglected. This is surprising, because in practice the assumption of correct specification of a model may be hard to justify. In this paper we derive the asymptotic normality of the full posterior distribution in the misspecified situation under conditions comparable to those obtained by Le Cam in the well-specified case.

This misspecified version of the Bernstein-Von Mises theorem has an important consequence for the interpretation of Bayesian credible sets. In the misspecified situation the posterior distribution of a parameter shrinks to the point within the model at minimum Kullback-Leibler divergence to the true distribution, a consis-
tency property that it shares with the maximum likelihood estimator. Consequently one can consider both the Bayesian procedure and the maximum likelihood estimator as estimates of this minimum Kullback-Leibler point. A confidence region for this minimum Kullback-Leibler point can be built around the maximum likelihood estimator based on its asymptotic normal distribution, involving the sandwich covariance. One might also hope that a Bayesian credible set automatically yields a valid confidence set for the minimum Kullback-Leibler point. However, the misspecified Bernstein-Von Mises theorem shows the latter to be false.

More precisely, let $B \mapsto \Pi_n(B \mid X_1, \ldots, X_n)$ be the posterior distribution of a parameter $\theta$ based on observations $X_1, \ldots, X_n$ sampled from a density $p_\theta$ and a prior measure $\Pi$ on the parameter set $\Theta \subset \mathbb{R}^d$. The Bernstein-Von Mises theorem asserts that if $X_1, \ldots, X_n$ is a random sample from the density $p_{\theta_0}$, the model $\theta \mapsto p_\theta$ is appropriately smooth and identifiable, and the prior puts positive mass around the parameter $\theta_0$, then,

$$P_{\theta_0}^n \sup_B \left| \Pi_n(B \mid X_1, \ldots, X_n) - N_{\hat{\theta}_n, (nV_{\theta_0})^{-1}}(B) \right| \to 0,$$

where $N_{x, \Sigma}$ denotes the (multivariate) normal distribution centred on $x$ with covariance matrix $\Sigma$, $\hat{\theta}_n$ may be any efficient estimator sequence of the parameter and $i_\theta$ is the Fisher information matrix of the model at $\theta$. It is customary to identify $\hat{\theta}_n$ as the maximum likelihood estimator in this context (correct under regularity conditions).

The Bernstein-Von Mises theorem implies that any random sets $\hat{B}_n$ such that $\Pi_n(\hat{B}_n \mid X_1, \ldots, X_n) = 1 - \alpha$ for each $n$ satisfy,

$$N_{0, \hat{\theta}_n, \sqrt{n}}((ni_{\theta_0})^{1/2}(\hat{B}_n - \hat{\theta}_n)) \to 1 - \alpha,$$

in probability. In other words, such sets $\hat{B}_n$ can be written in the form $\hat{B}_n = \hat{\theta}_n + (V_{\theta_0})^{-1/2} \hat{C}_n/\sqrt{n}$ for sets $\hat{C}_n$ that receive asymptotically probability $1 - \alpha$ under the standard Gaussian distribution. This shows that the $1 - \alpha$-credible sets $\hat{B}_n$ are asymptotically equivalent to the Wald $1 - \alpha$-confidence sets based on the asymptotically normal estimators $\hat{\theta}_n$, and consequently they are valid $1 - \alpha$ confidence sets.

In this paper we consider the situation that the posterior distribution is formed in the same way relative to a model $\theta \mapsto p_0$, but we assume that the observations are sampled from a density $p_0$ that is not necessarily of the form $p_{\theta_0}$ for some $\theta_0$. We shall show that the Bernstein-Von Mises can be extended to this situation, in the form,

$$P_{0}^n \sup_B \left| \Pi_n(B \mid X_1, \ldots, X_n) - N_{\theta^*, (nV_{\theta^*})^{-1}}(B) \right| \to 0,$$

where $\theta^*$ is the parameter value $\theta$ minimizing the Kullback-Leibler divergence $\theta \mapsto \theta_0 \log(p_0/p_\theta)$ (provided it exists and is unique, see corollary 5.2), $V_{\theta^*}$ is minus the second derivative matrix of this map, and $\hat{\theta}_n$ are suitable estimators.

Under regularity conditions the estimators $\hat{\theta}_n$ can again be taken equal to the maximum likelihood estimators (for the misspecified model), which typically sat-
isfy that the sequence $\sqrt{n}(\hat{\theta}_n - \theta^*)$ is asymptotically normal with mean zero and covariance matrix given by the “sandwich formula” $\Sigma_{\theta^*} = V_{\theta^*}(P_0 \ell_{\theta^*} \ell_{\theta^*}^T)^{-1}V_{\theta^*}$. (See, for instance, Huber (1967) [?] or Van der Vaart (1998) [90].) The usual confidence sets for the misspecified parameter take the form $\hat{\theta}_n + \Sigma_{\theta^*}^{1/2} C / \sqrt{n}$ for $C$ a central set in the Gaussian distribution. Because the covariance matrix $V_{\theta^*}$ appearing in the misspecified Bernstein-Von Mises theorem is not the sandwich covariance matrix, central posterior sets of probability $1 - \alpha$ do not correspond to these misspecified Wald sets. Although they are correctly centered, they may have the wrong width, and are in general not $1 - \alpha$-confidence sets. We show below by example that the credible sets may over- or under-cover, depending on the true distribution of the observations and the model, and to extreme amounts.

The first results concerning limiting normality of a posterior distribution date back to Laplace (1820) [63]. Later, Bernstein (1917) [6] and Von Mises (1931) [75] proved results to a similar extent. Le Cam used the term ‘Bernstein-Von Mises theorem’ in 1953 [66] and proved its assertion in greater generality. Walker (1969) [91] and Dawid (1970) [24] gave extensions to these results and Bickel and Yahav (1969) [14] proved a limit theorem for posterior means. A version of the theorem involving only first derivatives of the log-likelihood in combination with testability and prior mass conditions (compare with Schwartz’ consistency theorem, Schwartz (1965) [83]) can be found in Van der Vaart (1998) [90] which copies (and streamlines) the approach Le Cam presented in [71].

Weak convergence of the posterior distribution to the degenerate distribution at $\theta^*$ under misspecification was shown by Berk (1966,1970) [?, 10], while Bunke and Milhaud (1998) [?] proved asymptotic normality of the posterior mean. These authors also discuss the situation that the point of minimum Kullback-Leibler divergence may be non-unique, which obviously complicates the asymptotic behaviour considerably. Posterior rates of convergence in misspecified non-parametric models were considered in Kleijn and Van der Vaart (2006) [58].

In the present paper we address convergence of the full posterior under mild conditions comparable to those in Van der Vaart (1998) [90]. The presentation is split into two parts. In section 5.1 we derive normality of the posterior given that it shrinks at a $\sqrt{n}$-rate of posterior convergence (theorem 5.1). We actually state this result for the general situation of locally asymptotically normal (LAN) models, and next specify to the i.i.d. case. Next in section 5.2 we discuss results guaranteeing the desired rate of convergence, where we first show sufficiency of existence of certain tests (theorem 5.4), and next construct appropriate tests (theorem 5.6). We conclude with a lemma (applicable in parametric and non-parametric situations alike) to exclude testable model subsets, which implies a misspecified version of Schwartz’ consistency theorem.

In subsection 5.1.1 we work in a general locally asymptotically normal set-up, but in the remainder of the paper we consider the situation of i.i.d. observations, considered previously and described precisely in section 5.1.2.
5.1 Posterior limit distribution

5.1.1 Asymptotic normality in LAN models

Let $\Theta$ be an open subset of $\mathbb{R}^d$ parameterising statistical models $\{P^{(n)}_\theta : \theta \in \Theta\}$. For simplicity, we assume that for each $n$ there exists a single measure that dominates all measures $P^{(n)}_\theta$ as well as a “true measure” $P^{(n)}_0$, and we assume that there exist densities $p^{(n)}_\theta$ and $p^{(n)}_0$ such that the maps $(\theta, x) \mapsto p^{(n)}_\theta$ are measurable.

We consider models satisfying a stochastic local asymptotic normality (LAN) condition around a given inner point $\theta^* \in \Theta$ and relative to a given norming rate $\delta_n \rightarrow 0$: there exist random vectors $\Delta_{n, \theta^*}$ and nonsingular matrices $V_{\theta^*}$ such that the sequence $\Delta_{n, \theta^*}$ is bounded in probability, and for every compact set $K \subset \mathbb{R}^d$,

$$\sup_{h \in K} \left| \log \frac{p^{(n)}_{\theta^* + \Delta_n h}(X^{(n)}) - h^T V_{\theta^*} \Delta_{n, \theta^*} - \frac{1}{2} h^T V_{\theta^*} h}{p^{(n)}_{\theta^*}(X^{(n)})} \right| \rightarrow 0,$$

in (outer) $P^{(n)}_0$-probability. We state simple conditions ensuring this condition for the case of i.i.d. observations in section 5.1.2.

The prior measure $\Pi$ on $\Theta$ is assumed to be a probability measure with Lebesgue-density $\pi$, continuous and positive on a neighbourhood of a given point $\theta^*$. Priors satisfying these criteria assign enough mass to (sufficiently small) balls around $\theta^*$ to allow for optimal rates of convergence of the posterior if certain regularity conditions are met (see section 5.2).

The posterior based on an observation $X^{(n)}$ is denoted $\Pi_n(\cdot | X^{(n)})$: for every Borel set $A$,

$$\Pi_n(A \mid X^{(n)}) = \frac{\int_{\Theta} p^{(n)}_{\theta}(X^{(n)}) \pi(\theta) d\theta}{\int_{\Theta} p^{(n)}_{\theta}(X^{(n)}) \pi(\theta) d\theta}. \quad (5.2)$$

To denote the random variable associated with the posterior distribution, we use the notation $\vartheta$. Note that the assertion of theorem 5.1 below involves convergence in $P_0$-probability, reflecting the sample-dependent nature of the two sequences of measures converging in total-variation norm.

**Theorem 5.1.** Assume that (5.1) holds for some $\theta^* \in \Theta$ and let the prior $\Pi$ be as indicated above. Furthermore, assume that for every sequence of constants $M_n \rightarrow \infty$,

$$P^{(n)}_0 \Pi_n(\|\theta - \theta^*\| \geq \delta_n M_n \mid X^{(n)}) \rightarrow 0. \quad (5.3)$$

Then the sequence of posteriors converges to a sequence of normal distributions in total variation:

$$\sup_B \left| \Pi_n((\theta - \theta^*)/\delta_n \in B \mid X^{(n)}) - N_{\Delta_{n, \theta^*}, V_{\theta^*}}(B) \right| \xrightarrow{P_0} 0. \quad (5.4)$$
Proof. The proof is split into two parts: in the first part, we prove the assertion conditional on an arbitrary compact set \( K \subset \mathbb{R}^d \) and in the second part we use this to prove (5.4). Throughout the proof we denote the posterior for \( H = (\theta - \theta^*) / \delta_n \) given \( X(n) \) by \( \Pi_n \). The posterior for \( H \) follows from that for \( \theta \) by \( \Pi_n(H \in B | X(n)) = \Pi_n((\theta - \theta^/) / \delta_n \in B | X(n)) \) for all Borel sets \( B \). Furthermore, we denote the normal distribution \( N_{\Delta_n, \delta_n} \) by \( \Phi_n \). For a compact subset \( K \subset \mathbb{R}^d \) such that \( \Pi_n(H \in K | X(n)) > 0 \), we define a conditional version \( \Pi_n^K \) of \( \Pi_n \) by \( \Pi_n^K(B | X(n)) = \Pi_n(B \cap K | X(n)) / \Pi_n(K | X(n)) \). Similarly we defined a conditional measure \( \Phi_n^K \) corresponding to \( \Phi_n \).

Let \( K \subset \mathbb{R}^d \) be a compact subset of \( \mathbb{R}^d \). For every open neighbourhood \( U \subset \Theta \) of \( \theta^* \), \( \theta^* + K \delta_n \subset U \) for large enough \( n \). Since \( \theta^* \) is an internal point of \( \Theta \), for large enough \( n \) the random functions \( f_n : K \times K \rightarrow \mathbb{R} \),

\[
f_n(g, h) = \left( 1 - \frac{\phi_n(h) s_n(g)}{\phi_n(g) s_n(h)} \right) \pi_n(g),
\]

are well-defined, with \( \phi_n : K \rightarrow \mathbb{R} \) the Lebesgue density of the (randomly located) distribution \( N_{\Delta_n, \delta_n} \), \( \pi_n : K \rightarrow \mathbb{R} \) the Lebesgue density of the prior for the centred and rescaled parameter \( H \) and \( s_n : K \rightarrow \mathbb{R} \) the likelihood quotient \( s_n(h) = \frac{p_n(h)}{p_n(X(n))} \).

By the LAN assumption, we have for every random sequence \( (h_n) \subset K \), \( \log s_n(h_n) = h_n^T V \Delta_n \theta^* - \frac{1}{2} h_n^T V \theta^* h_n + o_P(1) \). For any two sequences \( (h_n), (g_n) \in K \), \( \pi_n(g_n) / \pi_n(h_n) \rightarrow 1 \) as \( n \rightarrow \infty \), leading to,

\[
\frac{\log \phi_n(h_n) s_n(g_n) \pi_n(g_n)}{\phi_n(g_n) s_n(h_n) \pi_n(h_n)} = (g_n - h_n)^T V \Delta_n \theta^* + \frac{1}{2} h_n^T V \theta^* h_n - \frac{1}{2} g_n^T V \theta^* g_n + o_P(1)
\]

\[
- \frac{1}{2} (h_n - \Delta_n \theta^*)^T V \theta^* (h_n - \Delta_n \theta^*) + \frac{1}{2} (g_n - \Delta_n \theta^*)^T V \theta^* (g_n - \Delta_n \theta^*)
\]

\[
= o_P(1),
\]

as \( n \rightarrow \infty \). Since all functions \( f_n \) depend continuously on \( (g, h) \) and \( K \times K \) is compact, we conclude that,

\[
\sup_{g, h \in K} f_n(g, h) \xrightarrow{P} 0, \quad (n \rightarrow \infty),
\]

(5.5)

where the convergence is in outer probability.

Assume that \( K \) contains a neighbourhood of 0 (to guarantee that \( \Phi_n(K) > 0 \)) and let \( \Xi_n \) denote the event that \( \Pi_n(K) > 0 \). Let \( \eta > 0 \) be given and based on that, define the events:

\[
\Omega_n = \left\{ \sup_{g, h \in K} f_n(g, h) \leq \eta \right\}_\star,
\]

where the * denotes the inner measurable cover set, in case the set on the right is not measurable. Consider the inequality (recall that the total-variation norm \( \| \cdot \| \) is bounded by 2):
\[ P_0^{(n)} \| \Pi_n^K - \Phi_n^K \|_{1_{\mathbb{Z}_n}} \leq P_0^{(n)} \| \Pi_n^K - \Phi_n^K \|_{1_{\Omega_n \cap \mathbb{Z}_n}} + 2 P_0^{(n)} (\mathbb{Z}_n \setminus \Omega_n). \] (5.6)

As a result of (5.5) the second term is \( o(1) \) as \( n \to \infty \). The first term on the r.h.s. is calculated as follows:

\[
\frac{1}{2} P_0^{(n)} \| \Pi_n^K - \Phi_n^K \|_{1_{\Omega_n \cap \mathbb{Z}_n}} = P_0^{(n)} \int K (1 - \frac{d\Phi_n}{d\Pi_n^K}) d\Pi_n^K 1_{\Omega_n \cap \mathbb{Z}_n} = P_0^{(n)} \int K (1 - \frac{s_n(g)\pi_n(g)\phi_n^K(h)}{s_n(h)\pi_n(h)\phi_n^K(g)} d\Phi_n^K(g)) \cdot d\Pi_n^K(h) 1_{\Omega_n \cap \mathbb{Z}_n},
\]

Note that for all \( g, h \in K \), \( \phi_n^K(h)/\phi_n^K(g) = \phi_n(h)/\phi_n(g) \), since on \( K \) \( \phi_n^K \) differs from \( \phi_n \) only by a normalisation factor. We use Jensen’s inequality (with respect to the \( \Phi_n^K \) expectation) for the (convex) function \( x \mapsto (1 - x)_+ \) to derive:

\[
\frac{1}{2} P_0^{(n)} \| \Pi_n^K - \Phi_n^K \|_{1_{\Omega_n \cap \mathbb{Z}_n}} \leq P_0^{(n)} \int K (1 - \frac{s_n(g)\pi_n(g)\phi_n(h)}{s_n(h)\pi_n(h)\phi_n(g)}) d\Phi_n^K(g) d\Pi_n^K(h) 1_{\Omega_n \cap \mathbb{Z}_n} \leq P_0^{(n)} \int K \sup_{g, h \in K} f_n(g, h) 1_{\Omega_n \cap \mathbb{Z}_n} |d\Phi_n^K(g) d\Pi_n^K(h)| \leq \eta.
\]

Combination with (5.6) shows that for all compact \( K \subset \mathbb{R}^d \) containing a neighbourhood of \( 0, P_0^{(n)} \| \Pi_n^K - \Phi_n^K \|_{1_{\mathbb{Z}_n}} \to 0 \).

Now, let \( (K_m) \) be a sequence of balls centred at \( 0 \) with radii \( M_m \to \infty \). For each \( m \geq 1 \), the above display holds, so if we choose a sequence of balls \( (K_m) \) that traverses the sequence \( K_m \) slowly enough, convergence to zero can still be guaranteed. Moreover, the corresponding events \( \mathbb{Z}_n = \{ \Pi_n(K_m) > 0 \} \) satisfy \( P_0^{(n)}(\mathbb{Z}_n) \to 1 \) as a result of (5.3). We conclude that there exists a sequence of radii \( (M_m) \) such that \( M_m \to \infty \) and \( P_0^{(n)} \| \Pi_n^K - \Phi_n^K \| \to 0 \) (where it is understood that the conditional probabilities on the l.h.s. are well-defined on sets of probability growing to one). The total variation distance between a measure and its conditional version given a set \( K \) satisfies \( \| \Pi - \Pi^K \| \leq 2\Pi(K^c) \). Combining this with (5.3) and lemma 5.10, we conclude that \( P_0^{(n)} \| \Pi_n - \Phi_n \| \to 0 \), which implies (5.4).

Condition (5.3) fixes the rate of convergence of the posterior distribution to be that occurring in the LAN property. Sufficient conditions to satisfy (5.3) in the case of i.i.d. observations are given in section 5.2.

### 5.1.2 Asymptotic normality in the i.i.d. case

Consider the situation that the observation is a vector \( X^{(n)} = (X_1, \ldots, X_n) \) and the model consists of \( n \)-fold product measures \( P_0^{(n)} = P_0^n \), where the components \( P_0 \) are given by densities \( p_\theta \) such that the maps \( (\theta, x) \mapsto p_\theta(x) \) are measurable and \( \theta \mapsto p_\theta \).
is smooth (in the sense of lemma 5.1). Assume that the observations form an \textit{i.i.d.} sample from a distribution \( P_0 \) with density \( p_0 \) relative to a common dominating measure. Assume that the Kullback-Leibler divergence of the model relative to \( P_0 \) is finite and minimized at \( \theta^* \in \Theta \), i.e.:

\[
-P_0 \log \frac{p_\theta}{p_0} = \inf_{\theta \in \Theta} -P_0 \log \frac{p_\theta}{p_0} < \infty. \tag{5.7}
\]

In this situation we set \( \delta_n = n^{-1/2} \) and use \( \Delta_n, \theta^* = V_{\theta^*}^{-1} G_n \hat{\ell}_{\theta^*} \) as the centering sequence (where \( \hat{\ell}_{\theta^*} \) denotes the score function of the model \( \theta \mapsto p_\theta \) at \( \theta^* \) and \( G_n = \sqrt{n}(P_n - P_0) \) is the empirical process).

Lemmas that establish the LAN expansion (5.1) (for an overview, see, for instance Van der Vaart (1998) [90]) usually assume a well-specified model, whereas current interest requires local asymptotic normality in misspecified situations. To that end we consider the following lemma which gives sufficient conditions.

**Lemma 5.1.** If the function \( \theta \mapsto \log p_\theta(X_1) \) is differentiable at \( \theta^* \) in \( P_0 \)-probability with derivative \( \ell_{\theta^*}(X_1) \) and:

(i) there is an open neighbourhood \( U \) of \( \theta^* \) and a square-integrable function \( m_{\theta^*} \) such that for all \( \theta_1, \theta_2 \in U \):

\[
|\log \frac{p_{\theta_1}}{p_{\theta_2}}| \leq m_{\theta^*} \|\theta_1 - \theta_2\|, \quad (P_0 - a.s.), \tag{5.8}
\]

(ii) the Kullback-Leibler divergence with respect to \( P_0 \) has a 2nd-order Taylor-expansion around \( \theta^* \):

\[
-P_0 \log \frac{p_\theta}{p_{\theta^*}} = \frac{1}{2}(\theta - \theta^*) V_{\theta^*}(\theta - \theta^*) + o(\|\theta - \theta^*\|^2), \quad (\theta \to \theta^*), \tag{5.9}
\]

where \( V_{\theta^*} \) is a positive-definite \( d \times d \)-matrix,

then (5.1) holds with \( \delta_n = n^{-1/2} \) and \( \Delta_n, \theta^* = V_{\theta^*}^{-1} G_n \hat{\ell}_{\theta^*} \). Furthermore, the score function is bounded as follows:

\[
\|\hat{\ell}_{\theta^*}(X)\| \leq m_{\theta^*}(X), \quad (P_0 - a.s.). \tag{5.10}
\]

Finally, we have:

\[
P_0 \ell_{\theta^*} = \frac{\partial}{\partial \theta} [P_0 \log p_\theta]_{\theta = \theta^*} = 0. \tag{5.11}
\]

**Proof.** Using lemma 19.31 in Van der Vaart (1998) [90] for \( \ell_\theta(X) = \log p_\theta(X) \), the conditions of which are satisfied by assumption, we see that for any sequence \( \langle h_n \rangle \) that is bounded in \( P_0 \)-probability:

\[
G_n \left( \sqrt{n}(\ell_{\theta^*} + h_n/\sqrt{n}) - \hat{\ell}_{\theta^*} \right) \xrightarrow{P_0} 0. \tag{5.12}
\]

Hence, we see that,
Using the second-order Taylor-expansion (5.9):

\[ P_0 \log \frac{p^{\theta^* + h_n / \sqrt{n}}}{p_0^\theta} - \frac{1}{2n} h_n^T V_{\theta^*} h_n = o_P(1), \]

and substituting the log-likelihood product for the first term, we find (5.1). The proof of the remaining assumptions is standard.

Regarding the centering sequence \( \Delta_n, \theta^* \) and its relation to the maximum-likelihood estimator, we note the following lemma concerning the limit distribution of maximum-likelihood sequences.

**Lemma 5.2.** Assume that the model satisfies the conditions of lemma 5.1 with non-singular \( V_{\theta^*} \). Then a sequence of estimators \( \hat{\theta}_n \) such that \( \hat{\theta}_n \overset{P}{\to} \theta^* \) and

\[ P_n \log p_{\hat{\theta}_n} \geq \sup_{\theta} P_n \log p_\theta - o_P(n^{-1}), \]

satisfies the asymptotic expansion:

\[ \sqrt{n}(\hat{\theta}_n - \theta^*) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} V_{\theta^*}^{-1} \hat{\ell}_\theta^*(X_i) + o_P(1). \]  

(5.13)

**Proof.** The proof of this lemma is a more specific version of the proof found in Van der Vaart (1998) [90] on page 54.

Lemma 5.2 implies that for consistent maximum-likelihood estimators (sufficient conditions for consistency are given, for instance, in theorem 5.7 of van der Vaart (1998) [90]) the distribution of \( \sqrt{n}(\hat{\theta}_n - \theta^*) \) has a normal limit with mean zero and covariance \( V_{\theta^*}^{-1} P_0[\hat{\ell}_\theta^* V_{\theta^*}^{-1} \hat{\ell}_\theta^*] V_{\theta^*}^{-1} \). More important for present purposes, however, is the fact that according to (5.13), this sequence differs from \( \Delta_n, \theta^* \) only by a term of order \( o_P(1) \). Since the total-variational distance \( \| N_{\mu, \Sigma} - N_{\nu, \Sigma} \| \) is bounded by a multiple of \( \| \mu - \nu \| \) as \( (\mu \to \nu) \), the assertion of the Bernstein-Von Mises theorem can also be formulated with the sequence \( \sqrt{n}(\hat{\theta}_n - \theta^*) \) as the locations for the normal limit sequence. Using the invariance of total-variation under rescaling and shifts, this leads to the conclusion that:

\[ \sup_{B} \left| \Pi_n( \theta \in B \mid X_1, \ldots, X_n ) - N_{\theta^*}^{-1} W_{\theta^*}(B) \right| \overset{P_0}{\to} 0, \]

which demonstrates the usual interpretation of the Bernstein-Von Mises theorem most clearly: the sequence of posteriors resembles more-and-more closely a sequence of ‘sharpening’ normal distributions centred at the maximum-likelihood estimators. More generally, any sequence of estimators satisfying (5.13) (i.e. any best-regular estimator sequence) may be used to centre the normal limit sequence on.
The conditions for lemma 5.2, which derive directly from a fairly general set of conditions for asymptotic normality in parametric $M$-estimation (see, theorem 5.23 in Van der Vaart (1998) [90]), are close to the conditions of the above Bernstein-Von Mises theorem. In the well-specified situation the Lipschitz condition (5.8) can be relaxed slightly and replaced by the condition of differentiability in quadratic mean.

It was noted in the introduction that the mismatch of the asymptotic covariance matrix $V_{\theta^*}^{-1}P_0[\ell_{\theta^*}^T]V_{\theta^*}^{-1}$ and the limiting covariance matrix $V_{\theta^*}^{-1}$ in the Bernstein-Von Mises theorem causes that Bayesian credible sets are not confidence sets at the nominal level. The following example shows that both over- and under-covering may occur.

**Example 5.1.** Let $P_\theta$ be the normal distribution with mean $\theta$ and variance 1, and let the true distribution possess mean zero and variance $\sigma^2 > 0$. Then $\theta^* = 0$, $P_0[\ell_{\theta^*}^2] = \sigma^2$ and $V_{\theta^*} = 1$. It follows that the radius of the $1 - \alpha$-Bayesian credible set is $z_\alpha / \sqrt{n}$, whereas a $1 - \alpha$-confidence set around the mean has radius $z_\alpha \sigma / \sqrt{n}$. Depending on $\sigma^2 \leq 1$ or $\sigma^2 > 1$, the credible set can have coverage arbitrarily close to 0 or 1.

### 5.1.3 Asymptotic normality of point-estimators

Having discussed the posterior distributional limit, a natural question concerns the asymptotic properties of point-estimators derived from the posterior, like the posterior mean and median.

Based on the Bernstein-Von Mises assertion (5.4) alone, one sees that any functional $f : \Theta \to \mathbb{R}$, continuous relative to the total-variational norm, when applied to the sequence of posterior laws, converges to $f$ applied to the normal limit distribution. Another general consideration follows from a generic construction of point-estimates from posteriors and demonstrate that posterior consistency at rate $\delta_n$ implies frequentist consistency at rate $\delta_n$.

**Theorem 5.2.** Let $X_1, \ldots, X_n$ be distributed i.i.d. $P_0$ and let $\Pi_n(\cdot \mid X_1, \ldots, X_n)$ denote a sequence of posterior distributions on $\Theta$ that satisfies (5.3). Then there exist point-estimators $\hat{\theta}_n$ such that:

$$
\delta_n^{-1}(\hat{\theta}_n - \theta^*) = O_P(1),
$$

i.e. $\hat{\theta}_n$ is consistent and converges to $\theta^*$ at rate $\delta_n$.

**Proof.** Define $\hat{\theta}_n$ to be the center of a smallest ball that contains posterior mass at least 1/2. Because the ball around $\theta^*$ of radius $\delta_n M_n$ contains posterior mass tending to 1, the radius of a smallest ball must be bounded by $\delta_n M_n$ and the smallest ball must intersect the ball of radius $\delta_n M_n$ around $\theta^*$ with probability tending to 1. This shows that $\|\hat{\theta}_n - \theta^*\| \leq 2\delta_n M_n$ with probability tending to one.
Consequently, frequentist restrictions and notions of asymptotic optimality have implications for the posterior too: in particular, frequentist bounds on the rate of convergence for a given problem apply to the posterior rate as well.

However, these general points are more appropriate in non-parametric context and the above existence theorem does not pertain to the most widely-used Bayesian point-estimators. Asymptotic normality of the posterior mean in a misspecified model has been analysed in Bunke and Milhaud (1998) [?]. We generalize their discussion and prove asymptotic normality and efficiency for a class of point-estimators defined by a general loss function, which includes the posterior mean and median.

Let \( \ell : \mathbb{R}^k \to [0, \infty) \) be a loss-function with the following properties: \( \ell \) is continuous and satisfies, for every \( M > 0 \),

\[
\sup_{\|h\| \leq M} \inf_{\|h\| > 2M} \ell(h),
\]

with strict inequality for some \( M \). Furthermore, we assume that \( \ell \) is subpolynomial, \textit{i.e.} for some \( p > 0 \),

\[
\ell(h) \leq 1 + \|h\|^p.
\]

Define the estimators \( \hat{\theta}_n \) as the (near-)minimizers of

\[
t \mapsto \int \ell(\sqrt{n}(t - \theta)) \, d\Pi_n(\theta|X_1, \ldots, X_n).
\]

The theorem below is the misspecified analog of theorem 10.8 in van der Vaart (1998) [90] and is based on general methods from \( M \)-estimation, in particular the argmax theorem (see, for example, corollary 5.58 in [90]).

**Theorem 5.3.** Assume that the model satisfies (5.1) for some \( \theta^* \in \Theta \) and that the conditions of theorems 5.4 are satisfied. Let \( \ell : \mathbb{R}^k \to [0, \infty) \) be a loss-function with the properties listed and assume that \( \int \|\theta\|^p \, d\Pi(\theta) < \infty \). Then under \( P_0 \), the sequence \( \sqrt{n}(\hat{\theta}_n - \theta^*) \) converges weakly to the minimizer of

\[
t \mapsto Z(t) = \int \ell(t - h) \, dN(t, V^{-1} \theta^* \Pi_0),
\]

where \( X \sim N(0, V^{-1} \Pi_0) \), provided that any two minimizers of this process coincide almost-surely. In particular, if the loss function is subconvex (e.g. \( \ell(x) = \|x\|^2 \) or \( \ell(x) = \|x\| \), giving the posterior mean and median), then \( \sqrt{n}(\hat{\theta}_n - \theta^*) \) converges weakly to \( X \) under \( P_0 \).

**Proof.** The theorem can be proved along the same lines as theorem 10.8 in [90]. The main difference is in proving that, for any \( M_n \to \infty \),

\[
U_n := \int_{\|h\| > M_n} \|h\|^p \, d\Pi_n(h|X_1, \ldots, X_n) \xrightarrow{P_0} 0.
\]

(5.16)
Here, abusing notation, we write \( d\Pi_n(h|X_1, \ldots, X_n) \) to denote integrals relative to the posterior distribution of the local parameter \( h = \sqrt{n}(\theta - \theta^*) \). Under misspecification a new proof is required, for which we extend the proof of theorem 5.4 below.

Once (5.16) is established, the proof continues as follows. The variable \( \hat{h}_n = \sqrt{n}(\hat{\theta}_n - \theta) \) is the maximizer of the process \( t \mapsto \int \ell(t-h) d\Pi_n(h|X_1, \ldots, X_n) \). Reasoning exactly as in the proof of theorem 10.8, we see that \( \hat{h}_n = O_P(1) \). Fix some compact set \( K \) and for given \( M > 0 \) define the processes

\[
\begin{align*}
t \mapsto Z_{n,M}(t) &= \int_{|h| \leq M} \ell(t-h) d\Pi_n(h|X_1, \ldots, X_n) \\
t \mapsto W_{n,M}(t) &= \int_{|h| \leq M} \ell(t-h) dN_{\Delta,\nu_{\theta^*}^{-1}}(h) \\
t \mapsto W_M(t) &= \int_{|h| \leq M} \ell(t-h) dN_{X,\nu_{\theta^*}^{-1}}(h)
\end{align*}
\]

Since \( \sup_{h \in K} |h| \leq M \), the continuous mapping theorem implies that \( W_{n,M} \Rightarrow W_M \) in \( \ell^\infty(K) \). Since \( \ell \) has subpolynomial tails, integrable with respect to \( N_{X,\nu_{\theta^*}^{-1}} \), \( W_M \Rightarrow Z \) in \( \ell^\infty(K) \) as \( M \to \infty \). Thus \( Z_{n,M} \Rightarrow W_M \) in \( \ell^\infty(K) \), for every \( M > 0 \), and \( W_M \Rightarrow Z \) as \( M \to \infty \). We conclude that there exists a sequence \( M_n \to \infty \) such that \( Z_{n,M_n} \Rightarrow Z \).

The limit (5.16) implies that \( Z_{n,M_n} - Z_n = o_P(1) \) in \( \ell^\infty(K) \) and we conclude that \( Z_n \Rightarrow Z \) in \( \ell^\infty(K) \). Due to the continuity of \( \ell \), \( t \mapsto Z(t) \) is continuous almost surely.

This, together with the assumed unicity of maxima of these sample paths, enables the Vapnik-Chervonenkis theorem (see, corollary 5.58 in [90]) and we conclude that \( \hat{h}_n \Rightarrow \hat{h} \), where \( \hat{h} \) is the minimizer of \( Z(t) \).

For the proof of (5.16) we adopt the notation of theorem 5.4. The tests \( \omega_n \) employed there can be taken nonrandomized without loss of generality (otherwise replace them for instance by \( 1_{\omega_n > 1/2} \)) and then \( U_n \omega_n \) tends to zero in probability by the only fact that \( \omega_n \) does so. Thus (5.16) is proved once it is established that, with \( \varepsilon_n = M_n/\sqrt{n} \),

\[
\begin{align*}
P_0(1 - \omega_n) 1_{\Omega_n} \int_{|\theta - \theta^*| < \varepsilon_n} \frac{n^{p/2} \|\theta - \theta^*\|^p d\Pi_n(\theta \mid X_1, \ldots, X_n)}{\int_{|\theta - \theta^*| < \varepsilon_n} d\Pi_n(\theta \mid X_1, \ldots, X_n)} &\to 0, \\
P_0(1 - \omega_n) 1_{\Omega_n} \int_{|\theta - \theta^*| > \varepsilon_n} \frac{n^{p/2} \|\theta - \theta^*\|^p d\Pi_n(\theta \mid X_1, \ldots, X_n)}{\int_{|\theta - \theta^*| > \varepsilon_n} d\Pi_n(\theta \mid X_1, \ldots, X_n)} &\to 0.
\end{align*}
\]

We can use bounds as in the proof of theorem 5.4, but instead of at (5.21) and (5.21) we arrive at the bounds

\[
\frac{\varepsilon^{p/2}(a_0^2(1-C) - D\varepsilon^2)}{\Pi(B(a_0, \theta^*; P_0))} n^{p/2} \int \|\theta - \theta^*\|^p d\Pi(\theta),
\]
5.2 Rate of convergence

In a Bayesian context, the rate of convergence is defined as the maximal pace at which balls around the point of convergence can be shrunk to radius zero while still capturing a posterior mass that converges to one asymptotically. Current interest lies in the fact that the Bernstein-Von Mises theorem of the previous section formulates condition (5.3) (with \( \delta_n = n^{-1/2} \)),

\[
\Pi_n(\| \vartheta - \theta^* \| \geq M_n/\sqrt{n} \mid X_1, \ldots, X_n) \xrightarrow{P} 0,
\]

for all \( M_n \to \infty \). A convenient way of establishing the above is through the condition that suitable test sequences exist. As has been shown in a well-specified context in Ghosal et al. (2000) [42] and under misspecification in Kleijn and Van der Vaart (2003) [58], the most important requirement for convergence of the posterior at a certain rate is the existence of a test-sequence that separates the point of convergence from the complements of balls shrinking at said rate.

This is also the approach we follow here: we show that the sequence of posterior probabilities in the above display converges to zero in \( P \)-probability if a test sequence exists that is suitable in the sense given above (see the proof of theorem 5.4). However, under the regularity conditions that were formulated to establish local asymptotic normality under misspecification in the previous section, more can be said: not complements of shrinking balls, but fixed alternatives are to be suitably testable against \( P_0 \), thus relaxing the testing condition considerably. Locally, the construction relies on score-tests to separate the point of convergence from complements of neighbourhoods shrinking at rate \( 1/\sqrt{n} \), using Bernstein’s inequality to obtain exponential power. The tests for fixed alternatives are used to extend those local tests to the full model.

In this section we prove that a prior mass condition and suitable test sequences suffice to prove convergence at the rate required for the Bernstein-Von Mises theorem formulated in section 5.1. The theorem that begins the next subsection summarizes the conclusion. Throughout the section we consider the i.i.d. case, with notation as in section 5.1.2.
5.2 Rate of convergence

5.2.1 Posterior rate of convergence

With use of theorem 5.6, we formulate a theorem that ensures $\sqrt{n}$-rate of convergence for the posterior distributions of smooth, testable models with sufficient prior mass around the point of convergence. The testability condition is formulated using measures $Q_\theta$, defined by,

$$Q_\theta(A) = P_0 \left( \frac{p_\theta}{p_{\theta^*}} \cdot 1_A \right),$$

for all $A \in \mathcal{A}$ and all $\theta \in \Theta$. Note that all $Q_\theta$ are dominated by $P_0$ and that $Q_{\theta^*} = P_0$.

Also note that if the model is well-specified, then $P_{\theta^*} = P_0$ and $Q_\theta = P_0$ for all $\theta$. Therefore the use of $Q_\theta$ instead of $P_\theta$ to formulate the testing condition is relevant only in the misspecified situation (see Kleijn and Van der Vaart (2006) [58] for more on this subject). The proof of theorem 5.4 makes use of Kullback-Leibler neighbourhoods of $\theta^*$ of the form:

$$B(\epsilon, \theta^*; P_0) = \{ \theta \in \Theta : -P_0 \log \frac{p_\theta}{p_{\theta^*}} \leq \epsilon^2, P_0 \left( \log \frac{p_\theta}{p_{\theta^*}} \right)^2 \leq \epsilon^2 \}, \quad (5.17)$$

for some $\epsilon > 0$.

**Theorem 5.4.** Assume that the model satisfies the smoothness conditions of lemma 5.1, where in addition, it is required that $P_0(p_\theta/p_{\theta^*}) < \infty$ for all $\theta$ in a neighbourhood of $\theta^*$ and $P_0(e^{sm_{\theta^*}}) < \infty$ for some $s > 0$. Assume that the prior possesses a density that is continuous and positive in a neighbourhood of $\theta^*$. Furthermore, assume that $P_0 \ell_\theta^* \ell_\theta^T$ is invertible and that for every $\epsilon > 0$ there exists a sequence of tests $(\phi_n)$ such that:

$$P_0^n \phi_n \rightarrow 0, \quad \sup_{\{\theta : \|\theta - \theta^*\| \geq \epsilon\}} Q_\theta^n(1 - \phi_n) \rightarrow 0. \quad (5.18)$$

Then the posterior converges at rate $1/\sqrt{n}$, i.e. for every sequence $(M_n)$, $M_n \rightarrow \infty$:

$$\Pi_n \left( \theta \in \Theta : \|\theta - \theta^*\| \geq M_n/\sqrt{n} \mid X_1, X_2, \ldots, X_n \right) \rightarrow 0, \quad P_\theta^0.$$ 

**Proof.** Let $(M_n)$ be given, and define the sequence $(\epsilon_n)$ by $\epsilon_n = M_n/\sqrt{n}$. According to theorem 5.6 there exists a sequence of tests $(\omega_n)$ and constants $D > 0$ and $\epsilon > 0$ such that (5.23) holds. We use these tests to split the $P_\theta^0$-expectation of the posterior measure as follows:

$$P_\theta^0 \Pi(\theta : \|\theta - \theta^*\| \geq \epsilon_n \mid X_1, X_2, \ldots, X_n) \leq P_\theta^0 \omega_n + P_\theta^0(1 - \omega_n) \Pi(\theta : \|\theta - \theta^*\| \geq \epsilon_n \mid X_1, X_2, \ldots, X_n).$$

The first term is of order $o(1)$ as $n \rightarrow \infty$ by (5.23). Given a constant $\epsilon > 0$ (to be specified later), the second term can be decomposed as:
\[ P_0^n (1 - \omega_n) \Pi(\theta : \|\theta - \theta^*\| \geq \varepsilon_n \mid X_1, X_2, \ldots, X_n) \]
\[ = P_0^n (1 - \omega_n) \Pi(\theta : \|\theta - \theta^*\| \geq \varepsilon \mid X_1, X_2, \ldots, X_n) \]
\[ + P_0^n (1 - \omega_n) \Pi(\theta : \varepsilon_n \leq \|\theta - \theta^*\| < \varepsilon \mid X_1, X_2, \ldots, X_n). \tag{5.19} \]

Given two constants \( M, M' \geq 0 \) (also to be specified at a later stage), we define the sequences \((a_n), a_n = M \sqrt{\log n/n} \) and \((b_n), b_n = M' \varepsilon_n\). Based on \( a_n \) and \( b_n \), we define two sequences of events:

\[ \Xi_n = \left\{ \int \prod_{i=1}^{n} \frac{p^\theta}{p^{\theta'}}(X_i) d\Pi(\theta) \leq \Pi(B(a_n, \theta^*; P_0)) e^{-na_2(1+C)} \right\}; \]
\[ \Omega_n = \left\{ \int \prod_{i=1}^{n} \frac{p^\theta}{p^{\theta'}}(X_i) d\Pi(\theta) \leq \Pi(B(b_n, \theta^*; P_0)) e^{-nb_2(1+C)} \right\}. \]

The sequence \((\Xi_n)\) is used to split the first term on the r.h.s. of (5.19) and estimate it as follows:

\[ P_0^n (1 - \omega_n) \Pi(\theta : \|\theta - \theta^*\| \geq \varepsilon \mid X_1, X_2, \ldots, X_n) \leq P_0(\Xi_n) + P_0^n (1 - \omega_n) 1_{\Omega, \Xi_n} \Pi(\theta : \|\theta - \theta^*\| \geq \varepsilon \mid X_1, X_2, \ldots, X_n). \]

According to lemma 5.3, the first term is of order \( o(1) \) as \( n \to \infty \). The second term is estimated further with the use of lemmas 5.3, 5.4 and theorem 5.6: for some \( C > 0, \)

\[ P_0^n (1 - \omega_n) 1_{\Omega, \Xi_n} \Pi(\theta : \|\theta - \theta^*\| \geq \varepsilon \mid X_1, X_2, \ldots, X_n) \leq \frac{e^{a_2^2 (1+C)}}{\Pi(B(a_n, \theta^*; P_0))} \int_{\{\theta : \|\theta - \theta^*\| \geq \varepsilon\}} Q_0^n (1 - \omega_n) d\Pi(\theta) \]
\[ \leq \frac{e^{a_2^2 (1+C) - De^2}}{\Pi(B(a_n, \theta^*; P_0))} \Pi(\theta : \|\theta - \theta^*\| \geq \varepsilon). \tag{5.20} \]

Note that \( a_2^2 (1+C) - De^2 \leq -a_2^2 (1+C) \) for large enough \( n \), so that:

\[ \frac{e^{a_2^2 (1+C) - De^2}}{\Pi(B(a_n, \theta^*; P_0))} \leq K^{-1} e^{-na_2^2 (1+C) (a_n)^{-d}} \leq \frac{1}{M^{d/2} K} (\log n)^{-d/2} n^{-M^2 (1+C) + \frac{d}{2}}, \]
for large enough \( n \), using (5.22). A large enough choice for the constant \( M \) then ensures that the expression on the l.h.s. in the next-to-last display is of order \( o(1) \) as \( n \to \infty \).

The sequence \((\Omega_n)\) is used to split the second term on the r.h.s. of (5.19) after which we estimate it in a similar manner. Again the term that derives from \( 1_{\Omega_n} \) is of order \( o(1) \), and

\[ P_0^n (1 - \omega_n) 1_{\Omega_n} \Pi(\theta : \varepsilon_n \leq \|\theta - \theta^*\| < \varepsilon \mid X_1, X_2, \ldots, X_n) \]
\[ \leq \frac{e^{b_2^2 (1+C)}}{\Pi(B(b_n, \theta^*; P_0))} \sum_{j=1}^{n} \int_{\Lambda_{n,j}} Q_0^n (1 - \omega_n) d\Pi(\theta), \]
where we have split the domain of integration into spherical shells $A_{n,j}$, $(1 \leq j \leq J$, with $J$ the smallest integer such that $(J + 1)e_n > \varepsilon$: $A_{n,j} = \{ \theta : j\varepsilon_n \leq \| \theta - \theta^* \| \leq ((J + 1)e_n) \wedge \varepsilon \}$. Applying theorem 5.6 to each of the shells separately, we obtain:

$$
\begin{align*}
P_0^n(1-\omega_n) \int_{\Omega_1} \prod (\theta : \epsilon_n \leq \| \theta - \theta^* \| < \varepsilon \mid X_1, X_2, \ldots, X_n) \\
= \sum_{j=1}^J e^{h\varepsilon_n(1+\varepsilon)} \sup_{\theta \in A_{n,j}} Q_\theta^n(1-\omega_n) \prod (A_{n,j}) \\
\leq \sum_{j=1}^J e^{h\varepsilon_n(1+\varepsilon)-nDj^2\varepsilon^2_n} \prod \{ \theta : \| \theta - \theta^* \| \leq (j+1)e_n \} \\
\leq \sum_{j=1}^J e^{h\varepsilon_n(1+\varepsilon)-nDj^2\varepsilon^2_n} \prod \{ \theta : \| \theta - \theta^* \| \leq (j+1)e_n \}.
\end{align*}
$$

For a small enough $\varepsilon$ and large enough $n$, the sets $\{ \theta : \| \theta - \theta^* \| \leq (j+1)e_n \}$ all fall within the neighbourhood $U$ of $\theta^*$ on which the prior density $\pi$ is continuous. Hence $\pi$ is uniformly bounded by a constant $R > 0$ and we see that $\Pi \{ \theta : \| \theta - \theta^* \| \leq (j+1)e_n \} \leq RV_j(j+1)^d \varepsilon^d_n$, where $V_j$ is the Lebesgue-volume of the $d$-dimensional ball of unit radius. Combining this with (5.22), there exists a constant $K' > 0$ such that, with $M' < \sqrt{D/2(1+\varepsilon)}$:

$$
P_0^n(1-\omega_n) \int_{\Omega_1} \prod (\theta : \epsilon_n \leq \| \theta - \theta^* \| < \varepsilon \mid X_1, \ldots, X_n) \\
\leq K'e^{-\varepsilon_n(1+\varepsilon)-nDj^2\varepsilon^2_n} \sum_{j=1}^J (j+1)^d \varepsilon^d_n,
$$

for large enough $n$. The series is convergent and we conclude that this term is also of order $o(1)$ as $n \to \infty$.

Consistent testability of the type (5.18) appears to be a weak requirement because the form of the tests is arbitrary. (It may be compared to “classical conditions” like (B3) in section 6.7, page 455, of [?], formulated in the well-specified case.) Consistent testability is of course one of Schwarz’ conditions for consistency ([83]) and appears to have been introduced in the context of the (well-specified) Bernstein-Von Mises theorem by Le Cam. To exemplify its power we show in the next theorem that the tests exist as soon as the parameter set is compact and the model is suitably continuous in the parameter.

**Theorem 5.5.** Assume that $\Theta$ is compact and that $\theta^*$ is a unique point of minimum of $\Theta \ni -P_0 \log p_\theta$. Furthermore assume that $P_0(p_\theta/p_{\theta^*}) < \infty$ for all $\theta \in \Theta$ and that the map

$$
\theta \mapsto P_0 \left( \frac{p_\theta}{p_{\theta^*}} \right),
$$

is continuous at $\theta_1$ for every $s$ in a left neighbourhood of $1$, for every $\theta_1$. Then there exist tests $\phi_n$ satisfying (5.18). A sufficient condition is that for every $\theta_1 \in \Theta$ the maps $\theta \mapsto p_\theta/p_{\theta_1}$ and $\theta \mapsto p_{\theta}/p_{\theta_1}$ are continuous in $L_1(P_0)$ at $\theta = \theta_1$.

**Proof.** For given $\theta_1 \neq \theta^*$ consider the tests,

$$
\phi_{n,\theta_1} = \{ \mathbb{P}_n \log (p_\theta/q_{\theta_1}) < 0 \}.
$$


Because \( P_0 \log(p_0/q_{\theta_1}) \rightarrow P_0 \log(p_0/q_{\theta_1}) \) in \( P_0 \)-probability by the law of large numbers, and \( P_0 \log(p_0/q_{\theta_1}) = P_0 \log(p_{\theta^*}/p_{\theta_1}) > 0 \) for \( \theta_1 \neq \theta^* \) by the definition of \( \theta^* \) we have that \( P_0^* \phi_{n, \theta_1} \rightarrow 0 \) as \( n \rightarrow \infty \). By Markov’s inequality we have that,

\[
Q_\theta^n(1 - \phi_{n, \theta_1}) = Q_\theta^n \left( e^{n \log[p_0/q_{\theta_1}]} > 1 \right) \\
\leq Q_\theta^n e^{n \log[p_0/q_{\theta_1}]} = \left( Q_\theta(p_0/q_{\theta_1}) \right)^n = \rho(\theta_1, \theta, s)^n
\]

for \( \rho(\theta_1, \theta, s) = \int p_0^* q_{\theta^*}^* q_\theta \, d\mu \). It is known from Kleijn and Van der Vaart (2006) [58] that the affinity \( s \mapsto \rho(\theta_1, \theta, s) \) tends to \( P_0(q_{\theta_1} > 0) = P_0(p_{\theta_1} > 0) \) as \( s \uparrow 1 \) and has derivative from the left equal to \( P_0 \log(q_{\theta_1}/p_0) 1_{q_{\theta_1} > 0} = P_0 \log[p_{\theta_1}/p_{\theta^*}] 1_{p_{\theta_1} > 0} \) at \( s = 1 \). We have that either \( P_0(p_{\theta_1} > 0) < 1 \) or \( P_0(p_{\theta_1} > 0) = 1 \) and \( P_0 \log[p_{\theta_1}/p_{\theta^*}] 1_{p_{\theta_1} > 0} = P_0 \log(p_{\theta_1}/p_{\theta^*}) < 0 \) (or both). In all cases there exists \( \theta_1 \) arbitrary close to 1 such that \( \rho(\theta_1, \theta, s_\theta_1) < 1 \). By assumption the map \( \theta \mapsto \rho(\theta_1, \theta, s_\theta_1) \) is continuous at \( \theta_1 \). Therefore, for every \( \theta_1 \) there exists an open neighbourhood \( G_{\theta_1} \) such that,

\[
r_{\theta_1} = \sup_{\theta \in G_{\theta_1}} \rho(\theta_1, \theta, s_\theta_1) < 1.
\]

The set \( \{ \theta \in \Theta : \|\theta - \theta^*\| \geq \varepsilon \} \) is compact and hence can be covered with finitely many sets of the type \( G_{\theta_1} \), say \( G_{\theta_1} \) for \( 1 = 1, \ldots, k \). We now define

\[
\phi_n = \max_{i=1, \ldots, k} \phi_{n, \theta_i}.
\]

This test satisfies

\[
P_0^n \phi_n \leq \sum_{i=1}^k P_0^n \phi_{n, \theta_i} \rightarrow 0
\]

\[
Q_\theta^n(1 - \phi_n) \leq \max_{i=1}^k Q_\theta^n(1 - \phi_{n, \theta_i}) \leq \max_{i=1}^k r_{\theta_i}^n \rightarrow 0
\]

uniformly in \( \theta \in \cup_{i=1}^k G_{\theta_i} \). Therefore the tests \( \phi_n \) satisfy the requirements.

To prove the last assertion we write \( \rho(\theta_1, \theta, s) = P_0(p_{\theta}/p_{\theta_1})^s(p_{\theta}/p_{\theta^*})^{1-s} \). Continuity of the maps \( \theta \mapsto (p_{\theta}/p_{\theta_1}) \) and \( \theta \mapsto (p_{\theta}/p_{\theta^*}) \) in \( L_1(P_0) \) can be seen to imply the required continuity of the map \( \theta \mapsto \rho(\theta_1, \theta, s) \).

Beyond compactness it appears impossible to give mere qualitative sufficient conditions, like continuity, for consistent testability. For “natural” parameterizations it ought to be true that distant parameters (outside a given compact) are the easy ones to test for (and a test designed for a given compact ought to be consistent even for points outside the compact), but this depends on the structure of the model. Alternatively, many models would allow a suitable compactification to which the preceding result can be applied, but we omit a discussion. The results in the next section allow to discard a “distant” part of the parameter space, after which the preceding results apply.
In the proof of theorem 5.4, lower bounds in probability on the denominators of posterior probabilities are needed, as provided by the following lemma.

**Lemma 5.3.** For given \( \epsilon > 0 \) and \( \theta^* \in \Theta \) such that \( P_0(\log(p_0/p_{\theta^*}) < \infty \) define \( B(\epsilon, \theta^*; P_0) \) by (5.17). Then for every \( C > 0 \) and probability measure \( \Pi \) on \( \Theta \):

\[
P_n \left( \int_{\Theta} \prod_{i=1}^{n} \frac{p_0}{p_{\theta^*}}(X_i) d\Pi(\theta) \leq \Pi \left( B(\epsilon, \theta^*; P_0) \right) \right) \leq \frac{1}{C^2 n \epsilon^2}.
\]

**Proof.** This lemma can also be found as lemma 7.1 in Kleijn and Van der Vaart (2003) [58]. The proof is analogous to that of lemma 8.1 in Ghosal et al. (2000) [42].

Moreover, the prior mass of the Kullback-Leibler neighbourhoods \( B(\epsilon, \theta^*; P_0) \) can be lower-bounded if we make the regularity assumptions for the model used in section 5.1 and the assumption that the prior has a Lebesgue density that is well-behaved at \( \theta^* \).

**Lemma 5.4.** Under the smoothness conditions of lemma 5.1 and assuming that the prior density \( \pi \) is continuous and strictly positive in \( \theta^* \), there exists a constant \( K > 0 \) such that the prior mass of the Kullback-Leibler neighbourhoods \( B(\epsilon, \theta^*; P_0) \) satisfies:

\[
\Pi \left( B(\epsilon, \theta^*; P_0) \right) \geq K \epsilon^d, \quad (5.22)
\]

for small enough \( \epsilon > 0 \).

**Proof.** As a result of the smoothness conditions, we have, for some constants \( c_1, c_2 > 0 \) and small enough \( \| \theta - \theta^* \| \), \( -P_0(\log(p_0/p_{\theta^*}) \leq c_1 \| \theta - \theta^* \|^2 \), and \( P_0(\log(p_0/p_{\theta^*}))^2 \leq c_2 \| \theta - \theta^* \|^2 \). Defining \( c = (1/c_1 \wedge 1/c_2)^{1/2} \), this implies that for small enough \( \epsilon > 0 \), \( \{ \theta \in \Theta : \| \theta - \theta^* \| \leq c \epsilon \} \subset B(\epsilon, \theta^*; P_0) \). Since the Lebesgue-density \( \pi \) of the prior is continuous and strictly positive in \( \theta^* \), we see that there exists a \( \delta' > 0 \) such that for all \( 0 < \delta \leq \delta' \), \( \Pi (\theta \in \Theta : \| \theta - \theta^* \| \leq \delta) \geq \frac{1}{4} V_d \pi(\theta^*) \delta^d > 0 \). Hence, for small enough \( \epsilon, c \epsilon \leq \delta' \) and we obtain (5.22) upon combination.

### 5.2.2 Suitable test sequences

In this subsection we prove that the existence of test sequences (under misspecification) of uniform exponential power for complements of shrinking balls around \( \theta^* \) versus \( P_0 \) (as needed in the proof of theorem 5.4), is guaranteed whenever asymptotically consistent test-sequences exist for complements of fixed balls around \( \theta^* \) versus \( P_0 \) and the conditions of lemmas 5.1 and 5.6 are met. The following theorem is inspired by lemma 10.3 in Van der Vaart (1998) [90].

**Theorem 5.6.** Assume that the conditions of lemma 5.1 are satisfied, where in addition, it is required that \( P_0(p_{\theta}/p_{\theta^*}) < \infty \) for all \( \theta \) in a neighbourhood of \( \theta^* \) and...
$P_0(e^{\eta \varphi^*}) < \infty$ for some $s > 0$. Furthermore, suppose that $P_0 \ell_\theta, P_0 \ell_\theta^*$ is invertible and for every $\epsilon > 0$ there exists a sequence of test functions $(\phi_n)$, such that:

$$P_0^n \phi_n \to 0, \quad \sup_{\{\theta: \|\theta - \theta^*\| \geq \epsilon\}} Q^*_\theta(1 - \phi_n) \to 0.$$  

Then for every sequence $(M_n)$ such that $M_n \to \infty$ there exists a sequence of tests $(\omega_n)$ such that for some constants $D > 0$, $\epsilon > 0$ and large enough $n$:

$$P_0^n \omega_n \to 0, \quad Q^*_\theta(1 - \omega_n) \leq e^{-nd\|\theta - \theta^*\|^2 \wedge \epsilon^2}, \quad (5.23)$$

for all $\theta \in \Theta$ such that $\|\theta - \theta^*\| \geq M_n / \sqrt{n}$.

**Proof.** Let $(M_n)$ be given. We construct two sequences of tests: one sequence to test $P_0$ versus $\{Q_\theta: \theta \in \Theta_1\}$ with $\Theta_1 = \{\theta \in \Theta: M_n / \sqrt{n} \leq \|\theta - \theta^*\| \leq \epsilon\}$, and the other to test $P_0$ versus $\{Q_\theta: \theta \in \Theta_2\}$ with $\Theta_2 = \{\theta: \|\theta - \theta^*\| > \epsilon\}$, both uniformly with exponential power (for a suitable choice of $\epsilon$). We combine these sequences to test $P_0$ versus $\{Q_\theta: \|\theta - \theta^*\| \geq M_n / \sqrt{n}\}$ uniformly with exponential power.

For the construction of the first sequence, a constant $L > 0$ is chosen to truncate the score-function component-wise (i.e., for all $1 \leq k \leq d$, $(\ell_\theta^* k)_k = 0$ if $\|\ell_\theta^* k\| \geq L$ and $(\ell_\theta^* k)_k = (\ell_\theta^* k)_k$ otherwise) and we define:

$$\omega_{1,n} = 1 \{\|\sqrt{n}(P_n - P_0)\ell_\theta^*\| > \sqrt{M_n / n}\},$$

Because the function $\ell_\theta^*$ is square-integrable, we can ensure that the matrices $P_0(\ell_\theta^* \ell_\theta^{*T})$, $P_0(\ell_\theta^* (\ell_\theta^*)^T)$ and $P_0(\ell_\theta^* (\ell_\theta^*)^T)$ are arbitrarily close (for instance in operator norm) by a sufficiently large choice for the constant $L$. We fix such an $L$ throughout the proof.

By the central limit theorem $P_0^\omega \omega_{1,n} = P_0^\omega (\|\sqrt{n}(P_n - P_0)\ell_\theta^*\|^2 > M_n) \to 0$. Turning to $Q^*_\theta(1 - \omega_{1,n})$ for $\theta \in \Theta_1$, we note that for all $\theta$:

$$Q^*_\theta (\|\sqrt{n}(P_n - P_0)\ell_\theta^*\| \leq \sqrt{M_n / n}) = Q^*_\theta (\sup_{v \in S} v^T (P_n - P_0)\ell_\theta^* \leq \sqrt{M_n / n})$$

$$\leq \inf_{v \in S} Q^*_\theta (v^T (P_n - P_0)\ell_\theta^* \leq \sqrt{M_n / n}),$$

where $S$ is the sphere of unity in $\mathbb{R}^d$. With the choice $v = (\theta - \theta^*) / \|\theta - \theta^*\|$ as an upper bound for the l.h.s. in the above display, we note that:

$$Q^*_\theta ((\theta - \theta^*)^T (P_n - P_0)\ell_\theta^* \leq \sqrt{M_n / n}) = Q^*_\theta ((\theta - \theta^*)^T (P_n - Q_\theta)\ell_\theta^* \geq (\theta - \theta^*)^T (Q_\theta - Q_{\theta^*})\ell_\theta^* - \sqrt{M_n / n} \|\theta - \theta^*\|),$$

where we have used the notation (for all $\theta \in \Theta_1$ with small enough $\epsilon > 0$) $Q_\theta = \|Q_\theta\|^{-1} Q_\theta$ and the fact that $P_0 = Q_\theta^* = Q_{\theta^*}$. By straightforward manipulation, we find:
In view of lemma 5.6 and conditions (5.8), (5.9), \( P_0(p_\theta/p_\theta^*) - 1 \) is of order \( O(\|\theta - \theta^*\|^2) \) as \( \theta \to \theta^* \), which means that if we approximate the above display up to order \( o(\|\theta - \theta^*\|^2) \), we can limit attention on the r.h.s. to the first term in the last factor and equate the first factor to 1. Furthermore, using the differentiability of \( \theta \to \log(p_\theta/p_\theta^*) \), condition (5.8) and lemma 5.6, we see that:

\[
\begin{align*}
R_0 \left\| \left( p_\theta/p_\theta^* - 1 - (\theta - \theta^*)^T \ell_\theta^* \right) \ell_\theta^* \right\|
\leq R_0 \left\| \left( p_\theta/p_\theta^* - 1 - \log p_\theta/p_\theta^* \right) \ell_\theta^* \right\| + R_0 \left\| \left( \log p_\theta/p_\theta^* - (\theta - \theta^*)^T \ell_\theta^* \right) \ell_\theta^* \right\|,
\end{align*}
\]

which is \( o(\|\theta - \theta^*\|) \). Also note that since \( M_n \to \infty \) and for all \( \theta \in \Theta_1, \|\theta - \theta^*\| \geq M_n/\sqrt{\tau_n} \geq -\|\theta - \theta^*\| \sqrt{M_n/n} \geq -\|\theta - \theta^*\|^2 (M_n)^{-1/2} \). Summarizing the above and combining with the remark made at the beginning of the proof concerning the choice of \( L \), we find that for every \( \delta > 0 \), there exist choices of \( \varepsilon > 0, L > 0 \) and \( N \geq 1 \) such that for all \( n \geq N \) and all \( \theta \in \Theta_1 \):

\[
(\theta - \theta^*)^T (\hat{Q}_{\theta} - \tilde{Q}_{\theta}) \ell_\theta^* - \sqrt{M_n/n}\|\theta - \theta^*\|
\geq (\theta - \theta^*)^T R_0(\ell_\theta^* \ell_\theta^*) (\theta - \theta^*) - \delta \|\theta - \theta^*\|^2.
\]

We denote \( \Delta(\theta) = (\theta - \theta^*)^T R_0(\ell_\theta^* \ell_\theta^*) (\theta - \theta^*) \) and since \( P_0(\ell_\theta^* \ell_\theta^*) \) is strictly positive definite by assumption, its smallest eigenvalue \( c \) is greater than zero. Hence, \( -\delta \|\theta - \theta^*\|^2 \geq -\delta/c \Delta(\theta) \). and there exists a constant \( r(\delta) \) (depending only on the matrix \( P_0(\ell_\theta^* \ell_\theta^*) \)) and with the property that \( r(\delta) \to 1 \) if \( \delta \to 0 \) such that:

\[
Q_\theta^*(1 - \omega_{1,n}) \leq Q_\theta^* \left( (\theta^* - \theta)^T (\bar{W}_n - \hat{Q}_{\theta} \ell_\theta^*) \right) \geq r(\delta) \Delta(\theta),
\]

for small enough \( \varepsilon \), large enough \( L \) and large enough \( n \), demonstrating that the type-II error is bounded above by the (unnormalized) tail probability \( Q_\theta^* (\bar{W}_n \geq r(\delta) \Delta(\theta)) \) of the mean of the variables \( W_i = (\theta^* - \theta)^T (\ell_\theta^* (X_i) - \hat{Q}_{\theta} \ell_\theta^*) \), \( 1 \leq i \leq n \), so that \( \hat{Q}_{\theta} \bar{W}_i = 0 \). The random variables \( W_i \) are independent and bounded since:

\[
|W_i| \leq \|\theta - \theta^*\| (\|\ell_\theta^* (X_i)\| + \|\hat{Q}_{\theta} \ell_\theta^*\|) \leq 2\sqrt{\ell} \|\theta - \theta^*\|.
\]

The variance of \( W_i \) under \( \hat{Q}_{\theta} \) is expressed as follows:

\[
\text{Var}_{\hat{Q}_{\theta}} W_i = (\theta - \theta^*)^T \left[ Q_{\theta} (\ell_\theta^* (\ell_\theta^*)^T) - \hat{Q}_{\theta} \ell_\theta^* \hat{Q}_{\theta} (\ell_\theta^*)^T \right] (\theta - \theta^*).
\]

Using that \( P_0\ell_\theta^* = 0 \) (see (5.11)), the above can be estimated like before, with the result that there exists a constant \( s(\delta) \) (depending only on (the largest eigenvalue of) the matrix \( P_0\ell_\theta^* \ell_\theta^* \)) and with the property that \( s(\delta) \to 1 \) as \( \delta \to 0 \) such that:
Concerning the range \(u_x \in \mathbb{R}^d\) for small enough \(\varepsilon\) and large enough \(L\). We apply Bernstein’s inequality (see, for instance, Pollard (1984) [7], pp. 192–193) to obtain:

\[
Q_\delta^*(1 - \omega_{1,n}) = \|Q_\delta\|^n \frac{Q_\delta^*(W_1 + \ldots + W_n \geq nr(\delta)\Delta(\theta))}{\|Q_\delta\|^n} \leq \|Q_\delta\|^n \exp\left(-\frac{1}{2} \frac{r(\delta)^2 n \Delta(\theta)}{2 L \sqrt{d} ||\theta - \theta^*|| r(\delta)}\right). \tag{5.24}
\]

The factor \(t(\delta) = r(\delta)^2 (s(\delta) + \frac{1}{2 L \sqrt{d} ||\theta - \theta^*|| r(\delta)})^{-1}\) lies arbitrarily close to 1 for sufficiently small choices of \(\delta\) and \(\varepsilon\). As for the \(n\)-th power of the norm of \(Q_\delta\), we use lemma 5.6, (5.8) and (5.9) to estimate the norm of \(Q_\delta\) as follows:

\[
\|Q_\delta\| = 1 + R_\delta \log \frac{P_\theta}{P_{\theta^*}} + \frac{1}{2} R_\delta \left(\log \frac{P_\theta}{P_{\theta^*}}\right)^2 + o(||\theta - \theta^*||^2) \\
\leq 1 + R_\delta \log \frac{P_\theta}{P_{\theta^*}} + \frac{1}{2} (\theta - \theta^*)^T R_\delta \left(\theta - \theta^*\right) + o(||\theta - \theta^*||^2) \tag{5.25}
\]

for some constant \(u(\delta)\) such that \(u(\delta) \to 1\) if \(\delta \to 0\). Because \(1 + x \leq e^x\) for all \(x \in \mathbb{R}\), we obtain, for sufficiently small \(||\theta - \theta^*||\):

\[
Q_\delta^*(1 - \omega_{1,n}) \leq \exp\left(-\frac{n}{2} (\theta - \theta^*)^T V_{\theta^*} (\theta - \theta^*) + \frac{n}{2} \left(u(\delta) - t(\delta)\right) \Delta(\theta)\right). \tag{5.26}
\]

Note that \(u(\delta) - t(\delta) \to 0\) as \(\delta \to 0\) and \(\Delta(\theta)\) is upper bounded by a multiple of \(||\theta - \theta^*||^2\). Since \(V_{\theta^*}\) is assumed to be invertible, we conclude that there exists a constant \(C > 0\) such that for large enough \(L\), small enough \(\varepsilon > 0\) and large enough \(n\):

\[
Q_\delta^*(1 - \omega_{1,n}) \leq e^{-Cn||\theta - \theta^*||^2}. \tag{5.27}
\]

Concerning the range \(||\theta - \theta^*|| > \varepsilon\), an asymptotically consistent test-sequence of \(P_0\) versus \(Q_\theta\) exists by assumption, what remains is the exponential power; the proof of lemma 5.5 demonstrates the existence of a sequence of tests \(\omega_{2,n}\) such that (5.28) holds. The sequence \(\{\psi_n\}\) is defined as the maximum of the two sequences defined above: \(\psi_n = \omega_{1,n} \vee \omega_{2,n}\) for all \(n \geq 1\), in which case \(P_0^\psi \psi_n \leq P_0^\psi \omega_{1,n} + P_0^\psi \omega_{2,n} \to 0\) and:

\[
\sup_{\theta \in \Theta_n} Q_\delta^*(1 - \psi_n) = \sup_{\theta \in \Theta_1} Q_\delta^*(1 - \psi_n) \vee \sup_{\theta \in \Theta_2} Q_\delta^*(1 - \psi_n) \\
\leq \sup_{\theta \in \Theta_1} Q_\delta^*(1 - \omega_{1,n}) \vee \sup_{\theta \in \Theta_2} Q_\delta^*(1 - \omega_{2,n}).
\]

Combination of the bounds found in (5.27) and (5.28) and a suitable choice for the constant \(D > 0\) lead to (5.23).

The following lemma shows that for a sequence of tests that separates \(P_0\) from a fixed model subset \(V\), there exists a exponentially powerful version without further
5.2 Rate of convergence

conditions. Note that this lemma holds in non-parametric and parametric situations alike.

**Lemma 5.5.** Suppose that for given measurable subset \( V \) of \( \Theta \), there exists a sequence of tests \( (\phi_n) \) such that:

\[
P_n^0 \phi_n \to 0, \quad \sup_{\theta \in V} Q_n^0 (1 - \phi_n) \to 0.
\]

Then there exists a sequence of tests \( (\omega_n) \) and strictly positive constants \( C, D \) such that:

\[
P_n^0 \omega_n \leq e^{-\eta C}, \quad \sup_{\theta \in V} Q_n^0 (1 - \omega_n) \leq e^{-nD}.
\]  

(5.28)

**Proof.** For given \( 0 < \zeta < 1 \), we split the model subset \( V \) in two disjoint parts \( V_1 \) and \( V_2 \) defined by \( V_1 = \{ \theta \in V : ||Q_\theta|| \geq 1 - \zeta \} \), \( V_2 = \{ \theta \in V : ||Q_\theta|| < 1 - \zeta \} \). Note that for every test-sequence \( (\omega_n) \),

\[
\sup_{\theta \in V} Q_n^0 (1 - \omega_n) \leq \sup_{\theta \in V_1} Q_n^0 (1 - \omega_n) \vee (1 - \zeta)^n.
\]  

(5.29)

Let \( \delta > 0 \) be given. By assumption there exists an \( N \geq 1 \) such that for all \( n \geq N + 1 \), \( P_n^0 \phi_n \leq \delta \) and \( \sup_{\theta \in V} Q_n^0 (1 - \phi_n) \leq \delta \). Every \( n \geq N + 1 \) can be written as an \( m \)-fold multiple of \( N \) (\( m \geq 1 \)) plus a remainder \( 1 \leq r \leq N : n = mN + r \). Given \( n \geq N \), we divide the sample \( X_1, X_2, \ldots, X_n \) into \( (m - 1) \) groups of \( N \) consecutive \( X \)'s and a group of \( N + r \) \( X \)'s and apply \( \phi_N \) to the first \( (m - 1) \) groups and \( \phi_N + r \) to the last group, to obtain:

\[
\begin{align*}
Y_{1,n} &= \phi_N (X_1, X_2, \ldots, X_N), \\
Y_{2,n} &= \phi_N (X_{N+1}, X_{N+2}, \ldots, X_{2N}), \\
&\vdots \\
Y_{m-1,n} &= \phi_N (X_{(m-2)N+1}, X_{(m-2)N+2}, \ldots, X_{(m-1)N}), \\
Y_{m,n} &= \phi_N + r (X_{(m-1)N+1}, X_{(m-1)N+2}, \ldots, X_{mN+r}),
\end{align*}
\]

which are bounded, \( 0 \leq Y_{j,n} \leq 1 \) for all \( 1 \leq j \leq m \) and \( n \geq 1 \). From that we define the test-statistic \( \bar{Y}_{m,n} = (1/m) (Y_{1,n} + \ldots + Y_{m,n}) \) and the test-function \( \omega_n = 1 \{ \bar{Y}_{m,n} \geq \eta \} \), based on a critical value \( \eta > 0 \) to be chosen at a later stage. The \( P_0^0 \)-expectation of the test-function can be bounded as follows:

\[
P_0^0 \omega_n = P_0^0 (Y_{1,n} + \ldots + Y_{m,n} \geq m \eta)
\]

\[
= P_0^0 (Z_{1,n} + \ldots + Z_{m,n} \geq m \eta - \sum_{j=1}^{m-1} P_0^0 Y_{j,n} - P_0^0 Y_{m,n})
\]

\[
\leq P_0^0 (Z_{1,n} + \ldots + Z_{m,n} \geq m(\eta - \delta)),
\]

where \( Z_{j,n} = Y_{j,n} - P_0^0 Y_{j,n} \) for all \( 1 \leq j \leq m - 1 \) and \( Z_{m,n} = Y_{m,n} - P_0^0 Y_{m,n} \). Furthermore, the variables \( Z_{j,n} \) are bounded \( a_j \leq Z_{j,n} \leq b_j \) where \( b_j - a_j = 1 \). Imposing
η > δ we may use Hoeffding’s inequality to conclude that:
\[ P_0^\omega \omega_n \leq e^{-2m(\eta - \delta)^2}. \]  

(5.30)

A similar bound can be derived for \( Q_\theta(1 - \omega_n) \) as follows. First we note that:
\[ Q_\theta^0(1 - \omega_n) = Q_0^0 \left( Z_{1,n} + \ldots + Z_{m,n} > -m\eta + \sum_{j=1}^{m-1} Q_\theta^N Y_{j,n} + Q_\theta^{N+r} Y_{m,n} \right), \]

where, in this case, we have used the following definitions for the variables \( Z_{j,n} \):
\[ Z_{j,n} = -Y_{j,n} + Q_\theta^N Y_{j,n}, \quad Z_{m,n} = -Y_{m,n} + Q_\theta^{N+r} Y_{m,n}, \]

for \( 1 \leq j \leq m - 1 \). We see that \( a_j \leq Z_{j,n} \leq b_j \) with \( b_j - a_j = 1 \). Choosing \( \zeta \leq 1 - (4\delta)^{1/N} \) (for small enough \( \delta > 0 \)) and \( \eta \) between \( \delta \) and \( 2\delta \), we see that for all \( \theta \in V_1 \):
\[ \sum_{j=1}^{m-1} Q_\theta^N Y_{j,n} + Q_\theta^{N+r} Y_{m,n} - m\eta \geq m((1 - \zeta)^N - 3\delta) \geq m\delta > 0. \]

Hoeffding’s inequality then provides the bound,
\[ Q_\theta^0(1 - \omega_n) \leq \exp\left( -\frac{1}{2}m(\|Q_\theta\| - 3\delta)^2 + m\log \|Q_\theta\|^N \right). \]

In the case that \( \|Q_\theta\| < 1 \), we see that \( Q_\theta^0(1 - \omega_n) \leq e^{-\frac{1}{2}m\delta^2} \). In the case that \( \|Q_\theta\| \geq 1 \), we use the identity \( \log q \leq q - 1 \) and the fact that \( -\frac{1}{2}(q - 3\delta)^2 + (q - 1) \) has no zeroes for \( q \in [1, \infty) \) if we choose \( \delta < 1/6 \), to conclude that the exponent is negative and bounded away from 0: \( Q_\theta^0(1 - \omega_n) \leq e^{-mc} \). for some \( c > 0 \). Combining the two bounds leads to the assertion, if we notice that \( m = (n - r)/N \geq n/N - 1 \), absorbing eventual constants multiplying the exponential factor in (5.23) by a lower choice of \( D \).

The following lemma is used in the proof of theorem 5.6 to control the behaviour of \( \|Q_\theta\| \) in neighbourhoods of \( \theta^* \).

**Lemma 5.6.** Assume that \( P_0(p_\theta/p_{\theta^*}) \) and \( -P_0(\log(p_\theta/p_0)) \) are finite for all \( \theta \) in a neighbourhood \( U' \) of \( \theta^* \). Furthermore, assume that there exist a measurable function \( m \) such that,
\[ \left| \log \frac{p_\theta}{p_{\theta^*}} \right| \leq m\|\theta - \theta^*\|, \quad (P_0 - a.s.). \]  

(5.31)

for all \( \theta \in U' \) and such that \( P_0(e^{sm}) < \infty \) for some \( s > 0 \). Then,
\[ P_0 \left| \frac{p_\theta}{p_{\theta^*}} - 1 - \log \frac{p_\theta}{p_{\theta^*}} - \frac{1}{2} \left( \log \frac{p_\theta}{p_{\theta^*}} \right)^2 \right| = o\left( \|\theta - \theta^*\|^2 \right). \]
5.3 Consistency and testability

Proof. The function $R(x)$ defined by $e^x = 1 + x + \frac{1}{2}x^2 + x^2 R(x)$ increases from $-\frac{1}{2}$ in the limit ($x \to -\infty$) to $\infty$ as ($x \to \infty$), with $R(x) \to R(0) = 0$ if ($x \to 0$). We also have $|R(-x)| \leq R(x) \leq e^x/x^2$ for all $x > 0$. The l.h.s. of the assertion of the lemma can be written as

$$P_0 \left( \log \frac{p_{\theta}}{p_{\theta^*}} \right)^2 \left| R \left( \log \frac{p_{\theta}}{p_{\theta^*}} \right) \right| \leq \|\theta - \theta^*\|^2 P_0 \left( m^2 R(m\|\theta - \theta^*\|) \right).$$

The expectation on the r.h.s. of the above display is bounded by $P_0 m \phi R(\phi m)$ if $\|\theta - \theta^*\| \leq \varepsilon$. The functions $m^2 R(\phi m)$ are dominated by $e^{\varepsilon}$ for sufficiently small $\varepsilon$ and converge pointwise to $m^2 R(0) = 0$ as $\varepsilon \downarrow 0$. The lemma then follows from the dominated convergence theorem.

5.3 Consistency and testability

The conditions for the theorems concerning rates of convergence and limiting behaviour of the posterior distribution discussed in the previous sections include several requirements on the model involving the true distribution $P_0$. Depending on the specific model and true distribution, these requirements may be rather stringent, disqualifying for instance models in which $-P_0 \log p_{\theta}/p_{\theta^*} = \infty$ for $\theta$ in neighbourhoods of $\theta^*$. To drop this kind of condition from the formulation and nevertheless maintain the current proof(s), we have to find other means to deal with ‘undesirable’ subsets of the model. In this section we show that if Kullback-Leibler neighbourhoods of the point of convergence receive enough prior mass and asymptotically consistent uniform tests for $P_0$ versus such subsets exist, they can be excluded from the model beforehand. As a special case, we derive a misspecified version of Schwartz’s consistency theorem (see Schwartz (1965) [83]). Results presented in this section hold for the parametric models considered in previous sections, but are also valid in non-parametric situations.

5.3.1 Exclusion of testable model subsets

We start by formulating and proving the lemma announced above, in its most general form.

Lemma 5.7. Let $V \subset \Theta$ be a (measurable) subset of the model $\Theta$. Assume that for some $\varepsilon > 0$:

$$\Pi \left( \theta \in \Theta : -P_0 \log \frac{p_{\theta}}{p_{\theta^*}} \leq \varepsilon \right) > 0, \quad (5.32)$$

and there exist constants $\gamma > 0, \beta > \varepsilon$ and a sequence $(\phi_n)$ of test-functions such that:

$$P_0 \phi_n \leq e^{-n\gamma}, \quad \sup_{\theta \in V} Q^0_n(1 - \phi_n) \leq e^{-n\beta}, \quad (5.33)$$
for large enough \( n \geq 1 \). Then \( \Pi(V|X_1, X_2, \ldots, X_n) \to 0 \) \( P_0 \) almost-surely.

**Proof.** Due to the first inequality of (5.33), Markov's inequality and the first Borel-Cantelli lemma suffice to show that \( \phi_n \to 0 \), \( P_0 \) almost-surely. We split the posterior measure of \( V \) with the test function \( \phi_n \) and calculate the limes superior,

\[
\limsup_{n \to \infty} \Pi(V|X_1, X_2, \ldots, X_n) = \limsup_{n \to \infty} \Pi(V|X_1, X_2, \ldots, X_n) (1 - \phi_n),
\]

\( P_0 \) almost-surely. Next, consider the subset \( K_\varepsilon = \{ \theta \in \Theta : -P_0 \log(p_\theta / p_{\theta^*}) \leq \varepsilon \} \).

For every \( \varepsilon > 0 \) and all \( \theta \in K_\varepsilon \), there exists an \( N \geq 1 \) such that for all \( n \geq N \), \( \Pi^*\{p_\theta / p_{\theta^*}(X_i) \geq e^{-n\alpha}, P_0 \} \) almost-surely. Therefore,

\[
\liminf_{n \to \infty} e^{\alpha n} \int_{\Theta} \prod_{i=1}^{n} \frac{p_\theta}{p_{\theta^*}} (X_i) d\Pi(\theta) \geq \liminf_{n \to \infty} e^{\alpha n} \int_{K_\varepsilon} \prod_{i=1}^{n} \frac{p_\theta}{p_{\theta^*}} (X_i) d\Pi(\theta)
\]

\[
\geq \liminf_{n \to \infty} e^{\alpha n} \int_{K_\varepsilon} \prod_{i=1}^{n} \frac{p_\theta}{p_{\theta^*}} (X_i) d\Pi(\theta) \geq \Pi(K_\varepsilon),
\]

by Fatou's lemma. Since by assumption, \( \Pi(K_\varepsilon) > 0 \) we see that:

\[
\limsup_{n \to \infty} \Pi(V|X_1, X_2, \ldots, X_n) (1 - \phi_n)
\]

\[
\leq \limsup_{n \to \infty} e^{\alpha n} \int_{V} \prod_{i=1}^{n} \frac{p_\theta}{p_{\theta^*}} (X_i) (1 - \phi_n) (X_1, X_2, \ldots, X_n) d\Pi(\theta)
\]

\[
\leq \frac{1}{\Pi(K_\varepsilon)} \limsup_{n \to \infty} f_n(X_1, X_2, \ldots, X_n),
\]

where we use the notation \( f_n : \mathcal{X}^n \to \mathbb{R} \):

\[
f_n(X_1, X_2, \ldots, X_n) = e^{\alpha n} \prod_{i=1}^{n} \frac{p_\theta}{p_{\theta^*}} (X_i) (1 - \phi_n) (X_1, X_2, \ldots, X_n) d\Pi(\theta).
\]

Fubini's theorem and the assumption that the test-sequence is uniformly exponential, guarantee that for large enough \( n \), \( P_0 f_n \leq e^{-n(\beta - \alpha)} \). Markov's inequality can then be used to show that:

\[
P_0 (f_n > e^{-\frac{n}{2}(\beta - \varepsilon)}) \leq e^{n(\alpha - \frac{1}{2}(\beta + \varepsilon))}.
\]

Since \( \beta > \varepsilon \), we can choose \( \alpha \) such that \( \varepsilon < \alpha < \frac{1}{2}(\beta + \varepsilon) \) so that the series \( \sum_{n=1}^{\infty} P_0 (f_n > \exp -\frac{n}{2}(\beta - \varepsilon)) \) converges. The first Borel-Cantelli lemma then leads
to the conclusion that:

\[
P_0^\infty \left( \bigcap_{N=1}^{\infty} \bigcup_{n \geq N} \{ f_n > e^{-\frac{n}{2}(\beta - \epsilon)} \} \right) = P_0^\infty \left( \limsup_{n \to \infty} (f_n - e^{-\frac{n}{2}(\beta - \epsilon)}) > 0 \right) = 0.
\]

Since \( f_n \geq 0 \), we see that \( f_n \to 0 \), \( P_0 \)-almost-surely, to conclude the proof.

In many situations, (5.32) is satisfied for every \( \epsilon > 0 \). In that case the construction of uniform exponentially powerful tests from asymptotically consistent tests (as demonstrated in the proof of lemma 5.5) can be used to fulfill (5.33) under the condition that an asymptotically consistent uniform test-sequence exists.

**Corollary 5.1.** Let \( V \subset \Theta \) be a (measurable) subset of the model \( \Theta \). Assume that for all \( \epsilon > 0 \) (5.32) is satisfied and that there exists a test-sequence \((\phi_n)\) such that:

\[
P_0^\infty \phi_n \to 0, \quad \sup_{\theta \in V} Q_n^\theta (1 - \phi_n) \to 0.
\]  

(5.35)

Then \( \Pi(V|X_1, X_2, \ldots, X_n) \to 0 \), \( P_0 \)-almost-surely.

In this corollary form, the usefulness of lemma 5.7 is most apparent. All subsets \( V \) of the model that can be distinguished from \( P_0 \) based on a characteristic property (formalised by the test functions above) in a uniform manner (c.f. (5.35)) may be discarded from proofs like that of theorem 5.4. Hence the properties assumed in the statement of (for instance) theorem 5.4, can be left out as conditions if a suitable test sequence exist.

Whether or not a suitable test sequence can be found depends on the particular model and true distribution in question and little can be said in any generality. The likelihood ratio test is one possibility. The following lemma is comparable to the classical condition, as in [?].

**Lemma 5.8.** Let \( V \in \Theta \) be a (measurable) subset of the model \( \Theta \). Assume that for all \( \epsilon > 0 \) (5.32) is satisfied and suppose that there exists a sequence \((M_n)\) of positive numbers such that \( M_n \to \infty \) and

\[
P_0^\infty \left( \inf_{\theta \in V} -P_n \log \frac{p_\theta}{p_\theta^*} < \frac{1}{n} M_n \right) \to 0.
\]  

(5.36)

Then \( \Pi(V|X_1, X_2, \ldots, X_n) \to 0 \), \( P_0 \)-almost-surely.

**Proof.** Define the sequence of test functions:

\[
\psi_n = 1 \left\{ \inf_{\theta \in V} -P_n \log \frac{p_\theta}{p_\theta^*} < \frac{1}{n} M_n \right\}.
\]

According to assumption (5.36), \( P_0^\infty \psi_n \to 0 \). Let \( \theta \in V \) be given.
\[ Q_n^\theta (1 - \psi_n) = P_n^\theta \left( \frac{dP_n^\theta}{dP_0^\theta} (1 - \psi) \right) = P_n^\theta \left( \frac{dP_n^\theta}{dP_0^\theta} \sup_{\theta \in V} \log \frac{dP_n^\theta}{dP_0^\theta} \leq -M_n \right) \]
\[ \leq e^{-M_n} P_n^\theta \left( \frac{\sup_{\theta \in V} \log \frac{dP_n^\theta}{dP_0^\theta}}{\sup_{\theta \in V} \log \frac{\sup_{\theta \in \Theta} \log \frac{dP_n^\theta}{dP_0^\theta}}{\sup_{\theta \in V} \log \frac{dP_n^\theta}{dP_0^\theta}} \leq -M_n} \right) \leq e^{-M_n} \to 0. \]

Since \( M_n \) does not depend on \( \theta \), convergence to 0 is uniform over \( V \). Corollary 5.1 then gives the assertion.

Finally, we note that lemma 5.7 can also be used to prove consistency. Presently, we do not assume the existence of a **unique** minimizer of the Kullback-Leibler divergence; we define \( \Theta^* \) to be the set of points in the model at minimal Kullback-Leibler divergence with respect to the true distribution \( P_0 \), 
\[ \Theta^* = \{ \theta \in \Theta : -P_0 \log \frac{p_\theta}{p_0} = \inf_{\theta \in \Theta} -P_0 \log \frac{p_\theta}{p_0} \} \]
and we consider the posterior probability of this set under the conditions of corollary 5.1. We write 
\[ d(\theta, \Theta^*) \] for the infimum of \( \| \theta - \theta^* \| \) over \( \theta^* \in \Theta^* \).

**Corollary 5.2.** (Schwartz consistency) Assume that for all \( \varepsilon > 0 \) (5.32) is satisfied and that for all \( \eta > 0 \) there exists a test-sequence \( (\phi_n) \) such that:
\[ P_n^\theta \phi_n \to 0, \quad \sup_{\theta, d(\theta, \Theta^*) > \eta} Q_n^\theta (1 - \phi_n) \to 0. \]

Then \( \Pi (d(\theta, \Theta^*) > \eta | X_1, X_2, \ldots, X_n) \to 1 \), \( P_0 \)-almost-surely, for every \( \eta > 0 \).

### 5.4 Appendix: technical lemmas

The first lemma used in the proof of theorem 5.1 shows that given two sequences of probability measures, a sequence of balls that grows fast enough can be used conditionally to calculate the difference in total-variational distance, even when the sequences consist of random measures.

**Lemma 5.9.** Let \( (\Pi_n) \) and \( (\Phi_n) \) be two sequences of random probability measures on \( \mathbb{R}^d \). Let \( (K_n) \) be a sequence of subsets of \( \mathbb{R}^d \) such that,
\[ \Pi_n (\mathbb{R}^d \setminus K_n) \overset{P_0}{\to} 0, \quad \Phi_n (\mathbb{R}^d \setminus K_n) \overset{P_0}{\to} 0. \]  
(5.37)

Then,
\[ ||\Pi_n - \Phi_n|| \to ||\Pi_n^{K_n} - \Phi_n^{K_n}|| \overset{P_0}{\to} 0. \]  
(5.38)

**Proof.** Let \( K \), a measurable subset of \( \mathbb{R}^d \) and \( n \geq 1 \) be given and assume that \( \Pi_n (K) > 0 \) and \( \Phi_n (K) > 0 \). Then for any measurable \( B \subset \mathbb{R}^d \) we have:
\[ ||\Pi_n (B) - \Pi_n^{K_n} (B)|| \leq 2 \Pi_n (\mathbb{R}^d \setminus K). \]

and hence also:
\[ \left| (\Pi_n(B) - \Pi^n_k(B)) - (\Phi_n(B) - \Phi^{\infty}_n(B)) \right| \leq 2 (\Pi_n(\mathbb{R}^d \setminus K) + \Phi_n(\mathbb{R}^d \setminus K)). \] (5.39)

As a result of the triangle inequality, we then find that the difference in total-variation distances between \( \Pi_n \) and \( \Phi_n \) on the one hand and \( \Pi^n_k \) and \( \Phi^{\infty}_n \) on the other is bounded above by the expression on the right in the above display (which is independent of \( B \)).

Define \( A_n, B_n \) to be the events that \( \Pi_n(K_n) > 0, \Phi_n(K_n) > 0 \) respectively. On \( \Xi_n = A_n \cap B_n, \Pi^n_k \) and \( \Phi^{\infty}_n \) are well-defined probability measures. Assumption (5.37) guarantees that \( P^0_\delta(\Xi_n) \) converges to 1. Restricting attention to the event \( \Xi_n \) in the above upon substitution of the sequence \( (K_n) \) and using (5.37) for the limit of (5.39) we find (5.38), where it is understood that the conditional probabilities on the l.h.s. are well-defined with probability growing to 1.

The second lemma demonstrates that the sequence of normals satisfies the condition of lemma 5.9 when the sequence of centre points \( \Delta_n, \theta_n \) is uniformly tight.

**Lemma 5.10.** Let \( K_n \) be a sequence of balls centred on the origin with radii \( M_n \to \infty \). Let \( (\Phi_n) \) be a sequence of normal distributions (with fixed covariance matrix \( V \)) located respectively at the (random) points \( \Delta_n \subset \mathbb{R}^d \). If the sequence \( \Delta_n \) is uniformly tight, then \( \Phi_n(\mathbb{R}^d \setminus K_n) = N_{\Delta_n, V}(\mathbb{R}^d \setminus K_n) \to 0 \).

**Proof.** Let \( \delta > 0 \) be given. Uniform tightness of the sequence \( (\Delta_n) \) implies the existence of a constant \( L > 0 \) such that:

\[ \sup_{n \geq 1} P^0_\delta(\|\Delta_n\| \geq L) \leq \delta. \]

For all \( n \geq 1 \), call \( A_n = \{\|\Delta_n\| \geq L\} \). Let \( \mu \in \mathbb{R}^d \) be given. Since \( N(\mu, V) \) is tight, there exists for every given \( \varepsilon > 0 \) a constant \( L' \) such that \( N_{\mu, V}(B(\mu, L')) \geq 1 - \varepsilon \) (where \( B(\mu, L') \) defines a ball of radius \( L' \) around the point \( \mu \)). Assuming that \( \mu \leq L, B(\mu, L') \subset B(0, L + L') \) so that with \( M = L + L', N_{\mu, V}(B(0, M)) \geq 1 - \varepsilon \) for all \( \mu \) such that \( \|\mu\| \leq L \). Choose \( N \geq 1 \) such that \( M_n \geq M \) for all \( n \geq N \). Let \( n \geq N \) be given. Then:

\[ P^0_\delta(\Phi_n(\mathbb{R}^d \setminus B(0, M_n)) > \varepsilon) \leq P^0_\delta(A_n) + P^0_\delta(\Phi_n(\mathbb{R}^d \setminus B(0, M_n)) > \varepsilon) \cap A_n^c \]
\[ \leq \delta + P^0_\delta(\{N_{\Delta_n, V}(B(0, M_n)^c) > \varepsilon\} \cap A_n^c). \]

Note that on the complement of \( A_n, \|\Delta_n\| < L \), so:

\[ N_{\Delta_n, V}(B(0, M_n)^c) \leq 1 - N_{\Delta_n, V}(B(0, M)) \leq 1 - \inf_{\|\mu\| \leq L} N_{\mu, V}(B(0, M)) \leq \varepsilon, \]

and we conclude that the last term on the r.h.s. of the previous display equals zero.
Appendix A
Measure theory

In this appendix we collect some important notions from measure theory. The goal is not a self-contained presentation but rather to establish the basic definitions and theorems from the theory for reference in the main text. As such, the presentation omits certain existence theorems and many of the proofs of other theorems (although references are given). The focus is strongly on finite (e.g. probability-)measures, in places at the expense of generality. Some background in elementary set-theory and analysis is required. As a comprehensive reference we note Kingman and Taylor (1966) [57], alternatives being Dudley (1989) [29] and Billingsley (1986) [15].

A.1 Sets and sigma-algebras

It is assumed that the reader is familiar with the following notions in set theory: set, subset, empty set, union, intersection, complement, set difference and disjointness. Let \( \Omega \) be a set. The powerset \( \mathcal{P}(\Omega) \) is the collection of all subsets of \( \Omega \). A partition of \( \Omega \) is a \( \mathcal{A} \subset \mathcal{P}(\Omega) \) such that \( \Omega = \bigcup_{A \in \mathcal{A}} A \) and \( A \cap A' = \emptyset \) for any \( A, A' \in \mathcal{A} \) such that \( A \neq A' \). Let \( (A_n) \) be a sequence of subsets of \( \Omega \). We say that \( (A_n) \) is monotone decreasing (resp. monotone increasing) if \( A_{n+1} \subseteq A_n \) (resp. \( A_n \subseteq A_{n+1} \)) for all \( n \geq 1 \). A monotone decreasing (resp. increasing) sequence \( (A_n) \) has a set-theoretic limit \( \lim A_n \) defined as \( \bigcap_{n \geq 1} A_n \) (resp. \( \bigcup_{n \geq 1} A_n \)). For any sequence of subsets \( (A_n) \), the sequence \( (\bigcup_{m \geq n} A_m)_{n \geq 1} \) (resp. \( (\bigcap_{m \geq n} A_m)_{n \geq 1} \)) is monotone decreasing (resp. increasing) and, accordingly, for any sequence \( (A_n) \) we define

\[
\lim\sup A_n = \bigcap_{n \geq 1} \bigcup_{m \geq n} A_m, \quad \lim\inf A_n = \bigcup_{n \geq 1} \bigcap_{m \geq n} A_m.
\]

The sequence \( (A_n) \) is said to converge, if \( \lim\sup A_n = \lim\inf A_n \).

**Definition A.1.** Let \( \Omega \) be a set. A collection \( \mathcal{F} \) of subsets of \( \Omega \) is called a \( \sigma \)-algebra, if \( \mathcal{F} \) has the following properties.

1. \( \emptyset \in \mathcal{F} \),
2. If \( A \in \mathcal{F} \), then \( \Omega \setminus A \in \mathcal{F} \).

3. If \((A_n) \subset \mathcal{F}\), then \( \bigcup_{n \geq 1} A_n \in \mathcal{F} \).

**Definition A.2.** A measurable space \((\Omega, \mathcal{F})\) consists of a set \(\Omega\) and a \(\sigma\)-algebra \(\mathcal{F}\) of subsets of \(\Omega\).

A subset \(A\) of a measurable space \((\Omega, \mathcal{F})\) is called measurable if \(A \in \mathcal{F}\). It can be shown that a \(\sigma\)-algebra is a monotone class which means that if \((A_n) \subset \mathcal{F}\) is a monotone sequence, then \(\lim A_n \in \mathcal{F}\).

**Definition A.3.** Let \(\Omega\) be a non-empty set and let \(\mathcal{C}\) be a collection of subsets of \(\Omega\). The \(\sigma\)-algebra generated by \(\mathcal{C}\), denoted \(\sigma(\mathcal{C})\) is the smallest \(\sigma\)-algebra that contains \(\mathcal{C}\).

**Lemma A.1.** Let \(\Omega\) be a non-empty set and let \(\mathcal{C}\) be a collection of subsets of \(\Omega\). Then,

\[
\sigma(\mathcal{C}) = \bigcap \{ \Sigma \subset 2^\Omega : \mathcal{C} \subset \Sigma, \Sigma \text{ is a } \sigma\text{-algebra} \}
\]

**Example A.1.** Let \(X\) be a topological space. The Borel \(\sigma\)-algebra is the \(\sigma\)-algebra \(\sigma(\mathcal{T})\) generated by the open (or closed) sets. The Borel \(\sigma\)-algebra on \(X\) is denoted \(B(X)\).

### A.2 Measures

From here on, let \((\Omega, \mathcal{F})\) denote a measurable space. A set-function \(\nu\) is any mapping \(\mathcal{F} \rightarrow \mathbb{R}\).

**Definition A.4.** A set-function \(\nu : \mathcal{F} \rightarrow \mathbb{R}\) is said to be additive if, for any \(k \geq 1\) and any \(\mathcal{A} = \{A_1, \ldots, A_k\} \subset \mathcal{F}\) such that \(A_i \cap A_j = \emptyset\) for all \(1 \leq i < j \leq k\),

\[
\nu\left( \bigcup_{i=1}^{k} A_i \right) = \sum_{i=1}^{k} \nu(A_i).
\]

A set-function \(\nu\) is said to be countably additive (or \(\sigma\)-additive) if the above holds for any countable \(\mathcal{A} = \{A_n : n \geq 1\} \subset \mathcal{F}\) such that \(A_i \cap A_j = \emptyset\) for all \(i, j \geq 1, i \neq j\).

**Definition A.5.** Given a measurable space \((\Omega, \mathcal{F})\), a set-function \(\mu : \mathcal{F} \rightarrow \mathbb{R}\) is a signed measure if \(\mu\) is countably additive and \(\mu\) is a measure if \(\mu\) is countably additive and \(\mu \geq 0\). A measure with a Borel \(\sigma\)-algebra for a domain is called a Borel measure. If \(\mu\) is a measure, \((\Omega, \mathcal{F}, \mu)\) is called a measure space. If \(\mu\) is finite (resp. \(\sigma\)-finite), \((\Omega, \mathcal{F}, \mu)\) is called a finite (resp. \(\sigma\)-finite) measure space.

**Definition A.6.** Let \((\mathcal{Y}, \mathcal{B})\) be a measurable space. Given a set-function \(\nu : \mathcal{B} \rightarrow \mathbb{R}\), the total-variation norm of \(\nu\) is defined:

\[
\|\nu\| = \sup_{\mathcal{A}} \sum_{A \in \mathcal{A}} |\nu(A)|,
\]  
(A.1)
where the supremum is taken over all countable, measurable partitions \( \mathcal{A} \). Alternatively, we may decompose \( v = v_+ - v_- \) uniquely into two positive measures \( v_+, v_- \) (the so-called Hahn-Jordan decomposition), define the total variation measure \( |v| = v_+ + v_- \) and note that \( \|v\| = |v|(\mathcal{Y}) \). A set-function \( v \) is said to be finite if its total variation is finite. A \( \sigma \)-additive set-function \( v : \mathcal{F} \to \mathbb{R} \) is said to be \( \sigma \)-finite if there exists a measurable countable partition \( \{A_n\} \) of \( \Omega \) such that \( |v|(A_n) < \infty \) for all \( n \geq 1 \). A positive measure \( \nu \) such that \( \|\nu\| = \nu(\mathcal{Y}) = 1 \) is a probability measure. Then \( (\mathcal{Y}, \mathcal{B}, \nu) \) is called a probability space.

A null-set of a measure \( \mu \) on \( (\mathcal{Y}, \mathcal{B}) \) is an \( A \in \mathcal{B} \) such that \( \mu(A) = 0 \). If a property holds for all points in \( \mathcal{Y} \), except in a null-set \( A \subset \mathcal{Y} \) of a measure \( \mu \), we say that the property holds \( (\mu)\text{-almost-everywhere} \) (notation: \( \mu \text{-a.e.} \)) or, if \( \mu \) is a probability measure, \( (\mu)\text{-almost-surely} \) (notation: \( \mu \text{-a.s.} \)). For any two positive measures \( \mu \) and \( \nu \) on \( (\mathcal{Y}, \mathcal{B}) \), we say that \( \mu \) dominates \( \nu \) (notation: \( \nu \ll \mu \)), if \( \mu(A) = 0 \) implies \( \nu(A) = 0 \) for all \( A \in \mathcal{B} \). We say that \( \mu \) and \( \nu \) are (mutually) singular (notation: \( \mu \perp \nu \)), if there exists a measurable partition \( \{A, B\} \) of \( \mathcal{Y} \) such that \( \mu(C) = 0 \) for any measurable \( C \subset B \) and \( \nu(D) = 0 \) for any measurable \( D \subset A \).

**Proposition A.1.** Let \( (\Omega, \mathcal{F}) \) be a measurable space. The collection of all finite signed measures on \( \mathcal{F} \) forms a linear space \( \mathcal{M}(\Omega, \mathcal{F}) \) which is a Banach space for the total variation norm.

As a result of \( \sigma \)-additivity, measures display a form of continuity expressed by the following theorem.

**Theorem A.1.** Let \( (\Omega, \mathcal{F}) \) be a measurable space with measure \( \mu : \mathcal{F} \to [0, \infty] \). Then,

(i) for any monotone decreasing sequence \( (F_n)_{n \geq 1} \) in \( \mathcal{F} \) such that \( \mu(F_n) < \infty \) for some \( n \),

\[
\lim_{n \to \infty} \mu(F_n) = \mu(\bigcap_{n=1}^{\infty} F_n),
\]

(ii) for any monotone increasing sequence \( (G_n)_{n \geq 1} \) in \( \mathcal{F} \),

\[
\lim_{n \to \infty} \mu(G_n) = \mu(\bigcup_{n=1}^{\infty} G_n).
\]

Theorem A.1 is sometimes referred to as the continuity theorem for measures, because if we view \( \cap_n F_n \) as the monotone limit \( \lim F_n \), (A.2) can be read as \( \lim_n \mu(F_n) = \mu(\lim_n F_n) \), expressing continuity from below. Similarly, (A.3) expresses continuity from above. Note that theorem A.1 does not guarantee continuity for arbitrary sequences in \( \mathcal{F} \). It should also be noted that theorem A.1 is presented here in simplified form: the full theorem states that continuity from below is equivalent to \( \sigma \)-additivity of \( \mu \) (for a more comprehensive formulation and a proof of theorem A.1, see [57], theorem 3.2).

**Example A.2.** Let \( \Omega \) be a discrete set and let \( \mathcal{F} \) be the powerset \( 2^\Omega \) of \( \Omega \), i.e. \( \mathcal{F} \) is the collection of all subsets of \( \Omega \). The counting measure \( n : \mathcal{F} \to [0, \infty] \) on \( (\Omega, \mathcal{F}) \)
A Measure theory

is defined simply to count the number \( n(F) \) of points in \( F \subseteq \Omega \). If \( \Omega \) contains a finite number of points, \( n \) is a finite measure; if \( \Omega \) contains a countably infinite number of points, \( n \) is \( \sigma \)-finite. The counting measure is \( \sigma \)-additive.

**Example A.3.** We consider \( \mathbb{R} \) with any \( \sigma \)-algebra \( \mathcal{F} \), let \( x \in \mathbb{R} \) be given and define the measure \( \delta_x : \mathcal{F} \to [0,1] \) by

\[
\delta_x(A) = 1 \{ x \in A \},
\]

for any \( A \in \mathcal{F} \). The probability measure \( \delta_x \) is called the Dirac measure (or delta measure, or atomic measure) degenerate at \( x \) and it concentrates all its mass in the point \( x \). Clearly, \( \delta_x \) is finite and \( \sigma \)-additive. Convex combinations of Dirac measures, \( i.e. \) measures of the form

\[
P = \sum_{j=1}^{m} \alpha_j \delta_{x_j},
\]

for some \( m \geq 1 \) with \( \alpha_1, \ldots, \alpha_m \) such that \( \alpha_j \geq 0 \) and \( \sum_{j=1}^{m} \alpha_j = 1 \), can be used as a statistical model for an observation \( X \) that take values in a discrete (but unknown) subset \( \{ x_1, \ldots, x_m \} \) of \( \mathbb{R} \). The resulting model (which we denote \( D(\mathbb{R}, \mathcal{B}) \) for reference) is not dominated.

Often, one has a sequence of events \( (A_n) \) and one is interested in the probability of a limiting event \( A \), for example the event that \( A_n \) occurs infinitely often. The following lemmas pertain to this situation.

**Lemma A.2.** (First Borel-Cantelli lemma)
Let \( (\Omega, \mathcal{F}, P) \) be a probability space with a sequence \( (A_n) \subset \mathcal{F} \) and denote \( A = \limsup A_n \). If \( \sum_{n \geq 1} P(A_n) < \infty \), then \( P(A) = 0 \).

In the above lemma, the sequence \( (A_n) \) is general. To draw the converse conclusion, the sequence needs to exist of independent events: \( A, B \in \mathcal{F} \) are said to be independent under \( P \) if \( P(A \cap B) = P(A)P(B) \).

**Lemma A.3.** (Second Borel-Cantelli lemma)
Let \( (\Omega, \mathcal{F}, P) \) be a probability space and let \( (A_n) \subset \mathcal{F} \) be independent and denote \( A = \limsup A_n \). If

\[
\sum_{n \geq 1} P(A_n) = \infty,
\]

then \( P(A) = 1 \).

Together, the Borel-Cantelli lemmas assert that for a sequence of independent events \( (A_n) \), \( P(A) \) equals zero or one, according as \( \sum_n P(A_n) \) converges or diverges. As such, this corollary is known as a zero-one law.

To conclude this section, we consider a property of random vectors called exchangeability.

**Definition A.7.** A random vector \( (X_1, \ldots, X_n) \in \mathbb{R}^n \) with distribution \( P_n \) is said to be exchangeable, if, for any permutation \( \pi \) of \( \{1, \ldots, n\} \), the random vector \( (X_{\pi(1)}, \ldots, X_{\pi(n)}) \) also has distribution \( P_n \).
This property is a generalization of *i.i.d.*-ness: note that if \((X_1, \ldots, X_n) \sim P^n\) then \((X_1, \ldots, X_n)\) is exchangeable. The converse does not hold but exchangeable distributions can be characterized in terms of *i.i.d.* distributions, as the following result demonstrates.

**Theorem A.2.** (De Finetti’s theorem) The random vector \((X_1, \ldots, X_n) \in \mathbb{R}^n\) distributed according to a probability measure \(P_n\) is exchangeable if and only if there exists a (unique) probability measure \(\Pi\) on the collection \(\mathcal{M}_1^+ (\mathbb{R})\) of all Borel probability on \(\mathbb{R}\) such that,

\[
P_n(A_1 \times \ldots \times A_n) = \int_{\mathcal{M}(\mathbb{R})} \prod_{i=1}^n P(A_i) \, d\Pi(P),
\]

for all \(A_1, \ldots, A_n \in \mathcal{B}(\mathbb{R})\).

### A.3 Measurability, random variables and integration

In this section we consider random variables and their expectation values. Throughout this section, let \((\Omega, \mathcal{F}, P)\) denote a probability space.

**Definition A.8.** Given a map \(X : A \to B\) and a subset \(C \subset B\), the pre-image of \(C\) under \(X\), is defined as,

\[X^{-1}(C) = \{ a \in A : X(a) \in C \} \subset A.\]

Given two measurable spaces \((\Omega, \mathcal{F})\) and \((\mathcal{X}, \mathcal{B})\), a map \(X : \Omega \to \mathcal{X}\) is called measurable if, for all \(B \in \mathcal{B}\), \(X^{-1}(B) \in \mathcal{F}\). These subsets form a sub-\(\sigma\)-algebra \(\sigma(X) = \{ X^{-1}(B) : B \in \mathcal{B} \} \) called the \(\sigma\)-algebra generated by \(X\).

Essentially, measurability makes it possible to speak of “the probability that \(X\) lies in \(B\)”:

\[P(X \in B) = P(\{ \omega \in \Omega : X(\omega) \in B \}),\]

is well-defined only if \(X^{-1}(B)\) belongs to the domain of \(P\). Specializing to real-valued measurable maps, it follows from elementary manipulation of set-limits that suprema of sequences of measurable maps are again measurable. This statement can be framed in the following central theorem in measure theory.

**Theorem A.3.** (Monotone class theorem) For every \(n \geq 1\), let \(f_n : \Omega \to \overline{\mathbb{R}}\) be measurable and assume that \(f_{n+1}(\omega) \geq f_n(\omega)\) for all \(n \geq 1\) and \(\omega \in \Omega\). Then \(f(\omega) = \lim_{n \to \infty} f_n(\omega)\) defines a measurable map \(f : \Omega \to \overline{\mathbb{R}}\).

This means that the set of all measurable \(f : \Omega \to \overline{\mathbb{R}}\) forms what is know as a monotone class, an partially ordered set that is closed for limits over monotone sequences. Although measurability is preserved under linear combinations, the space of all measurable \(f : \Omega \to \overline{\mathbb{R}}\) is not a linear space because if, for some \(\omega \in \Omega\),
$f(\omega) = \infty$ and $g(\omega) = -\infty$, then $(f + g)(\omega) = \infty - \infty$ is ill-defined. No such problems arise when we restrict to the set of all measurable $f \geq 0$, which form a cone. Restriction to measurable $f: \Omega \rightarrow \mathbb{R}$, on the other hand, invalidates the monotone class theorem.

**Definition A.9.** Let $(\Omega, \mathcal{F}, P)$ be a probability space. A random variable is a measurable map $X: \Omega \rightarrow \mathbb{R}$ with the property that $P(|X| = \infty) = 0$. Therefore, every random variable can be represented by a real-valued $X': \Omega \rightarrow \mathbb{R}$, up to null-sets of $P$, i.e. $P(X = X') = 1$.

Note that random variables do not form a monotone class (take $f_n = n$), but they do form a linear space. To define expectations (integrals with respect to $P$), we extend by monotone limit starting from the following definition.

**Definition A.10.** A measurable map $f: \Omega \rightarrow \mathbb{R}$ is called simple if there exists a $k \geq 1$, a $k$-set partition $A_1, \ldots, A_k$ of $\Omega$ and $a_1, \ldots, a_k \in \mathbb{R}$ such that,

$$f(\omega) = \sum_{i=1}^{k} a_i 1_{A_i}(\omega).$$

The integral of a simple $f$ with respect to $P$ is defined as,

$$\int f \, dP = \sum_{i=1}^{k} a_i P(A_i).$$

A straightforward construction shows that for every measurable $f \geq 0$, there exists an increasing sequence $(f_n)$ of non-negative, simple functions such that $f_n(\omega) \uparrow f(\omega)$ for all $\omega \in \Omega$. By the monotony of $(f_n)$, this defines an integral for every non-negative, measurable $f$,

$$\int f \, dP = \lim_{n \to \infty} \int f_n \, dP,$$

(after one demonstrates that the l.h.s. does not depend on the particular $(f_n)$ we choose to approximate $f$). Extension to real-valued measurable functions that take on negative values as well is done by treating negative $f_-$ and non-negative $f_+$ parts of $f$ separately. Extension to $\mathbb{R}^d$ with $d > 1$ proceeds component-wise. The most important result in integration theory is the following elementary theorem.

**Theorem A.4.** (Monotone convergence) Let $(f_n)$ be a monotone sequence of measurable maps $\Omega \rightarrow \mathbb{R}$. Then $\lim_{n} \int f_n \, dP = \int (\lim_{n} f_n) \, dP$.

Before we can state Fatou’s lemma and the dominated convergence theorem, we define integrability of measurable maps.

**Definition A.11.** Let $(\Omega, \mathcal{F}, P)$ be a probability space. A real-valued measurable function $f: \Omega \rightarrow \mathbb{R}$ is said to be integrable with respect to $P$ if

$$\int_{\Omega} |f| \, dP < \infty.$$  \hfill (A.4)
It follows immediately from the definition that an integrable \( f \) is a random variable. Note that any sequence of measurable \( f_n \) is dominated by the sequence \( (\sup_{m \geq n} f_m) \). By the monotone class theorem the suprema are measurable and the resulting sequence of maps is monotone decreasing.

**Lemma A.4.** *(Fatou’s lemma)* Let \( f_n : \Omega \rightarrow \mathbb{R} \) be a sequence of measurable maps such that \( f_n \leq g \), \( P \)-almost-surely for all \( n \geq 1 \), for some \( P \)-integrable \( g : \Omega \rightarrow \mathbb{R} \). Then,

\[
\limsup_{n \to \infty} \int f_n \, dP \leq \int (\limsup_{n \to \infty} f_n) \, dP.
\]

An obvious extension provides an inequality for the limes inferior. When combined, the \( \limsup \) and \( \liminf \) versions of Fatou’s lemma imply the following result, known as Lebesgue’s (dominated convergence) theorem.

**Theorem A.5.** *(Dominated convergence)* Let \( f_n : \Omega \rightarrow \mathbb{R} \) be a sequence of measurable maps such that \( \lim_n f_n : \Omega \rightarrow \mathbb{R} \) exists and \( |f_n| \leq g \), \( P \)-almost-surely for all \( n \geq 1 \), for some \( P \)-integrable \( g : \Omega \rightarrow \mathbb{R} \). Then,

\[
\lim_{n \to \infty} \int f_n \, dP = \int (\lim_{n \to \infty} f_n) \, dP.
\]

For any two probability spaces \( (\Omega_1, \mathcal{F}_1, P_1) \) and \( (\Omega_2, \mathcal{F}_2, P_2) \), the set \( \Omega_1 \times \Omega_2 \) can be endowed with the \( \sigma \)-algebra generated by products of the form \( A_1 \times A_2 \) where \( A_1 \in \mathcal{F}_1, A_2 \in \mathcal{F}_2 \), which is called the product \( \sigma \)-algebra, denoted \( \mathcal{F} = \sigma(\mathcal{F}_1 \times \mathcal{F}_2) \) and a product measure \( P = P_1 \times P_2 \), to arrive at a probability space \( (\Omega, \mathcal{F}, P) \), for which the following elementary theorem on the interchangelability of integrals applies.

**Theorem A.6.** *(Fubini’s theorem)* Let \( (\Omega_1, \mathcal{F}_1, P_1) \) and \( (\Omega_2, \mathcal{F}_2, P_2) \) be probability spaces and denote their product by \( (\Omega, \mathcal{F}, P) \). For any non-negative, \( \mathcal{F} \)-measurable \( f : \Omega \rightarrow \mathbb{R} \) and any \( \omega_1 \in \Omega_1 \), \( f(\omega_1, \cdot) : \Omega_2 \rightarrow \mathbb{R} \) is \( \mathcal{F}_2 \)-measurable. Furthermore, for any \( A_1 \in \mathcal{F}_1 \) and \( A_2 \in \mathcal{F}_2 \),

\[
\int_{A_1 \times A_2} f(\omega_1, \omega_2) \, dP(\omega) = \int_{A_1} \left( \int_{A_2} f(\omega_1, \omega_2) \, dP_2(\omega_2) \right) \, dP_1(\omega_1)
\]

\[
= \int_{A_2} \left( \int_{A_1} f(\omega_1, \omega_2) \, dP_1(\omega_1) \right) \, dP_2(\omega_2).
\]

Another central result from integration theory forms the foundation for the probability density we associate with many distributions.

**Theorem A.7.** *(Radon-Nikodym theorem)* Let \( (\Omega, \mathcal{F}) \) be a measurable space and let \( \mu, \nu : \mathcal{F} \rightarrow [0, \infty] \) be two \( \sigma \)-finite measures on \( (\Omega, \mathcal{F}) \). There exists a unique decomposition

\[
\mu = \mu_\| + \mu_\perp,
\]

such that \( \nu_\| \ll \nu \) and \( \mu_\perp \) and \( \nu \) are mutually singular. Furthermore, there exists a finite-valued, \( \mathcal{F} \)-measurable function \( f : \Omega \rightarrow \mathbb{R} \) such that for all \( F \in \mathcal{F} \),
\[ \mu(F) = \int_{F} f \, d\nu. \]  
\[ \text{(A.5)} \]

The function \( f \) is \( \nu \)-almost-everywhere unique.

The function \( f : \Omega \to \mathbb{R} \) in the above theorem is called the Radon-Nikodym derivative of \( \mu \) with respect to \( \nu \). If \( \mu \) is a probability distribution, then \( f \) is called the (probability) density for \( \mu \) with respect to \( \nu \). The Radon-Nikodym derivative is sometimes denoted \( d\mu/d\nu \). The assertion that \( f \) is “\( \nu \)-almost-everywhere unique” means that if there exists a measurable function \( g : \Omega \to \mathbb{R} \) such that (A.5) holds with \( g \) replacing \( f \), then \( f = g, \) (\( \nu \)-a.e.), i.e. \( f \) and \( g \) may differ only on a set of \( \nu \)-measure equal to zero. Through a construction involving increasing sequences of simple functions, we see that the Radon-Nikodym theorem has the following implication.

**Corollary A.1.** Assume that the conditions for the Radon-Nikodym theorem are satisfied. Let \( X : \Omega \to [0, \infty] \) be measurable and \( \mu \)-integrable. Then the product \( X f \) is \( \nu \)-integrable and

\[ \int X \, d\mu = \int X f \, d\nu. \]

**Remark A.1.** Integrability is not a necessary condition here, but the statement of the corollary becomes rather less transparent if generalized.

### A.4 Existence of stochastic processes

A stochastic process has the following broad definition.

**Definition A.12.** Let \( (\Omega, \mathcal{F}, P) \) be a probability space, let \( T \) be an arbitrary set. A collection of \( \mathcal{F} \)-measurable random variables \( (X_t : \Omega \to \mathbb{R} : t \in T) \) is called a stochastic process indexed by \( T \).

When using this definition, one often starts from a collection of (possibly dependent) random quantities without the certainty that there exists a coupling, that is, a probability space like \( (\Omega, \mathcal{F}, P) \) above, on which all random quantities can be represented simultaneously as random variables.

Kolmogorov’s existence theorem provides an explicit construction of \( (\Omega, \mathcal{F}, P) \). Clearly, if the \( X_t \) take their values in a measurable space space \( (\mathcal{X}, \mathcal{B}) \), the obvious choice for \( \Omega \) is the product \( \mathcal{X}^T \) in which the process takes its values. The question remains how to characterize \( P \) and its domain \( \mathcal{F} \). Kolmogorov assumes that for any finite subset \( S = \{t_1, \ldots, t_k\} \subset T \), the distribution \( P_{t_1, \ldots, t_k} \) of the \( k \)-dimensional stochastic vector \( (X_{t_1}, \ldots, X_{t_k}) \) is given.

**Example A.4.** Choose \( T = [0, 1] \) and define random quantities \( f(t) \) for each \( t \in T \). For any finite subset \( S \subset T \), we may specify the distribution \( P_S \) of the random vector,

\[ (f(s) : s \in S) \sim P_S. \]
A.4 Existence of stochastic processes

For example, we may consider multivariate normal distributions $P$ with the property that, for any $s, t \in S$, the expectation $P(f(s) - f(t)) = 0$ and the variance of $f(s) - f(t)$ is proportional to $|s - t|$ (which gives rise to Brownian motion). If a coupling exists, the resulting stochastic process $(f(t) : t \in [0, 1])$ describes random functions $f : [0, 1] \to \mathbb{R}$.

Since the distributions $P_{t_1 \ldots t_k}$ are as yet unrelated and given for all finite subsets of $T$, consistency requirements are implicit if they are to serve as marginals to the probability distribution $P$: if two finite subsets $S_1, S_2 \subset T$ satisfy $S_1 \subset S_2$, then the distribution of $\{X_t : t \in S_1\}$ should be marginal to that of $\{X_t : t \in S_2\}$. Similarly, permutation of the components of the stochastic vector in the above display should be reflected in the respective distributions as well. The requirements for consistency are formulated in two requirements called Kolmogorov’s consistency conditions:

(K1) Let $k \geq 1$ and $\{t_1, \ldots, t_{k+1}\} \subset T$ be given. For any $C \in \sigma(\mathcal{B}^k)$,

$$P_{t_1 \ldots t_k}(C) = P_{t_1 \ldots t_{k+1}}(C \times \mathcal{G}),$$

(K2) Let $k \geq 1$, $\{t_1, \ldots, t_k\} \subset T$ and a permutation $\pi$ of $k$ elements be given. For any $A_1, \ldots, A_k \in \mathcal{B}$,

$$P_{(\pi(1) \ldots \pi(k))}(A_1 \times \ldots \times A_k) = P_{t_1 \ldots t_k}(A_{\pi^{-1}(1)} \times \ldots \times A_{\pi^{-1}(k)}).$$

Theorem A.8. (Kolmogorov’s existence theorem)

Let a collection of random quantities $\{X_t : t \in T\}$ be given. Suppose that for any $k \geq 1$ and all $t_1, \ldots, t_k \in T$, the finite-dimensional marginal distributions

$$(X_{t_1}, \ldots, X_{t_k}) \sim P_{t_1 \ldots t_k}, \quad (A.6)$$

are defined and satisfy conditions (K1) and (K2). Then there exists a probability space $(\Omega, \mathcal{F}, P)$ and a stochastic process $\{X_t : \Omega \to \mathcal{G} : t \in T\}$ such that all distributions of the form (A.6) are marginal to $P$.

Kolmogorov’s approach to the definition and characterization of stochastic processes in terms of finite-dimensional marginals is of great practical value: it allows one to restrict attention to finite-dimensional marginal distributions when characterising the process. The drawback of the construction becomes apparent only upon closer inspection of the $\sigma$-algebra $\mathcal{F}$: the $\sigma$-algebra generated by the so-called cylinder sets, which implies that measurability of events restricting an uncountable number of $X_t$’s simultaneously can not be guaranteed. This is the ever-recurring trade-off between generality and strength of a mathematical result: Kolmogorov’s existence theorem always works but it does not give rise to a comfortably ‘large’ domain for the resulting $P : \mathcal{F} \to [0, 1]$. 
A.5 Conditional distributions

In this section, we consider conditioning of probability measures. In first instance, we consider straightforward conditioning on events and illustrate Bayes’s rule, but we also cover conditioning on $\sigma$-algebras and random variables, to arrive at the posterior distribution and Bayes’s rule for densities.

**Definition A.13.** Let $(\Omega, \mathcal{F}, P)$ be a probability space and let $B \in \mathcal{F}$ be such that $P(B) > 0$. For any $A \in \mathcal{F}$, the conditional probability of the event $A$ given event $B$ is defined:

$$P(A|B) = \frac{P(A \cap B)}{P(B)}. \quad (A.7)$$

Conditional probability given $B$ describes a set-function on $\mathcal{F}$ and one easily checks that this set-function is a probability measure that assigns probability one to $B$. The conditional probability measure $P(\cdot|B) : \mathcal{F} \to [0, 1]$ can be viewed as the restriction of $P$ to $\mathcal{F}$-measurable subsets of $B$, normalized to be a probability measure. Definition A.13 gives rise to a relation between $P(A|B)$ and $P(B|A)$ (in case both $P(A) > 0$ and $P(B) > 0$, of course), which is called Bayes’s Rule.

**Proposition A.2.** (Bayes’s Rule)

Let $(\Omega, \mathcal{F}, P)$ be a probability space and let $A, B \in \mathcal{F}$ be such that $P(A) > 0$, $P(B) > 0$. Then

$$P(A|B)P(B) = P(B|A)P(A).$$

However, only being able to condition on events $B$ of non-zero probability is too restrictive. Moreover, $B$ above is a definite event; it is desirable also to be able to discuss probabilities conditional on events that have not been measured yet, i.e. to condition on a whole $\sigma$-algebra of events like $B$ above.

**Definition A.14.** Let $(\Omega, \mathcal{F}, P)$ be a probability space, let $\mathcal{C}$ be a sub-$\sigma$-algebra of $\mathcal{F}$ and let $X$ be a real-valued $P$-integrable random variable. The conditional expectation of $X$ given $\mathcal{C}$ is any $\mathcal{C}$-measurable random variable $E[X|\mathcal{C}] : \Omega \to \mathbb{R}$ such that,

$$\int_C X \, dP = \int_C E[X|\mathcal{C}] \, dP,$$

for all $C \in \mathcal{C}$.

If we consider some $B \in \mathcal{F}$ with $P(B) > 0$ and the $\sigma$-algebra $\sigma_B = \{ \emptyset, B, \Omega \setminus B, \Omega \}$, and we consider definition A.14 for $X = 1_A$, we recover,

$$E[1_A|\sigma_B] = P(A|B)1_B + P(A|\Omega \setminus B)1_{\Omega \setminus B}.$$

The condition that $X$ be $P$-integrable is sufficient for existence and uniqueness of $E[X|\mathcal{C}]$ $P$-almost-surely, the proof being an application of the Radon-Nikodym theorem (see theorem 10.1.1 in Dudley (1989)). So conditional expectations are not unique but if we have two different random variables $e_1$ and $e_2$ satisfying the defining conditions for $E[X|\mathcal{C}]$, then $e_1 = e_2$, $P$-almost-surely. Often, the $\sigma$-algebra $\mathcal{C}$ is
the $\sigma$-algebra $\sigma(Z)$ generated by another random variable $Z$. In that case we denote the conditional expectation by $E[X|Z]$ and realizations are denoted $E[X|Z=z]$.

**Definition A.15.** Let $(\Omega, \mathcal{F}, P)$ be a probability space and let $\mathcal{C}$ be a sub-$\sigma$-algebra of $\mathcal{F}$. Furthermore, let $(\mathcal{Y}, \mathcal{B})$ be a measurable space and let $Y: \Omega \to \mathcal{Y}$ be a random variable. For each $A \in \mathcal{F}$, the conditional distribution of $Y$ given $\mathcal{C}$ is defined as follows:

$$P_{Y|\mathcal{C}}(A, \omega) = E\left[1\{Y \in A\}|\mathcal{C}\right](\omega), \quad (A.8)$$

$P$-almost-surely.

Although seemingly innocuous, the fact that conditional expectations are defined only $P$-almost-surely poses a rather subtle problem: for every $A \in \mathcal{B}$ there exists an $A$-dependent null-set on which $P_{Y|\mathcal{C}}(A, \cdot)$ is not defined. This is not a problem if we are interested only in $A$ (or in a countable number of sets). But usually, we wish to view $P_{Y|\mathcal{C}}$ as a probability measure, that is to say, it must be well-defined as a map on the $\sigma$-algebra $\mathcal{B}$ almost-surely. Since most $\sigma$-algebras are uncountable, there is no guarantee that the corresponding union of exceptional null-sets has measure zero as well. This means that definition A.15 only defines $P_{Y|\mathcal{C}}(A, \cdot)\rightarrow P_{Y|\mathcal{C}}(A, \omega)$ per individual $A$, and not as a map $A \mapsto P_{Y|\mathcal{C}}(A, \omega)$ for $P$-almost-all $\omega \in \Omega$. The extra property that the conditional distribution is well-defined $P$-almost-surely as a map is called regularity of the conditional distribution.

**Definition A.16.** If $\pi: \mathcal{B} \times \Omega \to [0, 1]$ is such that,

1. for every $B \in \mathcal{B}$, $\omega \mapsto \pi(B, \omega)$ is $\mathcal{C}$-measurable,
2. there is an $E \in \mathcal{C}$ with $P(E) = 0$ such that for all $\omega \in \Omega \setminus E$, $B \mapsto \pi(B, \omega)$ is a probability measure,
3. for all $C \in \mathcal{C}$,

$$\int_C \pi(B, \omega) dP(\omega) = P(B \cap C),$$

then $\pi$ is said to be a regular conditional distribution.

The existence of a regular conditional probability cannot be guaranteed without further conditions on the underlying probability space.

**Definition A.17.** A topological space $(S, \mathcal{T})$ is said to be a Polish space if $\mathcal{T}$ is metrizable, complete and separable. Any topological space $T$ that is the continuous image of a Polish space is called a Souslin space.

Polish spaces appear in many subjects in measure theory: the existence of a countable, dense subset in a metric setting allows constructions based countable covers by metric balls. In this manner Polish spaces allow countable formulations for properties that would involve uncountable collections of subsets otherwise, in correspondence with countability restrictions arising from measure theory. Such a construction occurs in a theorem that guarantees the existence of regular conditional distributions.

**Theorem A.9.** Let $(\Omega, \mathcal{F}, P)$ be a probability space and let $\mathcal{Y}$ be a Polish space. If $Y: \Omega \to \mathcal{Y}$ is a Borel measurable random variable taking values in $\mathcal{Y}$ and $\mathcal{C}$ is
any sub-σ-algebra of \( \mathcal{F} \), there exists a \((P\text{-almost-surely unique})\) regular conditional distribution \( \Pi_{Y|C} : \mathcal{B} \times \Omega \to [0, 1] \).

**Proof.** Proof For a proof of this theorem, the reader is referred to Dudley (1989) [29], theorem 10.2.2).

In Bayesian context we can be more specific regarding the sub-σ-algebra \( C \) since \( \Omega = \mathcal{X} \times \Theta \). To condition on \( \theta \) we choose \( C = \{ \mathcal{X} \times G : G \in \mathcal{G} \} \). Due to this special choice for \( C \), \( C \)-measurability implies that \( \Pi_{Y|C}(\cdot, \theta) \) is a \( \mathcal{G} \)-measurable function of \( \theta \) which we denote \( \Pi_{Y|\theta} : \mathcal{B} \times \Theta \to [0, 1] \). Similarly, since the data \( Y \) usually takes its values in \( \mathbb{R} \) or \( \mathbb{R}^n \) (and certainly in a Polish space), the existence of a regular version of the posterior \( \Pi_{\theta|Y} : \mathcal{G} \times \mathcal{Y} \to [0, 1] \) is guaranteed.

**A.6 Convergence in spaces of probability measures**

Let \( \mathcal{M}(\mathbb{R}, \mathcal{B}) \) denote the space of all probability measures on \( \mathbb{R} \) with Borel σ-algebra \( \mathcal{B} \).

**Definition A.18.** (topology of weak convergence) Let \( (Q_n) \) and \( Q \) in \( \mathcal{M}(\mathbb{R}, \mathcal{B}) \) be given. Denote the set of points in \( \mathbb{R} \) where \( f \to Q(\xi, t) \) is continuous by \( C \). We say that \( Q_n \) converges weakly to \( Q \) if, for all \( t \in C \), \( Q_n(\xi, t) \to Q(\xi, t) \).

Weak convergence has several equivalent definitions.

**Lemma A.5.** Portmanteau lemma

Let \( (Q_n) \) and \( Q \) in \( \mathcal{M}(\mathbb{R}, \mathcal{B}) \) be given. The following are equivalent:

(i) \( Q_n \) converges weakly to \( Q \).
(ii) For every bounded, continuous \( f : \mathbb{R} \to \mathbb{R} \), \( Q_n f \to Q f \).
(iii) For every bounded, Lipschitz \( g : \mathbb{R} \to \mathbb{R} \), \( Q_n g \to Q g \).
(iv) For all non-negative, continuous \( h : \mathbb{R} \to \mathbb{R} \), \( \inf_{n \to \infty} Q_n f \geq Q f \).
(v) For every open set \( F \subset \mathbb{R} \), \( \liminf_{n \to \infty} Q_n(F) \geq Q(F) \).
(vi) For every closed set \( G \subset \mathbb{R} \), \( \limsup_{n \to \infty} Q_n(G) \leq Q(G) \).
(vii) For every Borel set \( B \) such that \( Q(\partial B) = 0 \), \( Q_n(B) \to Q(B) \).

In (vii) above, \( \partial B \) denotes the boundary of \( B \), which is defined as the closure of \( B \) minus the interior of \( B \).

**Lemma A.6.** When endowed with the topology of weak convergence, the space \( \mathcal{M}(\mathbb{R}, \mathcal{B}) \) is Polish, i.e. complete, separable and metric.

**Definition A.19.** (topology of pointwise convergence) Let \( (Q_n) \) and \( Q \) in \( \mathcal{M}(\mathbb{R}, \mathcal{B}) \) be given. We say that \( Q_n \) converges pointwise to \( Q \) if, for all \( B \in \mathcal{B} \), \( Q_n(B) \to Q(B) \).
Definition A.20. (topology of total variation)
Let $(Q_n)$ and $Q$ in $\mathcal{M}(\mathbb{R}, \mathcal{B})$ be given. We say that $Q_n$ converges in total variation to $Q$ if,
\[ \|Q_n(B) - Q(B)\| = \sup_{B \in \mathcal{B}} |Q_n(B) - Q(B)| \to 0. \]

In exercise 4.6, it is shown that this distance can also be calculated as the $L_1$-difference between densities for $Q_n$ and $Q$.

Lemma A.7. (Scheffé’s lemma)
Let $(\Omega, \mathcal{F}, \mu)$ be a measure space. Given a sequence $(f_n)$ of integrable functions and a measurable function $f$ such that $f_n(\omega) \to f(\omega)$ for $\mu$-almost-all $\omega$, then
\[ \int |f_n - f| \, d\mu \to 0 \text{ if and only if } \int |f_n| \, d\mu \to \int |f| \, d\mu. \]

Corollary A.2. Let $(\Omega, \mathcal{F}, \mu)$ be a measure space. If a sequence of probability densities $(p_n)$ converges to a probability density $p$ $\mu$-almost-everywhere, then
\[ \|P_n - P\| \to 0. \]
References

References


Index

$R$-better, 54
$s$-algebra, 147
Borel, 148
$p$-value, 44
\textit{i.i.d.}, 3

action, 53
admissible, 54
almost-everywhere, 149
almost-surely, 149
alternative, \textit{see} alternative hypothesis
hypothesis, 43

Bayes factor, 50
Bayes’s billiard, 22
Bayes’s Rule, 19
belief, 14
bootstrap, 72

central limit theorem, 46
classification, 43, 60
classifier, 60
clusters, 22
complement, 147
completion, 32
conditional distribution, 18, 157
regular, 157
conditional expectation, 156
conditional independence, 27
conditional probability, 156
confidence level, 39, \textit{see} level, confidence
confidence set, 39
asymptotic, 40
asymptotically consistent, 40
conjugate family, 78, 96
consistency, 15
consistency conditions, 155

data, 3
categorical, 3
functional, 3
interval, 3
nominal, 3
ordinal, 3
ranked, 3
ratio, 3
data distribution
Bayesian, 19
frequentist, 4, 27
decision, 53
decision principle
minimax, 55
decision rule, 54
Bayes, 57
minimax, 55
randomized, 55
decision-space, 53
density, \textit{see} probability density
Dirichlet distribution, 90
Dirichlet family, 91
Dirichlet process, 92

continuity theorem, 149
corversion in total variation, 159
cornered hull
closed, 32
corvolution, 21
counting measure, 5, 7, 149
coupling, 154
corerable interval, 41
corerable region, 41
corerable set, 41
asymptotic, 42
HPD-, 42
critical set, 44

continuity theorem, 149
corversion in total variation, 159
cornered hull
closed, 32
corvolution, 21
counting measure, 5, 7, 149
coupling, 154
corerable interval, 41
corerable region, 41
corerable set, 41
asymptotic, 42
HPD-, 42
critical set, 44

continuity theorem, 149
corversion in total variation, 159
convex hull
closed, 32
corvolution, 21
counting measure, 5, 7, 149
coupling, 154
corerable interval, 41
corerable region, 41
corerable set, 41
asymptotic, 42
HPD-, 42
critical set, 44
Index

disintegration, 19
disjointness, 147
distribution
  posterior, see posterior distribution
  posterior predictive, 12
  sampling, 30
  unimodal, 31
domination, 149
distribution
empirical Bayes, 86
empty set, 147
entropy
  Lindley, 77
  Shannon, 77
estimate, 8
estimator, see pint-estimator
  \(M\), 37
  formal Bayes, 35
  MAP, 36
  maximum-a-posteriori, 36
  maximum-likelihood, 10, 15
  minimax, 57
  non-parametric ML, 97
  penalized maximum-likelihood, 37
  small-ball, 36
  unbiased, 98
exchangability, 150
expectation
  empirical, 9
expected loss, 35
exponential family
  canonical representation, 79
  of full rank, 79
feature vector, 60
hyperparameter, 83
hyperprior, 71, 83
hypothesis, 43
  composite, 43
  simple, 43
identifiability, 5
inadmissible, 54
independence, 150
inference, 53
infinite divisibility, 90
integrability, 152
integral, 152
intersection, 147
lemma
  Fatou’s, 153
First Borel-Cantelli, 150
Second Borel-Cantelli, 150
level, 41, 44
  confidence, 39
  significance, 44
likelihood principle, 10
likelihood-function, 10
limit
  set-theoretic, 147
limit distribution, 9
location, 30
location family, 43
loss, 34, see loss-function
  loss-function, 35, 54
  \(L_2\)-, 56
measurability, 151
  of a subset, 148
measure, 148
  atomic, 150
  Borel, 148
  delta, 150
  Dirac, 150
  probability, 149
  signed, 148
  total variation, 149
measure space, 148
minimax optimality, 49
minimax theorem, 49
misclassification, 60
mixture model, 21
ML-II estimator, 87
MLE, see estimator, maximum-likelihood
  model, 4
  Bayesian, 18, 24
  dimension, 6
  dominated, 4
  full, 4
  full non-parametric, 4
  hierarchical Bayes, 83
  identifiable, 5
  mis-specified, 6
  non-parametric, 7
  normal, 7
  parameterized, 5
  parametric, 6
  well-specified, 6
model distributions
  Bayesian, 18
  frequentist, 4
model selection, 87, 88
monotone class, 148, 151
monotony
  set-theoretic, 147
Index

norm
  total variation, 32
  total-variation, 4, 10, 148
NPMLE, see nn-parametric MLE
null
  hypothesis, 43
  null-set, 149
odds ratio
  posterior, 50
  prior, 50
optimality criteria, 10
over-fitting, 88
parameter
  nuisance, 9
  of interest, 9
parameter space, 5
partition, 147
point-estimator, 8
pointwise convergence, 158
Polish space, 157
Portmanteau lemma, 158
posterior, 19
posterior distribution, 12
posterior mean, 33
posterior median, 34
posterior mode, 36
power function, 44
  sequence, 48
power-set, 7
powerset, 147, 149
pre-image, 151
prediction, 12
predictive distribution
  posterior, 19, 31
  prior, 19
preferred
  Bayes, 57
  minimax, 55
  prior, 12, 18
  conjugate, 78
  Dirichlet process, 21
  improper, 73
informative, 68
Jeffreys, 75
non-informative, 72
objective, 72
reference, 77
subjective, 68
probability density, 153, 154
probability density function, 4
probability space, 149
Radon-Nikodym derivative, 154
random variable, 152
randomization, 46
randomized test, 46
rate of convergence, 9, 15
regularity, 157
residual, 26
risk
  Bayes, 57
  minimax, 55
  risk function
    Bayesian, 35, 57
sample-average, 9
samplespace, 3, 53
sampling distribution, 40
Scheffé’s lemma, 159
second countable, 25
set, 147
set difference, 147
set-function, 148
σ-additive, 148
σ-finite, 149
additive, 148
countably additive, 148
finite, 149
sigma-algebra, 3, 15
  generated, 148, 151
significance level, see level, see level, significance
  simple function, 152
  simplex, 7
  singularity, 149
Souslin space, 157
state, 53
state-space, 53
statistic, 8, 39
statistical decision theory, 53
statistics
  inferential, 53
stochastic process, 154
studentization, 41
subset, 147
support, 25
test
  asymptotic, 46
  uniformly asymptotically most powerful, 48
  uniformly most powerful, 45
test function, 46
test sequence, 48
  minimax, 49
  test statistic, 44
test-statistic, 44
<table>
<thead>
<tr>
<th>theorem</th>
<th>type-II error, 44</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bernstein-von Mises, 42</td>
<td></td>
</tr>
<tr>
<td>central limit, 9</td>
<td>union, 147</td>
</tr>
<tr>
<td>De Finetti’s, 151</td>
<td>utility, see utility-function</td>
</tr>
<tr>
<td>dominated convergence, 153</td>
<td>utility-function, 54</td>
</tr>
<tr>
<td>Fubini’s, 153</td>
<td></td>
</tr>
<tr>
<td>Glivenko-Cantelli, 9</td>
<td></td>
</tr>
<tr>
<td>minimax, 55</td>
<td></td>
</tr>
<tr>
<td>monotone class, 151</td>
<td></td>
</tr>
<tr>
<td>monotone convergence, 152</td>
<td></td>
</tr>
<tr>
<td>Radon-Nikodym, 153</td>
<td></td>
</tr>
<tr>
<td>type-I error, 44</td>
<td></td>
</tr>
<tr>
<td></td>
<td>version posterior, 20</td>
</tr>
<tr>
<td></td>
<td>weak convergence, 158</td>
</tr>
<tr>
<td></td>
<td>zero-one law, 150</td>
</tr>
</tbody>
</table>