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# STATISTICAL INFERENCE

STA 732 – Lecture Notes

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# Foreword

These lecture notes accompany the course STA 732 - Statistical Theory at Duke University. They provide an exposition of a mathematical theory of statistics. Sections and exercises with ♠ are more advanced and optional course material. This is a work in progress.

The text assumes students have a background in real analysis, measure theory, and linear algebra. Appendices A, B, and C provide condensed refreshers on the most important concepts. Some of the proofs (marked ♠) rely on techniques from functional analysis. To keep the notes self-contained, Appendix C introduces these techniques. For those familiar with the subject, it may be interesting to see how these tools are applied; for those who are not, it provides a helicopter overview but is not required for the course.

## Literature and Acknowledgments

Several sources have been used, but some so extensively that they deserve upfront acknowledgment. I am grateful for the course material shared by Peter Hoff, Surya Tokdar, Yuansi Chen, and Li Ma. These notes are largely based on their material and the source material from which they draw:

- Keener, *Theoretical Statistics: Topics for a Core Course* (2010).
- E.L. Lehmann and G. Casella, *Theory of Point Estimation* (1998).
- G. Casella and R.L. Berger, *Statistical Inference* (2002).
- J.H. van Zanten, *Statistics for High- and Infinite-Dimensional Models* (unpublished).

Part two of the notes draws significantly from A.W. van der Vaart, *Asymptotic Statistics* (1998). Harry van Zanten's lecture notes have been a stylistic model, which, for me personally, set a standard for how to write a brief but rigorous exposition that I have tried to emulate.

## Notation

- $\mathbb{N} = \{1, 2, \dots\}$  denotes the set of natural numbers, and  $\mathbb{N}_0 = \{0, 1, 2, \dots\}$ .
- For a set  $A$ , its power set is denoted as  $2^A = \{S : S \subseteq A\}$ , the set of all subsets of  $A$ .
- The indicator function of a set  $A$  is denoted as  $\mathbb{1}_A$  or  $x \mapsto \mathbb{1}\{x \in A\}$ , which takes value 1 if  $x \in A$  and 0 otherwise.
- Given measurable spaces  $(\mathcal{X}, \mathcal{X})$  and  $(\mathcal{Y}, \mathcal{Y})$ , a measurable map  $f : \mathcal{X} \rightarrow \mathcal{Y}$  is to be understood as being measurable with respect to the  $\sigma$ -algebras  $\mathcal{X}$  and  $\mathcal{Y}$ . If  $f$  is measurable and real valued, but no sigma-algebra is specified, the Borel  $\sigma$ -algebra  $\mathcal{B}(\mathbb{R})$  is what is meant.
- For probability measures, we will sometimes forego the set notation whenever no ambiguity arises: both  $P(X \in A)$  and  $P(x : X(x) \in A)$  are shorthand for  $P(\{x : X(x) \in A\})$ .
- We use  $X \sim P$  to denote that the random variable  $X$  has distribution  $P$ .
- The  $n$ -fold product measure of a probability measure  $P$  is denoted by  $P^{\otimes n}$ .
- For sequences  $a_n, b_n$  of positive numbers, we use the notation  $a_n \lesssim b_n$  to indicate that  $a_n \leq Cb_n$  for some constant  $C > 0$  independent of  $n$ . We write  $a_n \asymp b_n$  if both  $a_n \lesssim b_n$  and  $b_n \lesssim a_n$ .

# Part I

## Statistical Decision Theory

# 1 Models, Statistics and Decisions

Inference is the process of drawing conclusions from evidence. In deductive inference, the conclusions follow with certainty by reasoning from the premises. In inductive inference, the conclusions are uncertain; they are at best probable.

Statistical inference is inductive inference in which the evidence consists of data generated by some unknown data-generating process involving randomness. This randomness can arise from several sources: we may be randomly sampling a subset from a larger population, our measurements may contain error, or the phenomenon itself may be governed by inherently stochastic mechanisms.

To describe the data-generating process, we need to describe the randomness that underlies it. Probability theory provides a mathematical language for describing randomness. It allows us to formally reason about the question: given a data-generating process, what is the distribution of the observable data? In statistics, however, we wish to formally reason about probable cause based on observed effects. This concerns ‘the inverse’ of the previous question: what does the observed data tell us about certain unknown features of the data-generating process?

We pursue statistical inference about unknown features of a data-generating process because they govern the real-world consequences of our actions. Whether a treatment saves lives, whether an investment succeeds, or a policy achieves its intended effect – all depend on the true nature of that process. *Statistical decision theory* is a mathematical framework for reasoning about optimal actions when consequences depend on an uncertain process we can only observe indirectly.

## 1.1 Statistical Models

The central object of statistical decision theory is a *statistical model*, which is a collection of probability distributions. Each of these probability distributions is a possible description of the data-generating process.

**Definition 1.1.** A *statistical model* is a collection of probability measures  $\mathcal{P}$  defined on a measurable space  $(\mathcal{X}, \mathcal{X})$ :

for all  $P \in \mathcal{P}$ ,  $P : \mathcal{X} \rightarrow [0, 1]$  is a measure that satisfies  $P(\mathcal{X}) = 1$ .

The objects accompanying the statistical model typically carry the special names and interpretations in statistical literature.

- The space  $(\mathcal{X}, \mathcal{X})$  is the *sample space*. It represents the set of all possible data.
- The accompanying sigma-algebra  $\mathcal{X}$  are the *events*. The collections of outcomes to which the model can assign probabilities.
- The collection  $\mathcal{P}$  specifies the possible ‘theories’ that could have generated the data.
- The triple  $(\mathcal{X}, \mathcal{X}, \mathcal{P})$  can be referred to as the *statistical experiment* (or simply the *experiment*), we revisit this terminology in Definition 1.6 below.
- The *outcome* of the experiment is represented by an element  $x \in \mathcal{X}$ . Equivalently (and more informatively), it is the list of all  $A \in \mathcal{X}$  for which  $x \in A$ . In other words, the outcome tells us exactly which events have occurred and which have not.

Measure theory provides a rigorous framework ensuring the intuitive properties we expect from probabilities hold without exception. Some of these properties follow almost immediately from the definition of a probability measure and a sigma-algebra (see Definitions B.1 and B.2):

- If the event  $A$  implies the event  $B$  (i.e.  $A \subseteq B$ ), then  $P(A) \leq P(B)$  for every  $P \in \mathcal{P}$ .
- If we can assign probability to the event  $A$ , we can assign it to its complement  $A^c$  and we have  $P(A^c) = 1 - P(A)$ .

Less intuitive<sup>1</sup> but highly desirable mathematically, is the ability to assign probabilities to countable unions of events. Without it, paradoxes and inconsistencies can arise in uncountable sample spaces.

Besides its desirable properties in terms of formalizing probabilities, the sigma-algebra formalizes the information that can be extracted from the data. This allows us to compare models with the same underlying sample space but where different events are observable.

**Example 1.2.** Consider an experiment of rolling two six-sided dice and observing the eyes on top each die. Formally, we could model this as  $(\mathcal{X}, \mathcal{X}, \mathcal{P})$  where the sample space is given by

$$\mathcal{X} = \{1, 2, 3, 4, 5, 6\} \times \{1, 2, 3, 4, 5, 6\},$$

and its powerset  $\mathcal{X} = 2^{\mathcal{X}}$  are the observable events, and  $\mathcal{P}$  should consist of a subset of the probability measures on  $(\mathcal{X}, \mathcal{X})$ . The sum of the eyes on each die is observable:  $S : \mathcal{X} \rightarrow \mathbb{R}$  given by  $S(x, y) = x + y$  for  $(x, y) \in \mathcal{X}$ , and so is whether the first die is larger than the second die:  $L(x, y) = \mathbb{1}_{\{x > y\}}$ .

<sup>1</sup>and in the eyes of some, controversial Regazzini 2013.

Consider another statistical model which models the case where we only observe the sum of the eyes on each die:

$$(\mathcal{X}, \sigma(S), \mathcal{Q}),$$

where  $\sigma(S)$  is the sigma-algebra generated by  $S$  (see Definition B.9) and the collection  $\mathcal{Q}$  consists of the probability measures  $P \in \mathcal{P}$  restricted to  $\sigma(S)$ . The sample space is the same as in the first experiment, but the sigma-algebra is strictly smaller.

In the first experiment, we can determine the value of the first die, the second die, whether they are equal, whether the first is larger, etc. In the second experiment, the observables are a subset of the observables in the first experiment. That is, certain events that we could assign probabilities to in the first experiment, we cannot assign probabilities to in the second experiment, such as the event that the first die is larger than the second die.  $\diamond$

The two experiments in Example 1.2 model different observational scenarios of the same underlying random phenomenon. The first experiment provides more information: knowing the individual outcomes of each die, we can reconstruct their sum. Conversely, knowing only the sum, we cannot recover the individual outcomes. Whether the first experiment is more suitable of the inference problem at hand depends on the question we are interested in. For certain inferential goals, knowing the sum of the individual dice is all we need. We will formalize this idea in Section 1.2, where we will discuss the concept of sufficient statistics. For now, let us note that the sigma-algebra captures precisely which features of the outcome are observable, making it possible to formalize such comparisons. The definition of the sample space allows for a lot of freedom: it need not match the minimal description of the data; in principle, it could be the whole universe, provided the sigma-algebra correctly captures the information available in the experiment.

To close this section, we will discuss the idea of a parameter space. It is common that we are only interested in particular characteristics of the data-generating process, such as its mean, certain quantiles, and so on. These are typically functionals on  $\mathcal{P}$ : they map each  $P$  to some value, for example its mean  $\int x dP(x)$ . We will call these characteristics *parameters*. Consider a set  $\Theta$  of possible values of those parameters for our statistical model. We call this set the *parameter space*.

**Definition 1.3.** A *parameter space* for the model  $\mathcal{P}$  is a set  $\Theta$  together with a map  $P \mapsto \theta(P)$  from  $\mathcal{P}$  onto  $\Theta$ .

**Example 1.4.** Let  $(\mathcal{X}, \mathcal{X}) = (\mathbb{R}, \mathcal{B}(\mathbb{R}))$ , where  $\mathcal{B}(\mathbb{R})$  is the Borel  $\sigma$ -algebra on  $\mathbb{R}$  (see Definition B.10). Consider the collection of probability measures  $\mathcal{P} = \{N(\theta, 1) : \theta \in \mathbb{R}\}$ ,

where  $N(\theta, \sigma^2)$  denotes the normal distribution with mean  $\theta$  and variance  $\sigma^2$ :

$$N(\theta, \sigma^2)(A) := \int_A \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\theta)^2}{2\sigma^2}} dx.$$

Further, consider the collection

$$\mathcal{Q} = \{\text{all probability measures on } (\mathbb{R}, \mathcal{B}(\mathbb{R})) \text{ with finite mean}\}.$$

Both  $(\mathcal{X}, \mathcal{X}, \mathcal{P})$  and  $(\mathcal{X}, \mathcal{X}, \mathcal{Q})$  are valid statistical models. The set  $\Theta = \mathbb{R}$  is a valid parameter space for  $\mathcal{P}$  and  $\mathcal{Q}$  under the map  $Q \mapsto \int x dQ(x)$ . The set  $\Theta = [-1, 1]$  is not a valid parameter space for either  $\mathcal{P}$  or  $\mathcal{Q}$  under the same map (why?).  $\diamond$

There is an important distinction between the models  $\mathcal{P}$  and  $\mathcal{Q}$  in Example 1.4. In the first model, the mean uniquely identifies its distribution: there is a one-to-one correspondence between the parameter space and the collection of probability measures. In the second model, the mean does not uniquely identify its distribution: many different probability measures have the same mean. The same parameter (here the mean) can identify the entire distribution in one model but fail to do so in another.

**Definition 1.5.** A statistical model  $\mathcal{P}$  is *identifiable* by a parameter space  $\Theta$  if for all  $P, P' \in \mathcal{P}$ , it holds that if  $\theta(P) = \theta(P')$ , then  $P = P'$ .

The identifiability condition  $\theta(P) = \theta(P') \implies P = P'$  means that the parameter space  $\Theta$  forms a ‘coordinate system’ for the collection of probability measures  $\mathcal{P}$ . Since the map  $P \mapsto \theta(P)$  is surjective, it means that every probability measure in  $\mathcal{P}$  is uniquely determined by its parameter value in  $\Theta$ .

Every statistical model  $\mathcal{P}$  admits a trivial identifiable parameterization: simply take  $\Theta = \mathcal{P}$  and  $\theta(P) = P$ . Whilst always possible, this parametrization is not always the most useful. Typically, the introduced parameter space brings along useful extra structure on the model that the bare set  $\mathcal{P}$  does not ‘directly’ possess. In the vast majority of examples in this course we choose  $\Theta$  to be an open, convex subset of  $\mathbb{R}^d$ . This endows the model with the rich Euclidean structure: vector-space operations, a natural notion of a distance metric, an inner product, differentiability, and so on.

When a model is identifiable, we may (and usually do) identify the parameter value  $\theta$  with the distribution  $P_\theta$  itself, so that “knowing  $\theta$ ” is equivalent to “knowing which distribution generated the data”. That is, we can index the distributions by the parameter value:

$$\mathcal{P} = \{P_\theta : \theta \in \Theta\}.$$

where the subscript  $\theta$  uniquely labels the distribution  $P_\theta$ .

This type of parametrization is what we will mostly be concerned with in this course, leading us to the definition of a statistical experiment.

**Definition 1.6.** A *statistical experiment* is a tuple  $(\mathcal{X}, \mathcal{X}, \mathcal{P}, \Theta)$  where the parameter space  $\Theta$  indexes the collection of probability measures  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  on the sample space  $(\mathcal{X}, \mathcal{X})$ .

There is often an intricate interplay between the parametrization of the model and the formulation of the sample space, leading to multiple ways to write down what is effectively the same model. Sufficiency is one concept that allows us to formalize this idea, which we will discuss next.

*Remark 1.7* (But wait... isn't my data supposed to be a random variable?). In the current framework, there is no random variable explicitly representing 'the data' in the experiment. This may appear to differ from the typical introductory setting; where a statistical setting is defined by a random variable with a given distribution depending on some parameter: "let  $X \sim N(\theta, 1)$  for  $\theta \in [-1, 1]$ ". Alternatively, one may be used to the following formal setting from probability courses, in which one considers an (implicit) probability space  $(\Omega, \mathcal{F}, \mathbb{P})$  and defines a random variable (or rather a random element)  $X : \Omega \rightarrow \mathcal{X}$  representing 'the data before it is observed'. The law of  $X$  is then defined as  $P(A) = \mathbb{P}(\omega : X(\omega) \in A)$  for some unknown probability measure  $P \in \mathcal{P}$  on  $(\mathcal{X}, \mathcal{X})$ .

In our framework, we work directly with  $(\mathcal{X}, \mathcal{X}, \mathcal{P})$  without introducing any underlying probability space. We can always recover the setup in which 'the data is a random variable' (and it is often linguistically and pedagogically useful to do so). Simply take the target space  $(\mathcal{X}, \mathcal{X})$  of the random variable that is supposed to represent the data and consider the identity map  $X : \mathcal{X} \rightarrow \mathcal{X}$ ,  $X(x) = x$  for all  $x \in \mathcal{X}$ . It is easy to see that this map is measurable with respect to  $\mathcal{X}$ . Further, the collection  $\mathcal{P}$  describes the possible laws of this 'random element':  $P(A) = P(x : X(x) \in A)$  for all  $A \in \mathcal{X}$  in  $P \in \mathcal{P}$ .

With this understanding in place, we will frequently use the familiar language of random variables—for instance, "let  $X \sim N(\theta, 1)$  for  $\theta \in [-1, 1]$ " should be understood as shorthand for the statistical model  $(\mathbb{R}, \mathcal{B}(\mathbb{R}), \{N(\theta, 1) : \theta \in [-1, 1]\})$ . In this context, there can be little to no ambiguity which sigma-algebra we are referring to (recall the definition of the normal distribution in Example 1.4). Similarly — recalling that independent random variables are distributed according to the product measure (see Definition B.31 in Appendix B) —  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\theta, 1)$  with  $\theta \in \Theta$  is to be understood as shorthand for the statistical model  $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), \{N(\theta, 1)^{\otimes n} : \theta \in \Theta\})$ .

## 1.2 Statistics, Sufficiency and Likelihoods

In Example 1.2, we noted that knowing the sum of two dice provides less information than knowing each die individually: from the sum alone, we cannot recover the individual outcomes. Yet for certain inferential goals, the sum may contain all the information we need. This section makes precise the notion of a statistic that captures “all the information about the parameter.” This will allow us to compare different formulations of models and judge when they are effectively the same for all intents and purposes. We start by defining what a statistic is.

**Definition 1.8.** A *statistic* is a measurable map  $T$  from the sample space  $(\mathcal{X}, \mathcal{X})$  to some measurable space  $(\mathcal{T}, \mathcal{T})$ .

Given a statistical model  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  defined on a measurable space  $(\mathcal{X}, \mathcal{X})$ , a statistic is a measurable map  $T : \mathcal{X} \rightarrow \mathcal{T}$  into another measurable space  $(\mathcal{T}, \mathcal{T})$ . The statistic  $T$  induces a new statistical model on  $(\mathcal{T}, \mathcal{T})$ , which we denote  $\mathcal{P}^T = \{P_\theta^T : \theta \in \Theta\}$ , where each  $P_\theta^T$  is the push-forward measure of  $P_\theta$  under  $T$ :

$$P_\theta^T(B) = P_\theta(T^{-1}(B)) \quad \text{for all } B \in \mathcal{T}.$$

The map  $T : \mathcal{X} \rightarrow \mathcal{T}$  sends each possible outcome of an experiment to a ‘summary’ of the data. Ideally, the summary  $T(X)$  is more ‘compressed’ than the original data  $X$ , while retaining all relevant information about the parameter  $\theta$ .

This brings us to the idea of sufficiency. The key idea is that a statistic  $T(X)$  is sufficient if, once we know  $T(X)$ , the remaining randomness in  $X$  tells us nothing further about which  $P_\theta$  generated the data. Formally, the conditional distribution of  $X$  given  $T(X)$  should not depend on  $\theta$ .

**Definition 1.9** (Sufficiency). Consider an identifiable model  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  on a sample space  $(\mathcal{X}, \mathcal{X})$ . A statistic  $T : \mathcal{X} \rightarrow \mathcal{T}$  is *sufficient* for  $\mathcal{P}$  if for every  $A \in \mathcal{X}$ , the conditional probability  $P_\theta(A | T)$  admits a version that does not depend on  $\theta$ .

Recall that the conditional probability  $P_\theta(A | T)$  is formally defined as a conditional expectation  $\mathbb{E}_\theta[\mathbb{1}_A | T]$  (see Definition B.33 in Appendix B). This expectation is a random variable, measurable with respect to the  $\sigma$ -algebra generated by  $T$ , satisfying the condition

$$\int_B \mathbb{E}_\theta[\mathbb{1}_A | T](x) dP_\theta(x) = P_\theta(x : x \in A, x \in B)$$

for all  $B \in \sigma(T)$ .

Because conditional expectations are only unique up to  $P_\theta$ -null sets, saying that “ $P_\theta(A | T)$  admits a version that does not depend on  $\theta$ ” means: for each  $A \in \mathcal{X}$  there

exists a measurable function  $h_A : \mathcal{X} \rightarrow [0, 1]$ , independent of  $\theta$ , such that

$$\mathbb{E}_\theta[\mathbb{1}_A | T](x) = h_A(x) \quad P_\theta\text{-a.s. for all } \theta \in \Theta.$$

For ‘nice’  $\sigma$ -algebras (for example, the Borel  $\sigma$ -algebra), we can go a step further and find a measurable function  $h_A : \mathcal{T} \rightarrow [0, 1]$ , independent of  $\theta$ , such that for all  $C \in \mathcal{T}$ ,

$$\int_C h_A(t) dP_\theta^T(t) = P_\theta(A \cap T^{-1}(C)) = P_\theta(x : x \in A, T(x) \in C), \quad \forall \theta \in \Theta.$$

That is,  $\mathbb{E}_\theta[\mathbb{1}_A | T]$  can be represented as a function of  $T$  (a so called ‘regular’ conditional probability), not depending on  $\theta$ :  $E_\theta[\mathbb{1}_A | T](x) = h_A(T(x))$ . Regardless of the representation, the key point is that  $h_A$  does not depend on  $\theta$ : *after conditioning on the ‘information of  $T$ ’ (the  $\sigma(T)$ -algebra), whatever we know about the event  $A$  does not depend on  $\theta$*  (up to sets of zero measure).

Sufficiency is a property of how the parameter enters the distribution of the data. The same statistic may be sufficient for one model but not another, and crucially depends on how the model is parametrized (we will see an illustration of this in Example 1.13).

Before studying interesting cases, we note that sufficiency is trivially achieved when no information is discarded. A statistic that is appropriately invertible is sufficient: by inverting the map, we can recover the data from the statistic.

**Proposition 1.10.** *Consider a statistic  $T : \mathcal{X} \rightarrow \mathcal{T}$  that is bijective, and assume its inverse is also measurable. Then,  $T$  is sufficient.*

*Proof.* Consider the  $\sigma$ -algebra generated by  $T$ ,  $\sigma(T)$ . This is the smallest  $\sigma$ -algebra containing all the preimages  $T^{-1}(B)$  of the sets in  $B \in \mathcal{T}$ , so

$$\sigma(T) \subseteq \mathcal{X}.$$

As the inverse of  $T$  is measurable,  $T(A) \in \mathcal{T}$  for all  $A \in \mathcal{X}$ . Hence, for any event  $A \in \mathcal{X}$ , measurability of  $T$  and its inverse implies that  $A = T^{-1}(T(A)) \in \sigma(T)$ , so  $\mathbb{1}_A$  is  $\sigma(T)$ -measurable. Conclude that  $\sigma(T) = \mathcal{X}$ .

Hence, we have that for all  $A \in \mathcal{X}$ ,

$$P_\theta(A | T) = \mathbb{E}_\theta[\mathbb{1}_A | T] = \mathbb{1}_A,$$

where the second equality holds because conditioning a  $\sigma(T)$ -measurable random variable on  $T$  returns itself. Since  $\mathbb{1}_A$  does not depend on  $\theta$ ,  $T$  is sufficient.  $\square$

The interesting cases of sufficiency are when the statistic is not invertible: A non-

invertible statistics compresses the data in a strict sense, without losing information about the parameter.

If models have densities with respect to a common measure, we have a very useful characterization of sufficiency that allows us to check sufficiency by looking at the form of their *probability density functions*. We need these densities to be well-defined with respect to a common measure.

**Definition 1.11.** A statistical model  $\mathcal{P}$  on a measurable space  $(\mathcal{X}, \mathcal{X})$  is *dominated* by a  $\sigma$ -finite measure  $\mu$  on  $(\mathcal{X}, \mathcal{X})$  if every  $P \in \mathcal{P}$  is absolutely continuous with respect to  $\mu$  (denoted  $P \ll \mu$ ). That is, for every  $A \in \mathcal{X}$ , if  $\mu(A) = 0$ , then  $P(A) = 0$  for all  $P \in \mathcal{P}$ .

If a model is dominated by  $\mu$ , the Radon–Nikodym theorem (see Theorem B.29 in Appendix B) guarantees the existence of a non-negative measurable function  $p = dP/d\mu$ , called the *Radon–Nikodym derivative* of  $P$  with respect to  $\mu$ , such that for all  $A \in \mathcal{X}$ ,

$$P(A) = \int_A p(x) d\mu(x).$$

When the model is parameterized as  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ , we denote the density of  $P_\theta$  by  $p(\cdot | \theta)$  or  $p_\theta(\cdot)$ . The choice of dominating measure is not unique; if  $\mu$  dominates  $\mathcal{P}$ , then any measure equivalent to  $\mu$  also dominates  $\mathcal{P}$ .

For a fixed parameter value  $\theta$ , the map  $x \mapsto p(x | \theta)$  is the probability density function (with respect to  $\mu$ ). If we instead fix the observation  $x$ , the map  $\theta \mapsto p(x | \theta)$  is called the *likelihood function*. Note that since the density is defined only up to a set of  $\mu$ -measure zero, the likelihood function is also only defined up to a  $\mu$ -null set of  $x$ 's. For a fixed  $x$ , different versions of the density may yield different likelihood functions, but they will agree for  $\mu$ -almost all  $x$ . In practice, we usually work with a specific, canonical version of the density (e.g., one that is continuous in  $x$ ), which makes the likelihood unique.

The following theorem says that a statistic is sufficient if and only if the likelihood function can be factorized into a function of the statistic and a function of the data.

**Theorem 1.12** (Fisher–Neyman Factorization). *Let  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  be dominated by a  $\sigma$ -finite measure  $\mu$ , with densities  $p(x | \theta) = dP_\theta/d\mu$ . A statistic  $T$  is sufficient for  $\mathcal{P}$  if and only if*

$$p(x | \theta) = g(T(x), \theta) h(x) \quad \mu\text{-a.e.}, \quad \text{for all } \theta \in \Theta$$

for some non-negative measurable functions  $g : \mathcal{T} \rightarrow [0, \infty)$  and  $h : \mathcal{X} \rightarrow [0, \infty)$ .

(♠)*Proof.* ( $\Leftarrow$ ) If  $p(x | \theta) = g(T(x), \theta) \cdot h(x)$  for all  $\theta \in \Theta$ , then on the support of any  $P_{\theta'}$  (i.e. where  $h > 0$ ),

$$\frac{dP_{\theta}}{dP_{\theta'}} = \frac{g(T, \theta)}{g(T, \theta')}$$

is  $\sigma(T)$ -measurable. Hence, by Bayes formula (Theorem B.36 in Appendix B),

$$P_{\theta}(A | T) = E_{\theta}[\mathbb{1}_A | T] = \frac{E_{\theta'}[\mathbb{1}_A \frac{dP_{\theta}}{dP_{\theta'}} | T]}{E_{\theta'}[\frac{dP_{\theta}}{dP_{\theta'}} | T]} = E_{\theta'}[\mathbb{1}_A | T].$$

Since this is true all  $\theta' \in \Theta$ , we find that  $P_{\theta}(A | T)$  admits a version that is constant in  $\theta$ . Hence,  $T$  is sufficient.

( $\Rightarrow$ ) Fix any  $\theta_0 \in \Theta$ . By the Halmos–Savage theorem,  $T$  being sufficient implies that  $dP_{\theta}/dP_{\theta_0}$  is  $\sigma(T)$ -measurable. Setting  $g(T(x), \theta) := dP_{\theta}/dP_{\theta_0}(x)$  and  $h := dP_{\theta_0}/d\mu$  gives the factorization:

$$\frac{dP_{\theta}}{d\mu}(x) = \frac{dP_{\theta}}{dP_{\theta_0}}(x) \cdot \frac{dP_{\theta_0}}{d\mu}(x) = g(T(x), \theta) \cdot h(x), \quad \mu - \text{a.e.}$$

□

The factorization says: the likelihood splits into a part  $g$  that depends on  $\theta$  but only through  $T(x)$ , and a part  $h$  that depends on  $x$  directly but not on  $\theta$ . All the  $\theta$ -dependence is mediated by  $T$ .

Equipped with the Fisher–Neyman factorization theorem, we can revisit the example of two dice from Example 1.2.

**Example 1.13.** Consider again rolling two dice as in Example 1.2. We will discover that whether the sum  $S(x, y) = x + y$  is sufficient depends critically on the assumed model.

**Model 1 (Nonparametric):** Suppose both dice are i.i.d. with unknown probability density<sup>2</sup>  $p$  on  $\{1, \dots, 6\}$ , so the model is

$$\mathcal{P} = \{P_p : P_p(\{(x, y)\}) = p(x)p(y), p \text{ a probability density on } \{1, \dots, 6\}\}.$$

The sum is *not* sufficient for the above model (no matter which parameterization is used). Consider the conditional probability of  $(1, 6)$  given  $S = 7$ :

$$P_p((1, 6) | S = 7) = \frac{p(1)p(6)}{\sum_{k=1}^6 p(k)p(7-k)}.$$

This depends on  $p$ . If  $p$  is uniform, this equals  $1/6$ . If the die is loaded toward extreme

<sup>2</sup>A Radon-Nikodym derivative with respect to the counting measure.

faces, it is larger. Knowing the sum is 7 does not pin down the conditional distribution of the outcome; the particular realization (1, 6) versus (3, 4) carries information about  $p$ .

**Model 2 (A scalar family):** Suppose each die follows a tilted distribution

$$p_\theta(x) = \frac{e^{\theta x}}{\sum_{k=1}^6 e^{\theta k}}, \quad x \in \{1, \dots, 6\}, \quad \theta \in \mathbb{R}. \quad (1.1)$$

Here  $\theta = 0$  gives fair dice,  $\theta > 0$  biases toward higher faces, and  $\theta < 0$  biases toward lower faces. The joint density is

$$p_\theta(x, y) = \frac{e^{\theta(x+y)}}{\left(\sum_{k=1}^6 e^{\theta k}\right)^2} = \underbrace{\frac{e^{\theta(x+y)}}{\left(\sum_{k=1}^6 e^{\theta k}\right)^2}}_{g(x+y, \theta)} \cdot \underbrace{1}_{h(x, y)},$$

which factors through the sum. By the Fisher–Neyman factorization theorem,  $S$  is sufficient for  $\theta$ .

The contrast is instructive. Model 2 is indexed by a scalar parameter. Model 1 is nonparametric—a vastly larger model in which no reduction beyond the full data (the pair of eyes) is possible. Both models are identifiable (see Exercise 1.5), yet the sum is only sufficient in Model 2. Sufficiency is determined by the choice of the model.  $\diamond$

The example illustrates that sufficiency depends on the model  $\mathcal{P}$ : the same statistic can be sufficient for one family of distributions and insufficient for another.

Sometimes, two models may have sample spaces that look different, but they can be mapped to the same common sample space via sufficient statistics. This is called *observational equivalence*.

**Definition 1.14.** Two statistical models  $(\mathcal{X}, \mathcal{X}, \{P_\theta : \theta \in \Theta\})$  and  $(\mathcal{Y}, \mathcal{Y}, \{Q_\theta : \theta \in \Theta\})$  with a common parameter space  $\Theta$  are *observationally equivalent* if there exist sufficient statistics  $T : \mathcal{X} \rightarrow \mathcal{T}$  and  $S : \mathcal{Y} \rightarrow \mathcal{T}$  such that  $P_\theta^T = Q_\theta^S$  for all  $\theta \in \Theta$ .

Models being observationally equivalent means we can transform them to a common sample space, without losing information about the parameter. In particular, when one model can be mapped to the other, they are observationally equivalent.

**Example 1.15.** Let  $\mathcal{P} = \{N(\mu, \sigma^2)^{\otimes n} : \mu \in \mathbb{R}\}$  on  $\mathbb{R}^n$  and  $\mathcal{Q} = \{N(\mu, \sigma^2/n) : \mu \in \mathbb{R}\}$  on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$  for a fixed  $\sigma^2 > 0$ . Then  $\bar{X} = n^{-1} \sum_{i=1}^n X_i$  is sufficient for  $\mathcal{P}$ , the identity is sufficient for  $\mathcal{Q}$ , and both have distribution  $N(\mu, \sigma^2/n)$ . Thus, the two models are observationally equivalent.  $\diamond$

Intuitively, if two experiments are observationally equivalent, we should be able to simulate the outcome of one experiment using the outcome of the other (possibly

with some independent randomization), without knowing the true parameter value. However, under the notion of observational equivalence introduced in Definition 1.14, this is not always possible: it does not allow for randomization. Later, in Chapter 5, we will introduce a slightly more general notion of equivalence called *simulation equivalence* (sometimes called *Blackwell sufficiency*). This notion is more general than observational equivalence: it says that the two models are simulation equivalent if given the data of one model, we can simulate data as if it were generated by the other model. For most models (those defined on ‘nice’ sigma-algebras), observational equivalence implies simulation equivalence. For now, we will just illustrate this idea using the following example.

**Example 1.16** (Simulation Equivalence of Normal Models). Let  $\mathcal{P} = \{N(\mu, \sigma^2)^{\otimes n} : \mu \in \mathbb{R}\}$  on  $\mathbb{R}^n$  and  $\mathcal{Q} = \{N(\mu, \sigma^2/n) : \mu \in \mathbb{R}\}$  on  $\mathbb{R}$ . These models are simulation equivalent:

- From  $\mathcal{P}$  to  $\mathcal{Q}$ : Given  $(X_1, \dots, X_n) \sim P_\mu$ , output  $\bar{X} = n^{-1} \sum_{i=1}^n X_i$ .
- From  $\mathcal{Q}$  to  $\mathcal{P}$ : Given  $Y \sim Q_\mu$ , generate  $Z_1, \dots, Z_n \stackrel{\text{iid}}{\sim} N(0, \sigma^2)$  and output

$$X_i = Y + Z_i - \bar{Z}.$$

It can be shown that  $P_\mu(\bar{X} \in A) = Q_\mu(A)$  for all  $A \in \mathcal{B}(\mathbb{R})$  and  $\mu \in \mathbb{R}$ , and similarly, for  $Y \sim Q_\mu$ ,  $Y + Z_i - \bar{Z}$  can be shown to be distributed as  $i = 1, \dots, n$  i.i.d.  $N(\mu, \sigma^2)$  random variables (see Exercise 1.6).  $\diamond$

A sufficient statistic always exists: the identity map  $X(x) = x$  itself is trivially sufficient by Proposition 1.10. We typically seek a sufficient statistic that achieves maximal reduction of the data. This brings us to the notion of *minimal sufficiency*.

**Definition 1.17.** A sufficient statistic  $T$  is *minimal sufficient* for an experiment  $(\mathcal{X}, \mathcal{X}, \{P_\theta : \theta \in \Theta\})$  if for any other sufficient statistic  $S$ , it satisfies  $\sigma(T) \subseteq \sigma(S)$  modulo  $P_\theta$ -null sets:

$$\sigma(T) \subseteq \sigma(\sigma(S) \cup \mathcal{N}), \quad \mathcal{N} := \{N \in \mathcal{X} : P_\theta(N) = 0 \forall \theta \in \Theta\}.$$

Minimal sufficient statistics partition the sample space into the coarsest equivalence classes that preserve all information about  $\theta$ . Any other sufficient statistic  $S$  generates a larger  $\sigma$ -algebra than  $T$ , except for sets which have probability zero under all  $P_\theta$ .

Another way to think about minimal sufficiency is that a sufficient statistic  $T$  is *minimal sufficient* if it is a function of every other sufficient statistic. We can formalize this idea if  $T$  takes values in a measure space with a nice  $\sigma$ -algebra, like the Borel  $\sigma$ -algebra. For such nice  $\sigma$ -algebras, Definition 1.17 is equivalent to the following: for

any sufficient statistic  $S$ , there exists a measurable function  $f$  such that  $T = f(S)$  almost surely under all  $P_\theta$ ,  $\theta \in \Theta$  (Doob-Dynkin, Lemma B.37 in Appendix B).

Just as with sufficiency, minimal sufficiency can be difficult to verify. Luckily, we have the following useful tool to check minimal sufficiency.

**Proposition 1.18.** *Let  $(\mathcal{X}, \mathcal{X}, \{P_\theta : \theta \in \Theta\})$  be a dominated model. A statistic  $T$  is minimal sufficient if and only if  $T(x) = T(x')$  whenever the likelihood ratio  $p(x | \theta)/p(x' | \theta)$  is constant in  $\theta$  (except for a  $\mu$ -null set).*

♠ *Proof.* ( $\implies$ ) Define an equivalence relation  $\sim$  on  $\mathcal{X}$  by  $x \sim x'$  if and only if  $p(x | \theta)/p(x' | \theta)$  is constant in  $\theta$ , and let  $S(x)$  denote the equivalence class of  $x$ . We claim  $S$  is sufficient (it is measurable with respect to the quotient  $\sigma$ -algebra  $\mathcal{X}/\sim$ , see Definition B.16 in Appendix B). For each equivalence class  $s$ , fix a representative  $x_s$ . For any  $x$  with  $S(x) = s$ , we have  $p(x | \theta)/p(x_s | \theta) = h(x)$  for some function  $h$  not depending on  $\theta$ . Thus,

$$p(x | \theta) = p(x_s | \theta)h(x) = g(S(x), \theta)h(x).$$

By the factorization theorem,  $S$  is sufficient. Since  $T$  is minimal sufficient,  $T$  is a function of  $S$ , so  $S(x) = S(x')$  implies  $T(x) = T(x')$ . The equality  $S(x) = S(x')$  is precisely the condition that the likelihood ratio is constant in  $\theta$ .

( $\impliedby$ ) Suppose  $T(x) = T(x')$  whenever the likelihood ratio is constant in  $\theta$ . Let  $S$  be any sufficient statistic. By the factorization theorem,  $p(x | \theta) = \tilde{g}(S(x), \theta)\tilde{h}(x)$ . If  $S(x) = S(x')$ , then

$$\frac{p(x | \theta)}{p(x' | \theta)} = \frac{\tilde{h}(x)}{\tilde{h}(x')},$$

which is constant in  $\theta$ . We have found that  $S(x) = S(x')$  implies that  $T(x) = T(x')$ .

This aforementioned fact is sufficient to construct a function  $f : S(\mathcal{X}) \rightarrow \mathcal{T}$  such that  $f \circ S = T$ . For each  $s \in S(\mathcal{X})$ , choose any  $x_s \in S^{-1}(\{s\})$  and define  $f(s) := T(x_s)$ . This is well-defined: if  $x' \in S^{-1}(\{s\})$  is another choice, then  $S(x') = s = S(x_s)$ , so by assumption  $T(x') = T(x_s)$ . For any  $x \in \mathcal{X}$ , we have  $x \in S^{-1}(\{S(x)\})$ , hence  $f(S(x)) = T(x)$ . Moreover,  $f$  is measurable: we have  $S^{-1}(f^{-1}(A)) = T^{-1}(A) \in \mathcal{X}$ .

Thus,  $T$  is a measurable function of  $S$ . Since  $S$  was arbitrary,  $T$  is minimal sufficient.  $\square$

To illustrate minimal sufficiency, we consider the following examples.

**Example 1.19** (Minimal Sufficiency for Uniform). Let  $\text{Uniform}(0, \theta)$  be the uniform distribution on the interval  $[0, \theta]$  with  $\theta > 0$ , that is, probability measure on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$  defined through the Lebesgue density  $p(x | \theta) = \frac{1}{\theta}\mathbf{1}\{0 \leq x \leq \theta\}$ .

Consider the statistical model corresponding to  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Uniform}(0, \theta)$  with  $\theta > 0$ . The likelihood is

$$p(x | \theta) = \frac{1}{\theta^n} \mathbf{1}\{x_{(n)} \leq \theta\},$$

where  $x_{(n)}$  is the  $n$ -th order statistic. By Theorem 1.12, the  $n$ -th order statistic  $X_{(n)}$  is sufficient. The likelihood ratio is

$$\frac{p(x | \theta)}{p(y | \theta)} = \frac{\mathbf{1}\{x_{(n)} \leq \theta\}}{\mathbf{1}\{y_{(n)} \leq \theta\}}.$$

This is constant in  $\theta$  if and only if  $x_{(n)} = y_{(n)}$  (check this!). Thus,  $X_{(n)}$  is minimal sufficient.  $\diamond$

**Example 1.20** (Minimal Sufficiency via Likelihood Ratios). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$ .

*Case 1:  $\sigma^2$  known.* The likelihood ratio is

$$\frac{p(x | \mu)}{p(y | \mu)} = \exp \left( -\frac{1}{2\sigma^2} \left( \sum_i x_i^2 - \sum_i y_i^2 - 2\mu n(\bar{x} - \bar{y}) \right) \right).$$

This is constant in  $\mu$  if and only if  $\bar{x} = \bar{y}$ . Thus  $\bar{X}$  is minimal sufficient.

*Case 2: Both  $\mu$  and  $\sigma^2$  unknown.* The likelihood ratio is

$$\frac{p(x | \mu, \sigma^2)}{p(y | \mu, \sigma^2)} = \exp \left( -\frac{1}{2\sigma^2} \left( \sum_i x_i^2 - \sum_i y_i^2 \right) + \frac{\mu}{\sigma^2} n(\bar{x} - \bar{y}) \right).$$

This is constant in  $(\mu, \sigma^2)$  if and only if  $\bar{x} = \bar{y}$  and  $\sum_i x_i^2 = \sum_i y_i^2$ . Thus  $(\bar{X}, \sum_i X_i^2)$  is minimal sufficient.  $\diamond$

Next, we introduce an additional type of sufficiency called *completeness*. A property that rules out redundancy in a statistic completely.

**Definition 1.21.** A statistic  $T$  is *complete* for  $\mathcal{P}$  if for every  $\sigma(T)$ -measurable integrable random variable  $U$ ,

$$\mathbb{E}_P[U] = 0 \text{ for all } P \in \mathcal{P} \implies U = 0 \text{ } P\text{-a.s. for all } P \in \mathcal{P}.$$

The definition of completeness is of a technical nature: if  $T$  is complete, there is no non-trivial function of  $T$  whose expectation is constant across all  $P \in \mathcal{P}$ . Given an identified model  $\{P_\theta : \theta \in \Theta\}$ , the idea is this:  $T$  contains no component that varies with the data but carries zero information about  $\theta$  on average.

Completeness and sufficiency are logically independent properties: neither implies the other. Completeness is not in and of itself useful; the trivial statistic  $T : x \mapsto c$  for

a constant  $c$  is complete for any model (check). However, when combined, they yield a powerful result: a complete sufficient statistic is automatically minimal sufficient.

**Theorem 1.22** (Bahadur). *If  $T$  is complete and sufficient for  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ , then  $T$  is minimal sufficient.*

*Proof.* Let  $S$  be any sufficient statistic. Fix  $B \in \sigma(T)$ . By sufficiency of  $S$ , there exists  $H_B : \mathcal{X} \rightarrow \mathbb{R}$  such that

$$H_B := \mathbb{E}_\theta[\mathbb{1}_B \mid \sigma(S)] \quad P_\theta\text{-a.s. for all } \theta \in \Theta.$$

Fix such a version  $H_B$ , so  $H_B$  is  $\sigma(S)$ -measurable and note that  $0 \leq H_B \leq 1$ .

The random variable

$$U := \mathbb{E}_\theta[H_B \mid \sigma(T)] - \mathbb{1}_B$$

is  $\sigma(T)$ -measurable (for each  $\theta$ ), integrable, and satisfies  $\mathbb{E}_\theta[U] = 0$  for all  $\theta$ . By completeness of  $T$  (Definition 1.21), we conclude that  $U = 0$   $P_\theta$ -a.s. for all  $\theta$ , i.e.

$$\mathbb{E}_\theta[H_B \mid \sigma(T)] = \mathbb{1}_B \quad P_\theta\text{-a.s. for all } \theta.$$

Since  $0 \leq H_B \leq 1$ , this identity forces  $H_B = \mathbb{1}_B$   $P_\theta$ -a.s. (indeed, on  $B$  we have  $\mathbb{E}_\theta[1 - H \mid \sigma(T)] = 0$ , and on  $B^c$  we have  $\mathbb{E}_\theta[H \mid \sigma(T)] = 0$ ). Since  $H_B$  is  $\sigma(S)$ -measurable,  $H_B = \mathbb{1}_B$   $P_\theta$ -a.s. implies that  $\mathbb{1}_B$  is  $\sigma(S)$ -measurable modulo  $P_\theta$ -null sets. As  $B \in \sigma(T)$  was arbitrary,  $\sigma(T) \subseteq \sigma(S)$  modulo  $P_\theta$ -null sets for every  $\theta$ .  $\square$

The previous theorem shows that the notion of completeness is stronger than minimal sufficiency: every complete sufficient statistic is minimal sufficient. The converse is not true: the following example shows that minimal sufficiency does not imply completeness.

**Example 1.23.** Let  $X_1, \dots, X_n \sim \text{Uniform}(\theta, \theta + 1)$  for  $\theta \in \mathbb{R}$ . The likelihood function is

$$L(\theta) = \prod_{i=1}^n \mathbf{1}_{\{\theta \leq x_i \leq \theta+1\}} = \mathbf{1}_{\{x_{(n)} - 1 \leq \theta \leq x_{(1)}\}}.$$

The likelihood is non-zero if and only if the interval  $[x_{(n)} - 1, x_{(1)}]$  is non-empty and contains  $\theta$ . The pair  $T = (X_{(1)}, X_{(n)})$  determines the likelihood function (as a function of  $\theta$ ) and is therefore minimal sufficient.

However,  $T$  is not complete.

Consider the statistic  $R = X_{(n)} - X_{(1)}$ . The expectation of  $R$  is

$$\mathbb{E}_\theta[R] = \mathbb{E}_\theta[X_{(n)}] - \mathbb{E}_\theta[X_{(1)}] = \left(\theta + \frac{n}{n+1}\right) - \left(\theta + \frac{1}{n+1}\right) = \frac{n-1}{n+1} \quad (\text{check}).$$

Pick arbitrary  $\theta_0 \in \mathbb{R}$ . Since  $R$  is not a constant,  $g(T) = R - \mathbb{E}_{\theta_0}[R]$  is a non-zero function of  $T$ . However,  $g(T)$  has zero expectation for all  $\theta$ . Thus,  $T$  is not complete.  $\diamond$

Next, we introduce the concept of *ancillarity*. This is a property of a statistic that is independent of the parameter.

**Definition 1.24.** Consider statistic  $V$  mapping  $(\mathcal{X}, \mathcal{X})$  to  $(\mathcal{V}, \mathcal{V})$ .  $V$  is *ancillary* for  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  if  $P_\theta(x : V(x) \in A)$  does not depend on  $\theta$  for all  $A \in \mathcal{V}$ . That is, if the distribution of  $V(X)$  does not depend on  $\theta$ .

While a sufficient statistic carries all the information about  $\theta$ , an ancillary statistic carries none—its distribution is the same regardless of which  $P_\theta$  generated the data.

**Example 1.25** (Ancillary in Scale Families). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Uniform}(0, \theta)$  for unknown  $\theta > 0$ . The maximum  $X_{(n)}$  is sufficient for  $\theta$  (Example 1.19). The ratios

$$\left( \frac{X_1}{X_{(n)}}, \dots, \frac{X_{n-1}}{X_{(n)}} \right)$$

are ancillary: their joint distribution does not depend on  $\theta$ . To see this, write  $X_i = \theta U_i$  where  $U_i \stackrel{\text{iid}}{\sim} \text{Uniform}(0, 1)$ . Then  $X_i/X_{(n)} = U_i/U_{(n)}$ , which involves only the  $U_i$ .  $\diamond$

A sufficient statistic captures all information about  $\theta$ ; an ancillary statistic carries none. One might hope these two types of statistics are “orthogonal” in some sense — the sufficient part and the ancillary part of the data do not interact. This is not true in general: a minimal sufficient statistic can be dependent on an ancillary statistic. However, when the sufficient statistic is also complete, this independence is guaranteed. This is the content of Basu’s theorem.

**Theorem 1.26** (Basu). *Consider a statistical model  $(\mathcal{X}, \mathcal{X}, \mathcal{P})$  with  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ . Let  $T$  be complete and sufficient for  $\mathcal{P}$ , and let  $V$  be ancillary for  $\mathcal{P}$ . Then  $T$  and  $V$  are independent under every  $P_\theta \in \mathcal{P}$ .*

*Proof.* Fix  $B \in \mathcal{V}$  and set  $A := \{V \in B\}$ . By sufficiency of  $T$ , the conditional expectation

$$H_B := \mathbb{E}_\theta[\mathbb{1}_A \mid \sigma(T)]$$

admits a version that is the same for all  $\theta$  (i.e.  $H_B$  is  $\sigma(T)$ -measurable and does not depend on  $\theta$  up to  $P_\theta$ -a.s. equality). By ancillarity,  $c_B := P_\theta(A)$  is constant in  $\theta$ . Hence for every  $\theta$ ,

$$\mathbb{E}_\theta[H_B] = \mathbb{E}_\theta[\mathbb{1}_A] = c_B,$$

so with  $G_B := H_B - c_B$  we have  $G_B$   $\sigma(T)$ -measurable and  $\mathbb{E}_\theta[G_B] = 0$  for all  $\theta$ . By completeness of  $T$  (equivalently, of  $\sigma(T)$ ),  $G_B = 0$   $P_\theta$ -a.s. for all  $\theta$ , i.e.

$$\mathbb{E}_\theta[\mathbb{1}_{\{V \in B\}} \mid \sigma(T)] = P_\theta(V \in B) \quad P_\theta\text{-a.s.}$$

for all  $B \in \mathcal{V}$ . This is exactly the independence of  $V$  and  $\sigma(T)$ , hence of  $V$  and  $T$ .  $\square$

Basu's theorem is very useful for showing independence between statistics without deriving their joint distribution directly.

**Example 1.27.** Revisiting Example 1.25, where  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Uniform}(0, \theta)$ , we identified that  $X_{(n)}$  is sufficient and the ratios  $V = (X_1/X_{(n)}, \dots, X_{n-1}/X_{(n)})$  are ancillary.

It turns out that  $X_{(n)}$  is complete. Hence, by Basu's theorem,  $X_{(n)}$  and  $V$  are – perhaps surprisingly – independent.

To check completeness of  $T := X_{(n)}$ , note that its density is  $f_T(t) = nt^{n-1}/\theta^n$  for  $0 < t < \theta$ . Suppose  $\mathbb{E}_\theta[g(T)] = 0$  for all  $\theta > 0$ . Then

$$\int_0^\theta g(t)t^{n-1} dt = 0 \quad \text{for all } \theta > 0.$$

Differentiating with respect to  $\theta$  gives  $g(\theta)\theta^{n-1} = 0$ , which implies  $g(\theta) = 0$  for almost all  $\theta$ . Thus,  $X_{(n)}$  is complete.  $\diamond$

There is a particular class of models for which it is easy to check completeness of sufficient statistics: the class of exponential families, which we will introduce in the next section.

## Exponential Families

Many common statistical models share a structure that leads to elegant sufficiency and completeness results.

**Definition 1.28.** A family of distributions  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  on  $(\mathcal{X}, \mathcal{X})$  dominated by a  $\sigma$ -finite measure  $\mu$  is an *exponential family* if the densities can be written as

$$p(x \mid \theta) = \exp\{\eta(\theta)^\top T(x) - B(\theta)\}h(x), \quad (1.2)$$

where  $T : \mathcal{X} \rightarrow \mathbb{R}^k$  and  $h : \mathcal{X} \rightarrow [0, \infty)$  are measurable functions, and  $\eta : \Theta \rightarrow \mathbb{R}^k$ .

The map  $T : \mathcal{X} \rightarrow \mathbb{R}^k$  is the *natural sufficient statistic*: by the Fisher–Neyman factorization theorem,  $T$  is sufficient for  $\theta$  in any exponential family – the density (1.2) factors as  $g(T(x), \theta) \cdot h(x)$ . For i.i.d. observations  $X_1, \dots, X_n$  from a distribution in an exponential family, the sufficient statistic is the sum  $\sum_{i=1}^n T(X_i)$ .

**Proposition 1.29.** *If  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  is an exponential family with natural sufficient statistic  $T$ , then the model  $\{P_\theta^{\otimes n} : \theta \in \Theta\}$  is also an exponential family, with natural sufficient statistic  $(x_1, \dots, x_n) \mapsto \sum_{i=1}^n T(x_i)$ .*

*Proof.* The joint density is

$$\prod_{i=1}^n p(x_i | \theta) = \exp\left\{\eta(\theta)^\top \sum_{i=1}^n T(x_i) - nB(\theta)\right\} \prod_{i=1}^n h(x_i),$$

which is of the form (1.2) with  $\tilde{T}(x_1, \dots, x_n) = \sum_{i=1}^n T(x_i)$ ,  $\tilde{B}(\theta) = nB(\theta)$ , and  $\tilde{h}(x_1, \dots, x_n) = \prod_{i=1}^n h(x_i)$ .  $\square$

The exponential family is in *natural* (or *canonical*) *parameterization* if  $\Theta \subseteq \mathbb{R}^k$  and  $\eta(\theta) = \theta$  is the identity map. The *natural parameter space* is

$$\mathcal{H} = \left\{ \eta \in \mathbb{R}^k : \int_{\mathcal{X}} \exp\{\eta^\top T(x)\} h(x) d\mu(x) < \infty \right\}.$$

The set  $\mathcal{H}$  is convex (verify this). A naturally parameterized exponential family with  $\mathcal{H}$  is called *full-rank* if  $\mathcal{H}$  contains an open subset of  $\mathbb{R}^k$ . For full-rank exponential families, there is a convenient route to minimal sufficiency: we show that  $T$  is complete using the proposition below, after which minimality is implied by Theorem 1.22.

**Proposition 1.30.** *Let  $\mathcal{P} = \{P_\eta : \eta \in \mathcal{H}\}$  be an exponential family in natural parameterization with natural sufficient statistic  $T$ . If  $\mathcal{H}$  contains an open subset of  $\mathbb{R}^k$ , then  $T$  is complete.*

♠*Proof.* The density of  $T$  (note  $T$  takes values in a regular Borel space) with respect to some base measure  $\nu$  is

$$p_T(t | \eta) = \exp(\eta^\top t - B(\eta)).$$

Suppose  $E_\eta[g(T)] = 0$  for all  $\eta \in \mathcal{H}$ . Then

$$\int g(t) \exp(\eta^\top t - B(\eta)) d\nu(t) = 0$$

for all  $\eta \in \mathcal{H}$ . Since  $e^{-B(\eta)} \neq 0$ , this implies

$$\int g(t) \exp(\eta^\top t) d\nu(t) = 0$$

for all  $\eta$  in an open subset of  $\mathcal{H}$ . The left side is the Laplace transform of the (signed) measure  $g d\nu$ . Since Laplace transforms are analytic and this one vanishes on an open

set, it vanishes on its entire domain. By uniqueness of the Laplace transform,  $g d\nu = 0$ , so  $g(T) = 0$   $\nu$ -a.s., hence  $P_\eta$ -a.s. for all  $\eta \in \mathcal{H}$ .  $\square$

What if  $\{P_\theta : \theta \in \Theta\}$  is not a family in natural parameterization? If  $\eta$  is injective, we may re-index the family as follows. Set  $\Xi := \eta(\Theta)$  and define a re-parameterized family

$$Q_\xi := P_{\eta^{-1}(\xi)}, \quad \xi \in \Xi.$$

Then, by injectivity of  $\eta$ , we have

$$\{Q_\xi : \xi \in \Xi\} = \{P_\theta : \theta \in \Theta\}$$

as sets of probability measures. Given this re-indexing, if  $\eta(\Theta)$  has nonempty interior in  $\mathbb{R}^k$  (equivalently; contains an open set), Proposition 1.30 implies that the natural sufficient statistic  $T$  is complete for this family, hence also complete under the original parameterization. Indeed, completeness is a property of the family of distributions, not of the parameterization: if two parameterizations define the same collection of probability measures and  $T$  is complete for one, it is complete for the other as well.

The exponential family encompasses a wide range of models. Many of the models we will see in this course belong to this class.

**Example 1.31** (Common exponential families). Most identifiably-parameterized commonly-used exponential families are full rank.

- **Poisson model:** Consider the  $\text{Poisson}(\theta)$  distribution for  $\theta > 0$ , defined by its density with respect to the counting measure:

$$p(x | \theta) = \frac{\theta^x e^{-\theta}}{x!} = \frac{1}{x!} \exp(x \log \theta - \theta), \quad x \in \{0, 1, \dots\}.$$

This constitutes an exponential family with sufficient statistic  $T(x) = x$  and natural parameter  $\eta = \log \theta$ . Since  $\theta > 0$ , the natural parameter  $\eta$  ranges over all of  $\mathbb{R}$ , which is an open set, so Proposition 1.30 yields that  $T$  is complete.

Similarly, for a sample  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Poisson}(\theta)$ , the sum  $T = \sum_{i=1}^n X_i$  is a complete sufficient statistic.

- **Binomial model:** The  $\text{Bernoulli}(p)$  distribution for  $p \in (0, 1)$  has counting measure density

$$p(x | p) = p^x (1-p)^{1-x}, \quad x \in \{0, 1\}.$$

This is an exponential family with  $T(x) = x$  and natural parameter  $\eta(p) = \log(p/(1-p))$ . Since  $\eta(p)$  ranges over all of  $\mathbb{R}$  for  $p \in (0, 1)$ , the family is full-rank. For the  $n$  i.i.d. draws model –  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Bernoulli}(p)$  – the sum  $\sum_{i=1}^n X_i$

is complete and sufficient. Since the map  $p \mapsto \eta(p)$  is a bijection between the parameter space  $(0, 1)$  and the natural parameter space  $\mathbb{R}$ , the statistic is also complete and sufficient for the original parameterization.

- **Multinomial model:** Consider a categorical distribution on  $k$  categories with probabilities  $p = (p_1, \dots, p_k)$  satisfying  $p_j > 0$  and  $\sum_{j=1}^k p_j = 1$ . A single observation is a basis vector  $x = e_j$  indicating category  $j$ , equivalently represented as  $x \in \{0, 1\}^k$  with  $\sum_{j=1}^k x_j = 1$ . The density with respect to counting measure is

$$p(x | p) = \prod_{j=1}^k p_j^{x_j}.$$

Using the constraint  $p_k = 1 - \sum_{j=1}^{k-1} p_j$  and  $x_k = 1 - \sum_{j=1}^{k-1} x_j$ :

$$\log p(x | p) = \sum_{j=1}^{k-1} x_j \log p_j + \left(1 - \sum_{j=1}^{k-1} x_j\right) \log p_k = \sum_{j=1}^{k-1} x_j \log \frac{p_j}{p_k} + \log p_k.$$

This is an exponential family with sufficient statistic  $T(x) = (x_1, \dots, x_{k-1}) \in \mathbb{R}^{k-1}$  and natural parameter  $\eta_j = \log(p_j/p_k)$  for  $j = 1, \dots, k-1$ . Since  $p_j > 0$  for all  $j$ , the ratios  $p_j/p_k$  can take any positive value, so  $\eta \in \mathbb{R}^{k-1}$ . The natural parameter space is all of  $\mathbb{R}^{k-1}$ , which is open, so the family is full-rank.

For  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Categorical}(p)$ , the sufficient statistic is  $\sum_{i=1}^n T(X_i) = (N_1, \dots, N_{k-1})$ , where  $N_j = \sum_{i=1}^n X_{ij}$  counts observations in category  $j$ . This statistic is complete.

- **Gamma model:** Consider the Gamma( $a, b$ ) distribution with shape parameter  $a > 0$  and rate parameter  $b > 0$ : its density (with respect to Lebesgue measure on  $(0, \infty)$ ) is

$$p(x | a, b) = \frac{b^a}{\Gamma(a)} x^{a-1} e^{-bx} = \exp((a-1) \log x - bx + a \log b - \log \Gamma(a)).$$

This constitutes an exponential family with sufficient statistic  $T(x) = (\log x, x)$  and natural parameter  $\eta = (a-1, -b)$ . The natural parameter space is  $(-1, \infty) \times (-\infty, 0)$ , which is an open subset of  $\mathbb{R}^2$ .

For a sample  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Gamma}(a, b)$ , the statistic  $T = (\sum_{i=1}^n \log X_i, \sum_{i=1}^n X_i)$  is sufficient and complete.

- **Multivariate normal model:** Consider the  $N_d(\mu, \Sigma)$  distribution for  $\mu \in \mathbb{R}^d$  and  $\Sigma$  positive definite. The density with respect to Lebesgue measure on  $\mathbb{R}^d$  is

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

Expanding the quadratic form gives

$$p(x \mid \mu, \Sigma) = (2\pi)^{-d/2} |\Sigma|^{-1/2} \exp\left((\Sigma^{-1}\mu)^\top x - \frac{1}{2}x^\top \Sigma^{-1}x - \frac{1}{2}\mu^\top \Sigma^{-1}\mu\right).$$

This is an exponential family with sufficient statistic  $T(x) = (x, xx^\top)$  and natural parameters  $\eta_1 = \Sigma^{-1}\mu \in \mathbb{R}^d$  and  $\eta_2 = -\frac{1}{2}\Sigma^{-1}$ , a negative definite  $d \times d$  matrix. The natural parameter space is  $\mathbb{R}^d \times \{M \in \mathbb{R}_{\text{sym}}^{d \times d} : M < 0\}$ , which is open in  $\mathbb{R}^{d+d(d+1)/2}$ .

For i.i.d. observations  $X_1, \dots, X_n$ , the sufficient statistic is  $(\sum_{i=1}^n X_i, \sum_{i=1}^n X_i X_i^\top)$ . Since  $\sum_{i=1}^n X_i X_i^\top = S + n\bar{X}\bar{X}^\top$  where  $S = \sum_{i=1}^n (X_i - \bar{X})(X_i - \bar{X})^\top$ , the pair  $(\bar{X}, S)$  is an equivalent (and complete) sufficient statistic.

The map  $(\mu, \Sigma) \mapsto (\Sigma^{-1}\mu, -\frac{1}{2}\Sigma^{-1})$  is a bijection between the original parameter space  $\mathbb{R}^d \times \{M \in \mathbb{R}_{\text{sym}}^{d \times d} : M > 0\}$  and the natural parameter space, so  $(\bar{X}, S)$  is also complete for the original parameterization  $\mu \in \mathbb{R}^d$  and  $\Sigma > 0$ .

**A non-example (a curved exponential family):** An exponential family model can fail to have a complete sufficient statistic if the parameter space has a different dimension than the minimal sufficient statistic. For example, suppose  $X_1, \dots, X_n \sim$  i.i.d.  $N(\theta, \theta^2)$ . Then the density can be expressed as

$$p(x_1, \dots, x_n \mid \theta) = c(\theta)h(x_1, \dots, x_n) \exp\left\{-\sum x_i^2/[2\theta^2] + \sum x_i/\theta\right\}.$$

In this case,  $T(x) = (\sum x_i, \sum x_i^2)$  is a minimal sufficient statistic (why?), but  $\eta(\Theta)$  equals  $\{(-1/[2\theta^2], 1/\theta) : \theta \in \Theta\}$ , which is a curve in  $\mathbb{R}^2$  – it does not contain an open set.

◇

We have so far discussed sufficiency and completeness as properties of the statistical model, allowing us to identify when different mathematical formulations of models are the same ‘for all intents and purposes’. This development, however, has been independent of any specific statistical task. To proceed, we must define what we aim to achieve with the data—whether to estimate a parameter, test a hypothesis, or predict a future value—and how to evaluate our success. In the next section, we introduce the framework of decision theory, which allows us to formalize these goals and rigorously compare statistical procedures.

## 1.3 Decision Problems

Given all the possibilities in terms of writing down models, which one is the ‘correct’ one? One might be tempted to adopt a very large model on the grounds that it is “most

likely to contain the true data-generating process”. We will see that this reasoning is flawed. Larger models typically come with costs: more parameters to estimate, higher variance, etc. To compare models meaningfully, we must first specify *what we intend to do with the data*: what decision or action we will take, and how we quantify the consequences of making that decision under different possible states of nature. Only once the decision problem (and an associated utility or loss function) has been fixed can we meaningfully compare statistical procedures, models, or parameterizations according to their expected performance.

Given observed data  $x$  and a statistical model  $\mathcal{P}$ , we want to determine which decision to take. For example, we may want to infer which probability distribution in the collection  $\mathcal{P}$  is ‘most likely’ to have generated the data. Perhaps we are interested in testing whether a particular  $P_0 \in \mathcal{P}$  gave rise to the observed data versus it is more likely that the data was generated by distribution  $P_1 \in \mathcal{P} \setminus \{P_0\}$ . Perhaps we are interested in predicting a future observed data from the data-generating process, and we want to make sure that our prediction is ‘good’ in the sense that if given that the true data-generating process is  $P_0 \in \mathcal{P}$ , then the prediction is ‘close’ to future data drawn from  $P_0$ . We will develop the formal framework that encapsulates these different inferential goals in a unified way.

To formalize this, we first need to specify the ingredients of a decision problem. Besides a statistical experiment  $(\mathcal{X}, \mathcal{X}, \mathcal{P})$ , a decision problem consists of set of possible actions (decisions), and a way to quantify the consequences of each action under each possible data-generating process. The set of possible actions forms the *decision space*  $\mathcal{D}$ , equipped with a  $\sigma$ -algebra  $\mathcal{D}$  to ensure measurability when we later define expectations and integrals over decisions.

**Definition 1.32.** A *decision space* is a measurable space  $(\mathcal{D}, \mathcal{D})$ .

A (*deterministic*) *decision rule* is a measurable function that assigns an action to each possible data outcome.

**Definition 1.33.** A (*deterministic*) *decision rule* is a measurable function  $\delta$  mapping the sample space  $(\mathcal{X}, \mathcal{X})$  into  $(\mathcal{D}, \mathcal{D})$ .

Later on, we will also consider *randomized decision rules*, which allow for probabilistic mixing of different deterministic decision rules.

To evaluate the quality of decisions, we need a *loss function* that measures the penalty for choosing action  $d \in \mathcal{D}$  when the true data-generating process is  $P_\theta$ .

**Definition 1.34.** A *loss function* is a function  $L : \Theta \times \mathcal{D} \rightarrow [0, \infty)$  such that  $d \mapsto L(\theta, d)$  is measurable for each  $\theta \in \Theta$ .

The loss function  $L(\theta, d)$  quantifies the penalty incurred by taking decision  $d$  when the ‘true state of nature’ is  $\theta$ . The choice of decision space  $\mathcal{D}$  and loss function  $L$  depends on the inferential goal and the consequences of errors in the application at hand.

Two of the most common types of problems which we will study extensively with corresponding loss functions are estimation and hypothesis testing.

**Example 1.35** (Estimation). Suppose we wish to estimate an unknown parameter  $\theta \in \Theta \subseteq \mathbb{R}^k$ . A natural choice is to take the decision space  $\mathcal{D} = \Theta$  and to equip it with the Borel sigma-algebra  $\mathcal{D} = \mathcal{B}(\Theta)$ .

Examples of loss functions for estimation:

- Euclidean distance;  $L(\theta, d) = \|\theta - d\|$ .
- Squared Euclidean distance;  $L(\theta, d) = \|\theta - d\|^2$ .
- Sup-norm loss;  $L(\theta, d) = \|\theta - d\|_\infty = \max_i |\theta_i - d_i|$ .
- Zero-one loss;  $L(\theta, d) = \mathbb{1}_{\{\theta \neq d\}}$ .

◇

**Example 1.36** (Hypothesis Testing). Suppose we wish to test between two hypotheses:  $H_0 : \theta \in \Theta_0$  versus  $H_1 : \theta \in \Theta_1$ , where  $\Theta = \Theta_0 \cup \Theta_1$  and  $\Theta_0 \cap \Theta_1 = \emptyset$ . The decision space is  $\mathcal{D} = \{0, 1\}$ , where  $d = 0$  means “accept  $H_0$ ” and  $d = 1$  means “accept  $H_1$ ”. A simple loss function is:

$$L(\theta, d) = \begin{cases} 0 & \text{if } d = 0 \text{ and } \theta \in \Theta_0, \\ 0 & \text{if } d = 1 \text{ and } \theta \in \Theta_1, \\ a & \text{if } d = 0 \text{ and } \theta \in \Theta_1, \\ b & \text{if } d = 1 \text{ and } \theta \in \Theta_0, \end{cases}$$

where  $a, b > 0$  are the costs of Type II and Type I errors, respectively. When  $a = b = 1$ , this is the zero-one loss. When  $a \neq b$ , we reflect asymmetric consequences—for instance, in medical testing, falsely declaring a patient healthy might be far more costly than falsely declaring them sick.

◇

Combining all the ingredients, we can now define a decision problem.

**Definition 1.37.** A (statistical) *decision problem* is a tuple  $(\mathcal{X}, \mathcal{X}, \mathcal{P}, \Theta, (\mathcal{D}, \mathcal{D}), L)$  where  $(\mathcal{X}, \mathcal{X}, \mathcal{P}, \Theta)$  is a statistical experiment and  $(\mathcal{D}, \mathcal{D})$  is a decision space and  $L$  is a loss function.

For decision problems with identifiable models, the expected loss (under  $P_\theta$ ) of the decision rule  $\delta$  given the ‘true state of nature  $\theta$ ’ is called its *risk*.

**Definition 1.38** (Risk Function). Given an identifiable statistical model  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  on a measurable space  $(\mathcal{X}, \mathcal{X})$ , a decision space  $(\mathcal{D}, \mathcal{D})$  and a loss function  $L : \Theta \times \mathcal{D} \rightarrow \mathbb{R}$ , the *risk* of a decision rule  $\delta : \mathcal{X} \rightarrow \mathcal{D}$  is defined as

$$\mathcal{R}(\theta, \delta) := \int_{\mathcal{X}} L(\theta, \delta(x)) dP_\theta(x), \quad (1.3)$$

whenever this integral exists in  $[-\infty, \infty]$ .

Instead of the integral in Equation (1.3), we will frequently write

$$\mathcal{R}(\theta, \delta) = \mathbb{E}_{P_\theta}[L(\theta, \delta(X))] \equiv \mathbb{E}_\theta[L(\theta, \delta(X))],$$

where the expectation is to be understood as the expectation under the probability distribution  $P_\theta$  and the random element  $X$  is simply the identity map on  $\mathcal{X}$  (see Remark 1.7).

Throughout this course, we evaluate decision rules based on their risk, the expected loss. One might object that focusing on the first moment of the loss is a limiting choice made for mathematical convenience. However, there is considerable flexibility in the choice of loss function itself. For instance, if our goal is for an estimator to be  $\epsilon$ -close to the true parameter with high probability, the loss function  $L(\theta, d) = \mathbb{1}_{\{\|\theta - d\| > \epsilon\}}$  captures exactly this objective.

Beyond flexibility in  $L$ , there are deeper reasons to focus on expected loss. One appeals to frequency under (hypothetical) repetitions and betting interpretations: if we use a decision rule  $\delta$  repeatedly under the same conditions, the average loss converges to the risk  $\mathcal{R}(\theta, \delta)$  by the law of large numbers. A more philosophical justification, grounded in rational preferences over random outcomes, is given in Section 1.3.3.

So far, our decision rules  $\delta : \mathcal{X} \rightarrow \mathcal{D}$  have been deterministic: given data  $x$ , the action  $\delta(x)$  is fully determined. Just as mixed strategies in game theory allow players to randomize over actions, we can allow decision rules to incorporate auxiliary randomness independent of the data.

**Definition 1.39.** A *randomized decision rule* is a measurable function  $\delta : \mathcal{X} \times [0, 1] \rightarrow \mathcal{D}$ . Given data  $x \in \mathcal{X}$  and an independent random variable  $U \sim \text{Uniform}(0, 1)$ , the decision is  $\delta(x, U)$ .

The risk of a randomized rule averages over both the data and the auxiliary randomness:

$$\mathcal{R}(\theta, \delta) = \int_{\mathcal{X}} \int_0^1 L(\theta, \delta(x, u)) du dP_\theta(x) = \int_0^1 \int_{\mathcal{X}} L(\theta, \delta(x, u)) dP_\theta(x) du. \quad (1.4)$$

Often, we will simply write this as  $\mathbb{E}_\theta[L(\theta, \delta(X, U))]$ , but it is important to remember that  $U$  is ancillary to the model.

Why allow randomization? In most estimation problems, deterministic rules suffice—randomization cannot improve expected performance when the loss is convex (as we will see in Section 1.3.1 below). However, randomization becomes important in two settings we will study later:

- *Hypothesis testing* (Chapter 3): To achieve exactly a prescribed significance level  $\alpha$ , we may need to randomize when the test statistic falls on the boundary of the rejection region (see Exercise 1.14).
- *Bayesian decision theory* (Chapter 4).

Furthermore, for general (non-convex) loss functions, randomization can strictly reduce the *worst-case risk*, as shown in the following example.

**Example 1.40** (Matching pennies). Let  $X \in \{0, 1\}$  be a single observation from a model with  $\Theta = \{0, 1\}$  and

$$P_\theta(X = 1) = \begin{cases} 0.3 & \text{if } \theta = 0, \\ 0.6 & \text{if } \theta = 1. \end{cases}$$

The decision space is  $\mathcal{D} = \{0, 1\}$  with 0-1 loss  $L(\theta, d) = \mathbb{1}\{\theta \neq d\}$ . Consider the deterministic rule  $\delta(x) = x$ . Its risk is

$$R(0, \delta) = P_0(X = 1) = 0.3, \quad R(1, \delta) = P_1(X = 0) = 0.4.$$

The worst-case risk is  $\max_\theta R(\theta, \delta) = 0.4$ .

Now consider a randomized rule that follows  $\delta(x) = x$  except when  $X = 0$ , where it randomizes:

$$\delta(x, u) = \begin{cases} \mathbb{1}\{u \leq \gamma\} & \text{if } x = 0, \\ 1 & \text{if } x = 1. \end{cases}$$

The risks are  $R(0, \delta) = 0.3 + 0.7\gamma$  and  $R(1, \delta) = 0.4(1 - \gamma)$ . Setting these equal gives  $\gamma = 1/11$ , yielding

$$\max_\theta R(\theta, \delta) = \frac{4}{11} \approx 0.364 < 0.4.$$

Randomization strictly improves the risk for the worst-case  $\theta$ . ◇

The example above shows that randomization allows us to ‘hedge’ against the worst-case scenario. We will return to such worst-case analyses in later chapters.

For convex loss functions, however, randomized decision rules do not outperform deterministic decision rules. The theorem below makes this precise: for any randomized

decision rule, there exists a deterministic decision rule with at most the same risk if the loss is convex.

**Theorem 1.41.** *If  $d \mapsto L(\theta, d)$  is convex for all  $\theta \in \Theta$ , then for any randomized decision rule  $\delta$ , there exists a deterministic decision rule  $\delta^*$  with  $\mathcal{R}(\theta, \delta^*) \leq \mathcal{R}(\theta, \delta)$  for all  $\theta \in \Theta$ .*

*Proof.* Let  $\delta : \mathcal{X} \times [0, 1] \rightarrow \mathcal{D}$  be a randomized decision rule. Define the deterministic decision rule  $\delta^*(x) = \mathbb{E}^U[\delta(x, U)]$ . By convexity of  $d \mapsto L(\theta, d)$  and Jensen's inequality,

$$L(\theta, \delta^*(x)) = L(\theta, \mathbb{E}^U[\delta(x, U)]) \leq \mathbb{E}^U[L(\theta, \delta(x, U))].$$

Taking expectations over  $X \sim P_\theta$  yields

$$\mathcal{R}(\theta, \delta^*) = \mathbb{E}_\theta[L(\theta, \delta^*(X))] \leq \mathbb{E}_\theta[\mathbb{E}^U[L(\theta, \delta(X, U))]] = \mathcal{R}(\theta, \delta). \quad \square$$

*Remark 1.42* (Why a uniform random variable?). The choice of  $U \sim \text{Uniform}(0, 1)$  as the source of randomness may seem restrictive. Does a single uniform provide enough randomness? For decision spaces with standard measurability properties (e.g.,  $\mathcal{D} \subseteq \mathbb{R}^k$  with the Borel  $\sigma$ -algebra), the answer is yes: any conditional distribution on  $\mathcal{D}$  can be generated from a uniform random variable. We revisit this in Section ??.

### 1.3.1 Sufficiency and loss

Intuitively, a sufficient statistic  $T$  contains all the information about the parameter  $\theta$  that is relevant to making decisions. So, if we are able to attain a certain level of risk in one model, we should be able to attain the same level of risk in the forward model induced by sufficient statistic  $T$ .

The Rao-Blackwell theorem formalizes this intuition. It states that for any convex loss function, we can improve (or at least match) the performance of any decision rule by conditioning on a sufficient statistic.

**Theorem 1.43** (Rao-Blackwell, convex loss). *Let  $T$  be a  $(\mathcal{T}, \mathcal{F})$ -valued sufficient statistic for  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ , and let  $L : \Theta \times \mathcal{D} \rightarrow [0, \infty)$  be a loss function.*

*If  $d \mapsto L(\theta, d)$  is convex for each  $\theta$  and  $\mathcal{D} \subseteq \mathbb{R}^m$  is convex, closed and equipped with the Borel  $\sigma$ -algebra, then for any decision rule  $\delta : \mathcal{X} \rightarrow \mathcal{D}$  with  $\mathbb{E}_\theta[\|\delta(X)\|] < \infty$ , there exists a decision rule  $\delta^*$  satisfying  $\delta^*(X) = \mathbb{E}_\theta[\delta(X) \mid T]$   $P_\theta$ -a.s. for all  $\theta \in \Theta$  and*

$$\mathcal{R}(\theta, \delta^*) \leq \mathcal{R}(\theta, \delta) \quad \text{for all } \theta \in \Theta.$$

*If  $L$  is strictly convex, the inequality is strict unless  $\delta$  is already a function of  $T$ .*

*Proof.* Fix any  $\theta \in \Theta$ . The random vector  $\delta^*(X) = \mathbb{E}_\theta[\delta(X) \mid T]$  is  $\sigma(T)$ -measurable (and hence  $\mathcal{X}$ -measurable) and admits a version not depending on  $\theta$ ; meaning that there exists a version of the conditional expectation that does not depend on  $\theta$  (through similar arguments as in Exercise 1.13) and is  $\mathcal{D}$ -valued. Hence,  $\delta^*(X)$  is a valid decision rule.

By Jensen's inequality (see Lemma B.42 in Appendix B),

$$L(\theta, \delta^*(X)) = L(\theta, \mathbb{E}_\theta[\delta(X) \mid T]) \leq \mathbb{E}_\theta[L(\theta, \delta(X)) \mid T]$$

as  $d \mapsto L(\theta, d)$  is convex. Taking expectations gives  $\mathcal{R}(\theta, \delta^*) \leq \mathcal{R}(\theta, \delta)$ . If  $L(\theta, \cdot)$  is strictly convex and  $\delta$  is not  $\sigma(T)$ -measurable, then  $\delta(X)$  is non-constant conditional on  $T$  with positive probability, and Jensen's inequality is strict on that event, giving  $\mathcal{R}(\theta, \delta^*) < \mathcal{R}(\theta, \delta)$ .  $\square$

This theorem is powerful because it gives us a constructive way to improve estimators. If you have an estimator  $\delta$  and a sufficient statistic  $T$ , you should consider  $\delta^* = E[\delta \mid T]$ . For example, if  $T$  is minimal sufficient, this often leads to the “best” possible reduction. If  $T$  is complete and sufficient, and we restrict ourselves to unbiased estimators, the Lehman-Scheffé theorem (which we will cover later) tells us  $\delta^*$  is the unique best unbiased estimator.

For general loss functions, we have a randomized version of the Rao-Blackwell theorem. The theorem says: *we lose nothing by restricting to decision rules based on  $T$  alone.*

**Theorem 1.44** (Rao-Blackwell, general loss). *Let  $T$  be a  $(\mathcal{T}, \mathcal{F})$ -valued sufficient statistic for  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ , and let  $L : \Theta \times \mathcal{D} \rightarrow [0, \infty)$  be a loss function. Consider  $(\mathcal{D}, \mathcal{D})$  a standard Borel measurable space. Let  $\delta : \mathcal{X} \rightarrow \mathcal{D}$  be any decision rule. There exists a randomized decision rule  $\delta^*$  of the form  $\delta^*(X, U) = f(T(X), U)$  for some measurable function  $f : \mathcal{T} \times [0, 1] \rightarrow \mathcal{D}$  such that*

$$\mathcal{R}(\theta, \delta^*) = \mathcal{R}(\theta, \delta) \quad \text{for all } \theta \in \Theta.$$

*Proof.* By sufficiency, the conditional distribution of  $X$  given  $T(X)$  admits a version not depending on  $\theta$ : we denote its conditional expectation by  $\mathbb{E}[h(X) \mid T]$  for functions  $h : \mathcal{X} \rightarrow \mathbb{R}$ . Since  $(\mathcal{D}, \mathcal{D})$  is standard Borel, the conditional distribution of  $\delta(X)$  given  $T(X) = t$  can be represented via a measurable function (see Theorem B.39 in Appendix B). By sufficiency, this function does not depend on  $\theta$ : there exists  $f : \mathcal{T} \times [0, 1] \rightarrow \mathcal{D}$  such that for each  $t \in \mathcal{T}$ , the random variable  $f(t, U)$  with  $U \sim \text{Uniform}(0, 1)$  has the same distribution as  $\delta(X)$  given  $T(X) = t$ . Define  $\delta^*(x, u) = f(T(x), u)$ .

For each  $t \in \mathcal{T}$ , by construction,

$$\int_0^1 L(\theta, f(t, u)) du = \mathbb{E}[L(\theta, \delta(X)) \mid T = t].$$

Therefore,

$$\begin{aligned} \mathcal{R}(\theta, \delta^*) &= \mathbb{E}_\theta \left[ \int_0^1 L(\theta, f(T(X), u)) du \right] \\ &= \mathbb{E}_\theta \left[ \mathbb{E}[L(\theta, \delta(X)) \mid T] \right] \\ &= \mathbb{E}_\theta [L(\theta, \delta(X))] = \mathcal{R}(\theta, \delta). \end{aligned} \quad \square$$

Together, the Rao-Blackwell theorems can be summarized as follows. For convex losses, deterministic conditioning on a sufficient statistic improves performance. For general losses, a sufficient statistic combined with randomization based on the conditional distribution attains equally good performance. Sufficiency means all decision-relevant information is contained in  $T$ .

### 1.3.2 Comparing decision problems

Now that the key infrastructure of statistical decision theory is in place, we are able to formalize several fundamental questions.

1. **Comparing decision rules:** Given a model  $\mathcal{P}$  and loss function  $L$ , which decision rule  $\delta$  has the ‘best’ risk function  $\mathcal{R}(\theta, \delta)$ ?
2. **Comparing loss functions:** For a given model  $\mathcal{P}$ , how does the choice of loss function  $L$  affect which decision rules are optimal?
3. **Comparing models:** Given models  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  and  $\mathcal{Q} = \{Q_\theta : \theta \in \Theta\}$ , a decision space  $(\mathcal{D}, \mathcal{D})$  and loss function  $L : \Theta \times \mathcal{D} \rightarrow \mathbb{R}$ , how does the choice of model  $\mathcal{P}$  (or  $\mathcal{Q}$ ) affect inference?

We will do an in-depth study of each of these questions in this course in the order of the list above. To give a flavor, we now preview each of these questions in turn.

#### Comparing decision rules

Given a statistical model  $\mathcal{P}$  and a loss function  $L$ , we seek to identify decision rules with small risk. Ideally, we would find a rule  $\delta^*$  with *uniformly minimum risk*:

$$\mathcal{R}(\theta, \delta^*) \leq \mathcal{R}(\theta, \delta) \quad \text{for all } \theta \in \Theta \text{ and all decision rules } \delta.$$

It turns out that uniformly optimal rules rarely exist (see Exercise 1.15). Given that a uniformly optimal rule does not exist, the question “which rule has the best risk function?” is ill-posed. We must refine our criterion for comparing decision rules. In these notes, we will consider two main strategies:

1. **Global risk comparisons.** Compare rules based on summaries of their entire risk function:

- *Admissibility:* Eliminate rules that are uniformly dominated by another rule.
- *Bayes risk:* Average the risk over  $\theta \in \Theta$  with respect to a prior distribution (‘weighing’ the risk across the parameter space).
- *Minimax risk:* Find the best rule with respect to the worst-case risk; i.e.  $\delta^*$  such that

$$\sup_{\theta \in \Theta} \mathcal{R}(\theta, \delta^*) = \inf_{\delta \in \mathcal{C}} \sup_{\theta \in \Theta} \mathcal{R}(\theta, \delta). \quad (1.5)$$

where  $\mathcal{C}$  is the class of all decision rules.

2. **Restricted decision rules.** Impose additional structure or constraints:

- *Unbiasedness:* Require for example that  $\mathbb{E}_{P_\theta}[\delta(X)] = \theta$  for estimation problems.
- *Invariance:* Require decision rules to respect symmetries in the problem (e.g. translation invariance for location parameters, or invariant to scale: unit of measurement does not matter).
- *Level constraints:* For testing, consider tests with Type I error rate at most  $\alpha$  and find the most powerful test within this class.

These approaches are not mutually exclusive. In some problems, the best unbiased estimator coincides with a Bayes rule, or the minimax rule can be found within the class of invariant procedures. In other cases, we will see that we have to choose between being e.g. minimax or unbiased. There is a deep connection between admissibility and Bayes’ risk which we will explore in Chapter 4. In many problems, the best unbiased estimator coincides with a Bayes rule, or the minimax rule can be found within the class of invariant procedures. Understanding these connections is a central goal of this course.

## Comparing loss functions

Once we have a deepened understanding of optimal decision rules given statistical model, a decision space and a loss function, we can start to compare different loss functions and see how they affect the optimal decision rules. Different loss functions

encode different priorities: squared error loss heavily penalizes large errors and leads to estimators sensitive to outliers; absolute error loss treats all errors more equally and yields more robust estimators; zero-one loss distinguishes only between correct and incorrect decisions, ignoring the magnitude of errors entirely.

We will see that the quality of an inference depends fundamentally on the chosen loss function; what constitutes an optimal decision rule changes as the loss function changes. A decision rule that is optimal for one loss function may not be optimal for another. Understanding the interplay between loss function and model allows us to reflect on the consequences of errors in specific applications. A medical diagnostic test, a financial trading algorithm, and a scientific hypothesis test may all involve the same statistical model but call for different loss functions.

In some cases, it makes sense to study a model for a collection of loss functions. These considerations will not be the main focus of this course, but we will touch upon them here and there.

### Comparing models

After we have a deepened understanding of performance ‘within’ the context of a given statistical model, a decision space and loss function(s), we can revisit the question posed at the end of Section 1.1 (see Example 1.4): which model is the right one? The concept of sufficiency introduced in Section 1.2 allows us to say when models are effectively the *same for all intents and purposes*. However, in many cases of practical interest, we are interested in comparing models that are vastly different, and knowing which is better for a particular task at hand.

Given a parameter space  $\Theta$ , a decision space  $\mathcal{D}$  and a loss function  $L : \Theta \times \mathcal{D} \rightarrow \mathbb{R}$ , consider two models

$$\begin{aligned} \mathcal{P} &= \{P_\theta : \theta \in \Theta\} \quad \text{with each } P_\theta \text{ defined on sample space } (\mathcal{X}, \mathcal{X}) \\ \text{and } \mathcal{Q} &= \{Q_\theta : \theta \in \Theta\} \quad \text{with each } Q_\theta \text{ defined on sample space } (\mathcal{Y}, \mathcal{Y}). \end{aligned}$$

The parameter space  $\Theta$ , which represents the phenomenon of interest, is the same for both models. The distributions  $P_\theta$  and  $Q_\theta$  could be different. Their sample spaces  $(\mathcal{X}, \mathcal{X})$  and  $(\mathcal{Y}, \mathcal{Y})$  could be vastly different. When the two models are observationally equivalent, we expect there not to be any difference in terms of inference. But when they are not, how do we decide which model is “better”? Or more generally, how do we quantify how much information is lost by choosing one model over the other?

Le Cam and Yang 1986 gives the following example:

**Example 1.45** (Estimating the half-life of Carbon 14). A physicist wants to estimate the half-life of Carbon 14, assuming the lifetime of a  $C^{14}$  atom follows an exponential

distribution with rate parameter  $\theta > 0$ . To do so, the physicist considers two possible experimental designs.

In the first setup, the physicist takes a sample of  $n$  atoms and observes the number of disintegrations  $x \in \mathbb{N}_0$  over a fixed time period of 2 hours. Under this model,  $P_\theta = \text{Poisson}(2n(1 - e^{-2\theta}))$ : the distribution of the count in fixed time. This defines the statistical experiment  $\mathcal{P} = \{P_\theta : \theta \in (0, \infty)\}$ , where  $P_\theta$  is defined on the sample space of non-negative integers.

In the second setup, the physicist observes the waiting time  $y \geq 0$  until a fixed number of disintegrations, say  $m = 10^6$ , occurs. Here,  $Q_\theta = \text{Gamma}(m, \theta)$ , defining another experiment  $\mathcal{Q} = \{Q_\theta : \theta \in (0, \infty)\}$ , with  $Q_\theta$  on the positive real line. Which setup is more informative? Explore this further in Exercise 1.9.  $\diamond$

Given a loss function  $L : \Theta \times \mathcal{D} \rightarrow \mathbb{R}$ , we could compare best possible performance of the two models. We could find for example that one model has a strictly better performance in terms of minimax risk:

$$\inf_{\delta} \sup_{\theta \in \Theta} \mathbb{E}_{P_\theta}[L(\theta, \delta(X))] = \inf_{\delta} \sup_{\theta \in \Theta} \mathbb{E}_{Q_\theta}[L(\theta, \delta(Y))] + \epsilon$$

for some  $\epsilon > 0$ , which means that the model  $\mathcal{P}$  is ‘ $\epsilon$ -deficient’ for the loss function  $L$  compared to the model  $\mathcal{Q}$  in terms of its best worst-case performance. We could even go a step further and compare the best worst-case performance of the two models with respect to a large collection of loss functions, to see if the one model is deficient across loss functions compared to the other. In other cases, we might find that two models with different sample spaces and distributions lead to exactly the same best possible performance. Sometimes, we might find that this to be true for all loss functions.

The above notion of deficiency allows us to think about situations where models are *not* observationally equivalent: given that a statistic is not sufficient for a model, how much information is lost? Note that being ‘ $\epsilon$ -deficient’ might not mean that the model  $\mathcal{P}$  is ‘bad’; it might be the better model to work with for practical purposes. Finding its deficiency with respect to another model is a way to quantify how much information is lost when approximating one model by something that is perhaps more tractable, or more affordable in terms of experimental design.

This line of thinking extends to perhaps the most powerful theoretical tool developed in Part II: The ability to compare models asymptotically. Under certain regularity conditions, complicated models can be shown to ‘tend asymptotically’ —in various precise senses—to much simpler experiments whose performance is well understood. This allows us to reason about performance in complicated models by reasoning about performance in simpler models, enabling meaningful analysis of performance that would otherwise be intractable.

Lastly, another reason to compare models is *misspecification*. We might want to know how robust decision procedure is if in reality, the model  $\mathcal{Q}$  is the correct one, but we are using the model  $\mathcal{P}$  to make decisions.

### 1.3.3 ♠ Why (Expected) Loss?

One might reasonably ask: why focus on expected loss rather than, say, the median loss, or some quantile of the loss distribution, or the maximum loss? And why consider loss functions at all?

Suppose that if  $\theta$  were known, you could provide a preference ordering over possible decisions in  $\mathcal{D}$ . We write  $d_1 \leq d_2$  if we prefer decision  $d_1$  to decision  $d_2$  (or are indifferent between them) when the true parameter is  $\theta$ . For instance, in hypothesis testing with  $\theta \in \Theta_0$ , we would prefer deciding  $H_0$  over deciding  $H_1$ . In estimation, we typically prefer decisions closer to the true value of the estimand  $g(\theta)$ .

These preferences naturally extend to randomized decisions. Consider now a comparison between two randomized decision rules: We write  $\delta_1 \leq \delta_2$  if we prefer (or are indifferent to) the randomized decision rule  $\delta_1$  over  $\delta_2$ .

**A1 (Transitivity):** If  $\delta_1 \leq \delta_2$  and  $\delta_2 \leq \delta_3$ , then  $\delta_1 \leq \delta_3$ .

**A2 (Independence):** If  $\delta_1 \leq \delta_2$ , then

$$\lambda\delta_1 + (1 - \lambda)\delta_3 \leq \lambda\delta_2 + (1 - \lambda)\delta_3 \quad \text{for all } \lambda \in (0, 1], \delta_3.$$

**A3 (Continuity):** If  $\delta_1 < \delta_2 < \delta_3$ , then there exist  $\lambda_a, \lambda_b \in (0, 1)$  such that

$$\lambda_a\delta_1 + (1 - \lambda_a)\delta_3 \leq \delta_2 \leq \lambda_b\delta_1 + (1 - \lambda_b)\delta_3.$$

The first axiom says that if we prefer  $\delta_2$  over  $\delta_1$  and  $\delta_3$  over  $\delta_2$ , then we should also prefer  $\delta_3$  over  $\delta_1$ . This makes the comparison  $\leq$  a partial order on the space of decision rules. The second axiom says that mixing between decision rules in an irrelevant alternative should not reverse preferences. The third axiom says there is no decision rule that is infinitely preferable to another; every decision rule can be made comparable through appropriate randomization. We will skip the philosophical discussion of why these axioms could be considered ‘rational’.

These axioms are enough to guarantee that our preferences over the decision space can be represented by risk in the sense of Definition 1.38: there exists a loss function such that the corresponding risk function captures our preferences.

**Theorem 1.46** (Representation Theorem). *If the space of decision rules equipped with the comparison  $\leq$  satisfies axioms A1, A2 and A3, then there exists a measurable*

function  $L : \Theta \times \mathcal{D} \rightarrow [-\infty, \infty]$  such that

$$\delta_1 \leq \delta_2 \iff \mathcal{R}(\theta, \delta_1) \leq \mathcal{R}(\theta, \delta_2).$$

See Ferguson 1967 for a proof. In words, if our preferences over the decision space are rational in this sense, then they can be represented by minimizing expected loss for some loss function  $L$ .

## Exercises

*Exercise 1.1.* Consider an experiment in which we observe  $Y = \mu + \epsilon$ , where  $\mu \in \mathbb{R}^d$  is an unknown vector and  $\epsilon \sim N_d(0, \sigma^2 I_d)$  is independent noise with unknown  $\sigma > 0$ .

1. Write down a corresponding statistical model and verify that the set  $\Theta := \mathbb{R}^d \times (0, \infty)$  is identifiable under an appropriate parameterization.
2. Suppose we instead believe  $\mu$  lies on a ray through the origin:  $\mu = \alpha v$  for some unknown  $\alpha \in \mathbb{R}$  and direction  $v \in S^{d-1}$  in the unit sphere. Consider the statistical model  $\{N_d(\alpha v, \sigma^2 I_d) : \alpha \in \mathbb{R}, v \in S^{d-1}, \sigma > 0\}$  and the set  $\Theta_{\text{ray}} := \mathbb{R} \times S^{d-1} \times (0, \infty)$ .

Is there a parameterization  $\vartheta : \mathcal{P}_{\text{ray}} \rightarrow \Theta_{\text{ray}}$  such that for every  $P \in \mathcal{P}_{\text{ray}}$  with  $\vartheta(P) = (\alpha, v, \sigma)$  we have  $P = N_d(\alpha v, \sigma^2 I_d)$ ? If not, give a subset  $\Theta'_{\text{ray}} \subseteq \Theta_{\text{ray}}$  for which such a parameterization exists and is identifiable.

*Exercise 1.2.* In Example 1.2, show that the observable  $L$  (whether the first die is larger than the second) is not  $\sigma(S)$ -measurable. What is the smallest sigma-algebra containing  $\sigma(S)$  that makes  $L$  measurable?

*Exercise 1.3.* Consider  $\mathcal{X} = \mathbb{R}$ ,  $\mathcal{X} = \mathcal{B}(\mathbb{R})$ , and the model

$$\mathcal{P} = \left\{ \frac{1}{2}N(\theta_1, 1) + \frac{1}{2}N(\theta_2, 1) : (\theta_1, \theta_2) \in \mathbb{R}^2 \right\}.$$

- (a) Can we take the inverse of the indexing map  $(\theta_1, \theta_2) \mapsto P_{\theta_1, \theta_2}$  (as a well defined map) onto  $\mathbb{R}^2$  to obtain a valid parameter space for  $\mathcal{P}$ ?
- (b) Show that  $\Theta_{\leq} := \{(\theta_1, \theta_2) \in \mathbb{R}^2 : \theta_1 \leq \theta_2\}$  is a valid parameter space under the map  $\frac{1}{2}N(\theta_1, 1) + \frac{1}{2}N(\theta_2, 1) \mapsto (\theta_1, \theta_2)$  and that the induced parameterization is identifiable in the sense of Definition 1.5.

*Exercise 1.4.* Let  $x, z \in \mathbb{R}^n$  and consider statistical model  $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), \mathcal{P})$  where  $\mathcal{P} = \{P_{\alpha, \beta} : \alpha, \beta \in \mathbb{R}\}$  and  $P_{\alpha, \beta}$  is the multivariate normal distribution with mean  $\alpha x + \beta z$  and variance  $I_n$ . Find a sufficient condition on  $x$  and  $z$  and an explicit parameterization (a map from  $\mathcal{P}$  to  $\mathbb{R}^2$ ) that makes the model  $\mathcal{P}$  identifiable with  $\Theta = \mathbb{R}^2$ .

*Exercise 1.5.* Revisiting Example 1.13, prove that the sum  $S$  is not sufficient in Model 1 but is sufficient in Model 2. Specifically:

- (a) In Model 1 (nonparametric), show that the conditional distribution of the outcome given  $S = 7$  depends on the unknown distribution  $p$ .

- (b) In Model 2, use the definition of sufficiency (or the Factorization Theorem) to prove that  $S$  is sufficient for  $p_\theta$ .

*Exercise 1.6.* Verify the claims in Example 1.16.

- (a) Show that if  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$ , then  $\bar{X} \sim N(\mu, \sigma^2/n)$ .
- (b) Show that if  $Y \sim N(\mu, \sigma^2/n)$  and  $Z_1, \dots, Z_n \stackrel{\text{iid}}{\sim} N(0, \sigma^2)$  independent of  $Y$ , then the variables  $X_i = Y + Z_i - \bar{Z}$  are i.i.d.  $N(\mu, \sigma^2)$ .

*Exercise 1.7.* Verify the claims in Example 1.23. Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Uniform}(\theta, \theta + 1)$  for  $\theta \in \mathbb{R}$ .

1. Show that  $T = (X_{(1)}, X_{(n)})$  is minimal sufficient.
2. Show that  $T$  is not complete.

*Exercise 1.8.* Let  $\{P_\eta : \eta \in \Theta\}$ ,  $\Theta \subseteq \mathbb{R}^k$  be an exponential family with density  $p(x | \eta) = \exp\{\eta^\top T(x) - A(\eta)\}h(x)$  with respect to a  $\sigma$ -finite measure  $\mu$ .

1. Show that  $P_{\eta_1} = P_{\eta_2}$  if and only if  $(\eta_1 - \eta_2)^\top T(x)$  is constant  $\mu$ -a.e.
2. Conclude that  $P_\eta = P_{\eta'} \iff \eta = \eta'$  if and only if there do not exist distinct  $\eta_1, \eta_2 \in \Theta$  with  $(\eta_1 - \eta_2)^\top T(x)$  constant  $\mu$ -a.e.

*Exercise 1.9.* Revisiting Example 1.45, suppose we are interested in estimating the mean lifetime  $\tau = 1/\theta$ .

- (a) In the first setup, let  $X$  be the number of disintegrations in time  $t = 2$ . Show that the maximum likelihood estimator for  $\tau$  is  $\hat{\tau}_1 = \frac{-2}{\log(1 - X/(2n))}$ .
- (b) In the second setup, let  $Y$  be the time until  $m$  disintegrations. Show that the maximum likelihood estimator for  $\tau$  is  $\hat{\tau}_2 = Y/m$ .
- (c) Compare the variances of these two estimators (you may use a heuristic argument, considering what happens for  $m, n$  and  $\tau$ ). Which experiment seems more informative if we want to estimate  $\tau$ , particularly for large  $\tau$  (long lifetimes)?

*Exercise 1.10.* The *empirical distribution* of a sample  $X_1, \dots, X_n$  is given by  $\hat{P}$  satisfying

$$\hat{P}(A) = \sum_i \mathbf{1}(X_i \in A)/n$$

for all measurable sets  $A \subseteq \mathcal{X}$ . Suppose  $\mathcal{X} = \mathbb{R}$ .

- (a) Show that observing the empirical distribution  $\hat{P}$  is observationally equivalent to observing the sample cumulative distribution function

$$\hat{F}(x) = \sum_i \mathbf{1}(X_i \leq x)/n.$$

- (b) Show that observing the empirical distribution is observationally equivalent to observing the order statistics  $(X_{(1)}, \dots, X_{(n)})$ .

*Exercise 1.11.* Consider the following **definition**: A model  $\mathcal{P}_n$  on a product space  $(\mathcal{X}^n, \mathcal{A}^n)$  is *exchangeable* if for all  $P_n \in \mathcal{P}_n$ , sets  $A_1 \in \mathcal{A}, \dots, A_n \in \mathcal{A}$ , and permutation  $\pi$  of  $\{1, \dots, n\}$ ,

$$P_n(A_1 \times \dots \times A_n) = P_n(A_{\pi_1} \times \dots \times A_{\pi_n}).$$

Let  $\mathcal{P}_n$  be an exchangeable model on  $(\mathcal{X}^n, \mathcal{A}^n)$ , where  $\mathcal{X}$  is a finite set. Prove that the empirical distribution  $\hat{P}_n$ , defined by  $\hat{P}_n(A) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}_A(X_i)$ , is a sufficient statistic.

*Exercise 1.12.* Consider the statistical model  $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n), \mathcal{P})$  where  $\mathcal{P} = \{P_f : f \in \Theta\}$  and  $\Theta \subseteq L_2[0, 1]$  (see Definition B.25) is such that  $Y = (Y_1, \dots, Y_n) \sim P_f$  satisfies

$$Y_i = f(i/n) + \epsilon_i, \quad i = 1, \dots, n,$$

for  $f \in \Theta$  and  $\epsilon_1, \dots, \epsilon_n \stackrel{\text{iid}}{\sim} N(0, 1)$ .

- (a) Is the map  $\vartheta : \Theta \rightarrow \mathcal{P}, f \mapsto P_f$  injective?
- (b) Consider instead  $\Theta$  equal to the space  $L_2([0, 1], \mathcal{B}[0, 1], \mathbb{P}_n)$  where the measure  $\mathbb{P}_n : \mathcal{B}[0, 1] \rightarrow [0, 1]$  is to be understood as

$$\mathbb{P}_n(A) = \frac{|\{i \in \{1, \dots, n\} : i/n \in A\}|}{n}.$$

Show that this makes the previous map injective and provide a map from  $\mathcal{P}$  to  $\Theta$  that makes the parameterization identifiable.

*Exercise 1.13.* Let  $T$  be a sufficient statistic for the model  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ . Show that if  $h(X)$  is any bounded measurable function that does not depend on  $\theta$ , then the conditional expectation  $\mathbb{E}_\theta[h(X) | T]$  admits a version that does not depend on  $\theta$ .

*Hint: Use the definition of conditional expectation and the fact that  $T$  is sufficient and use the standard machine of measure theory (Appendix B Section B.2.1).*

*Exercise 1.14* (Deterministic and randomized tests). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Poisson}(\theta)$  with  $\theta > 0$  unknown, and consider testing  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta > \theta_0$ . The decision space is  $\mathcal{D} = \{0, 1\}$ , where  $d = 1$  means “reject  $H_0$ ”. A deterministic test is

$$\delta(x) = \mathbb{1}\{\sum_{i=1}^n x_i > c\}$$

for some threshold  $c \in \mathbb{N}$ .

1. Show that there may be no  $c$  such that  $P_{\theta_0}(\sum_{i=1}^n X_i > c) = \alpha$  for a given significance level  $\alpha$ .
2. Consider the randomized test

$$\delta(x, u) = \begin{cases} 1 & \text{if } \sum_{i=1}^n x_i > c, \\ \mathbb{1}\{u \leq \gamma\} & \text{if } \sum_{i=1}^n x_i = c, \\ 0 & \text{if } \sum_{i=1}^n x_i < c. \end{cases}$$

Show that  $c \in \mathbb{N}$  and  $\gamma \in [0, 1]$  can be chosen such that  $E_{\theta_0}[\delta(X, U)] = \alpha$ .

*Exercise 1.15* (Nonexistence of uniformly optimal rules). Consider the statistical model corresponding to  $X \sim P_\theta$  where  $P_{\theta_0} = N(0, 1)$  and  $P_{\theta_1} = N(1, 1)$  and let  $\Delta$  denote the set of all (possibly randomized) decision rules. Define the *risk set*

$$\mathcal{R} = \{(R(\theta_0, \delta), R(\theta_1, \delta)) : \delta \in \Delta\} \subseteq \mathbb{R}^2.$$

1. Consider estimating  $\theta$  under squared error loss. Compute the risk pair for:
  - (a) the estimator  $\delta_0(X) = 0$ ,
  - (b) the estimator  $\delta_1(X) = 1$ ,
  - (c) the estimator  $\delta_{1/2}(X) = 1/2$ .
  - (d) the estimator  $\delta(X) = X$ .

Which of these decision rules do you prefer? Can you think of a rule that is better than all of them?

2. A decision rule  $\delta^*$  is *uniformly optimal* if  $(R(\theta_0, \delta^*), R(\theta_1, \delta^*))$  is componentwise smaller than or equal to  $(R(\theta_0, \delta), R(\theta_1, \delta))$  for all  $\delta \in \Delta$ . Using the risk pairs (specifically,  $\delta_0$  and  $\delta_1$ ), argue that no uniformly optimal rule exists.

*Exercise 1.16* (♠). Consider an experiment of flipping a coin infinitely many times.

- (a) What should the sample space  $\mathcal{X}$  be? What is its cardinality?

- (b) What sigma-algebra  $\mathcal{X}$  would naturally represent the observable events (e.g., "the  $n$ -th flip is heads")?
- (c) Explain why it is impossible to define a countably additive probability measure on  $(\mathcal{X}, 2^{\mathcal{X}})$  that consistently assigns probabilities to cylinder sets  $C_n = \{x \in \mathcal{X} : x_n = 1\}$  as if the coin flips were independent.

*Hint: Consider what happens if all singleton sets have probability zero versus positive probability.*

*Exercise 1.17* ( $\spadesuit$  Empirical distribution equivalence). Let  $(\mathcal{X}, \mathcal{X}) = (\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$  and consider the i.i.d. model

$$\mathcal{P} = \{P^{\otimes n} : P \in \Theta\}, \quad \Theta := \mathcal{M}_1(\mathbb{R}),$$

where  $\mathcal{M}_1(\mathbb{R})$  denotes the set of all probability measures on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ . Equip  $\mathcal{M}_1(\mathbb{R})$  with the Borel  $\sigma$ -algebra generated by the total variation distance (see Definitions 2.2 and B.10 in the appendix).

For  $x = (x_1, \dots, x_n) \in \mathbb{R}^n$  define the *empirical measure*  $\hat{P}_x \in \mathcal{M}_1(\mathbb{R})$  by

$$\hat{P}_x(A) := \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{x_i \in A\}, \quad A \in \mathcal{B}(\mathbb{R}).$$

Let  $\mathcal{C}$  denote the set of all cumulative distribution functions (c.d.f.'s), and equip  $\mathcal{C}$  with the Borel  $\sigma$ -algebra generated by the sup-norm on  $\mathcal{C}$ , and define the *empirical c.d.f.*  $\hat{F}_x \in \mathcal{C}$  by

$$\hat{F}_x(t) := \hat{P}_x((-\infty, t]) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{x_i \leq t\}, \quad t \in \mathbb{R}.$$

Lastly, consider the order statistics  $T(X) = (X_{(1)}, \dots, X_{(n)})$  as a  $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$  valued statistic.

- (a) Show that  $\sigma(\hat{P}) = \sigma(\hat{F}) = \sigma(T)$ .
- (b) Show that the order statistics are complete.
- (c) Conclude that  $\hat{P}$  and  $\hat{F}$  are complete sufficient statistics for  $\mathcal{P}$ .

## 2 Point Estimation

In this chapter, we study the problem of *estimation*: constructing a decision rule that approximates an unknown parameter or functional of the parameter based on observed data. Recall from Chapter 1 that a statistical model is a family of probability distributions  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  indexed by a parameter  $\theta$  in a parameter space  $\Theta$ . Often, we wish to estimate either the parameter  $\theta$  itself or a functional of it,  $\theta \mapsto \phi(\theta)$ . An *estimator* is a decision rule  $\delta : \mathcal{X} \rightarrow \phi(\Theta)$  that maps the observed data  $X$  to an estimate  $\delta(X)$  of the target quantity. This means our decision space is the same as our parameter space (or a function thereof,  $\phi(\Theta)$ ).

The central questions of this chapter are: what makes an estimator good, and how do we construct estimators with desirable properties? And how do we compare estimators? Intuitively, good performance means that when we observe data  $X \sim P_\theta$ , the estimator  $\delta(X)$  is “close” to the true value  $\phi(\theta)$ . To formalize this, we could equip the target space  $\phi(\Theta)$  with a metric distance  $\mathbf{d}$  and define the loss as a function in terms of this distance, for example  $L(\delta(X), \theta) = \mathbf{d}(\delta(X), \phi(\theta))^2$ . In this sense, specifying the functional  $\phi$  is part of specifying the loss and the decision space: it fixes what quantity the estimator is judged against, and hence what counts as estimation error. Taking the Borel  $\sigma$ -algebra on  $\phi(\Theta)$  induced by  $\mathbf{d}$  ensures that loss functions and estimators can be defined as measurable functions. In the common setting where  $\phi(\Theta) \subseteq \mathbb{R}^k$ , the Euclidean metric is a natural choice.

**Example 2.1** (Estimation (and prediction) in a linear model). Suppose we observe a random vector  $Y$  in  $\mathbb{R}^n$  generated from the linear model

$$\mathcal{P} = \{N_d(X\beta, \sigma^2 I_n) : (\beta, \sigma^2) \in \Theta\},$$

with fixed design  $X \in \mathbb{R}^{n \times p}$  (with  $X^\top X$  invertible) and parameter space  $\Theta = \mathbb{R}^p \times (0, \infty)$ . If we wish to estimate  $\phi(\theta) = \beta$ , an estimator is any decision rule  $\delta : \mathbb{R}^n \rightarrow \mathbb{R}^p$ , e.g.

$$\delta(Y) := (X^\top X)^{-1} X^\top Y.$$

A sensible loss function is the squared Euclidean distance:

$$L((\beta, \sigma^2), \delta) = \|\delta - \beta\|^2.$$

If instead we wish to predict the mean response at a known new covariate  $x_{\text{new}} \in \mathbb{R}^p$ , the target is the functional  $\phi(\theta) = x_{\text{new}}^\top \beta \in \mathbb{R}$ . That means that our decision space is

$\mathbb{R}$ , and as a loss function, we could consider

$$L((\beta, \sigma^2), \delta) = |\delta - x_{\text{new}}^\top \beta|.$$

◇

However, estimation problems sometimes involve more abstract target spaces. For example, the target of estimation could be itself the probability distribution generating the data — i.e.  $\phi(\theta) = P_\theta$ . In this case, the loss function could be a metric on the space of probability measures. A possible choice for such a metric is the total variation distance.

**Definition 2.2.** The *total variation distance* between two probability measures  $P$  and  $Q$  on a measurable space  $(\mathcal{X}, \mathcal{X})$  is defined as

$$\mathbf{d}_{TV}(P, Q) = \sup_{A \in \mathcal{X}} |P(A) - Q(A)|.$$

The total variation metric allows us to study the parameter space where  $\Theta$  is (a subset of) the space of probability measures, equipped with the Borel sigma-algebra of the total variation metric. Given a statistical model  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ , we could take  $\phi$  to be the map  $\theta \mapsto P_\theta$  and the loss function to be the total variation distance:

$$L(\delta(X), \theta) = \mathbf{d}_{TV}(\delta(X), P_\theta).$$

For some models, various losses can be related to each other in a simple way. In other cases, they do not. For example, when  $P_\theta \mapsto \phi(\theta)$  does not identify the model, we cannot generally hope that estimating the functional  $\phi(\theta)$  allows for an estimate of  $P_\theta$ . The example below illustrates that in estimation problems, we are often not trying to estimate the entire distribution  $P_\theta$ , but rather a lower-dimensional summary such as the mean, variance, or quantile, depending on what we are interested in. Only in special cases, these lower-dimensional summaries translate back to the data generating process.

**Example 2.3** (Estimating a functional vs. the distribution). We revisit Example 1.4 from Chapter 1. Consider two statistical models on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ :

- (i)  $\mathcal{P} = \{P_\theta := N(\theta, 1) : \theta \in \mathbb{R}\}$ .
- (ii)  $\mathcal{Q} = \{\text{all probability measures on } (\mathbb{R}, \mathcal{B}(\mathbb{R})) \text{ with variance at most } 1\}$ .

For the model  $\mathcal{P}$ , it can be shown (see Exercise 2.18) that the total variation

distance is bounded by the distance between the means for  $\theta, \theta' \in \mathbb{R}$ :

$$d_{TV}(P_\theta, P_{\theta'}) \leq \frac{1}{2}|\theta - \theta'|.$$

This implies that estimating the parameter  $\theta$  well (in Euclidean distance) automatically ensures that we estimate the distribution  $P_\theta$  well (in total variation distance).

For the model  $\mathcal{Q}$ , the mean parameter  $\phi : Q \mapsto \int x dQ(x)$  does not identify the distribution in the sense of Definition 1.5. Estimating the mean  $\phi(Q) = \int x dQ(x)$  is still almost equally ‘doable’ as in the case of normals (we will see this in Example 2.51). However, estimating the distribution  $Q \in \mathcal{Q}$  itself turns out to be much more difficult: it is impossible to find a ‘good’ estimate of the distribution in total variation distance uniformly over  $\mathcal{Q}$ , even under repeated sampling (see Exercise 2.17). That is, for the model  $\mathcal{Q}$ , estimating the distribution  $Q \in \mathcal{Q}$  itself is a very different estimation problem compared to estimating  $\int x dQ(x)$ .  $\diamond$

This example also motivates a useful (informal) taxonomy of estimation problems. The labels *parametric*, *semiparametric*, and *nonparametric* are best thought of as describing the *complexity of the model in relation to the estimand*: the same model can lead to different types of problems depending on whether we aim to estimate a low-dimensional functional (like a mean) or a high/infinite-dimensional object (like an entire distribution).

- **Parametric estimation:** the model is indexed by a *finite-dimensional* parameter, typically  $\Theta \subseteq \mathbb{R}^d$  with fixed  $d$ , and the data-generating distribution is fully determined (up to  $\theta$ ). In Example 2.3(i),  $\mathcal{P} = \{N(\theta, 1) : \theta \in \mathbb{R}\}$  is a one-dimensional parametric model. In such settings, estimating  $\theta$  is often closely related to estimating  $P_\theta$  itself because the parameter identifies the distribution (and here even controls it in total variation).
- **Semiparametric estimation:** the model is *infinite-dimensional*, but the target  $\phi(\theta)$  is *finite-dimensional* (typically in  $\mathbb{R}^k$  for fixed  $k$ ). The remaining aspects of the distribution act as an infinite-dimensional *nuisance*. In Example 2.3(ii), if the goal is only to estimate the mean functional  $g(Q) = \int x dQ(x) \in \mathbb{R}$ , then we are in this regime: many different  $Q \in \mathcal{Q}$  share the same mean, yet the target itself is one-dimensional.
- **Nonparametric estimation:** the model is *infinite-dimensional* (e.g. a large class of distributions, densities, regression functions, etc.), and the target is typically itself an *infinite-dimensional object* such as the distribution  $P$ , its CDF, or its density. In Example 2.3(ii), if the goal is to estimate  $Q \in \mathcal{Q}$  (as a distribution), then this is a nonparametric estimation problem.

The example above illustrates that the labels *parametric*, *semiparametric*, and *nonparametric* are best understood as describing an *estimation problem*—in particular, the target  $g(\theta)$  and the loss function—and not only the “size” or complexity of the model class. Moreover, these labels are only *loose distinctions*: different statistics books (and different subfields) use them in slightly different and sometimes inconsistent ways.

There is also a fourth, even less sharply defined regime that we will encounter throughout the chapter: *high-dimensional* estimation problems, where the parameter is technically finite-dimensional (e.g.  $\Theta \subseteq \mathbb{R}^d$ ), but the dimension  $d$  is large relative to the other relevant aspects of the problem (such as the sample size  $n$ ) in a way that drastically changes which decision rules are reasonable. In this sense, high-dimensional problems often behave more like nonparametric problems than classical parametric ones, despite having a finite-dimensional parameter space. We return to this theme in Section 2.3.

Returning to the central question of this chapter: given a statistical model  $\mathcal{P}$ , a target quantity  $\phi(\theta)$  and a loss function  $L$ , what is a good estimator for  $\phi(\theta)$ ? For typical loss functions (e.g. if  $L$  is related to some distance metric) and a fixed  $\theta$ , we might observe that if we knew  $P_\theta$ , the “best estimator” would simply be the constant function  $\delta(x) = \phi(\theta)$  for all  $x$ . This estimator is measurable and achieves zero loss if  $\theta$  is the parameter underlying the data-generating process. However, since inference of  $\theta$  is the whole point, this is not a sensible estimator. The challenge of formulating what is ‘a good estimator’ is to construct a data-dependent rule that ‘performs well across the parameter space’. There are multiple criteria for measuring what ‘performance across the parameter space’ means, which we explore throughout this chapter.

## 2.1 Unbiasedness

Throughout this section, we consider a statistical model  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  and a target quantity  $\phi : \Theta \rightarrow \mathbb{R}^k$ . We will study estimators of  $\phi(\theta)$  satisfying the following property.

**Definition 2.4** (Unbiasedness). An estimator  $\delta : \mathcal{X} \rightarrow \mathbb{R}^k$  is an *unbiased estimator* of  $\phi(\theta)$  if for all  $\theta \in \Theta$ ,

$$\mathbb{E}_\theta[\delta(X)] = \phi(\theta).$$

Unbiasedness is an appealing property: on average, the estimator produces the correct value. If we, or others, were to repeat the experiment many times, the average of the estimates would converge to the true parameter value.

**Example 2.5** (Averaging i.i.d. estimators). Suppose we have  $m$  independent replications of a study, yielding estimators  $\delta_1, \dots, \delta_m$  of a parameter  $\theta \in \mathbb{R}$ . Assume these

are independent and identically distributed with unit variance (i.e.,  $\text{Var}(\delta_j) = 1$ ). A natural estimator is the average:

$$\delta(X) = \frac{1}{m} \sum_{j=1}^m \delta_j.$$

If the individual estimators are unbiased, then  $\delta(X)$  converges to  $\theta$  over repeat replications. However, if there is systematic bias ( $\mathbb{E}[\delta_j] \neq \theta$ ), the convergence fails. See Exercise 2.5.  $\diamond$

However, it does not guarantee that any single estimate is close to the true parameter. A large variance implies that the estimator fluctuates significantly, making individual estimates unreliable. By minimizing variance, we maximize the probability that the estimator is close to the target  $\phi(\theta)$ .

**Definition 2.6.** Let  $X$  and  $Y$  be random vectors in  $\mathbb{R}^k$  and  $\mathbb{R}^m$ , respectively, with means  $\mu_X = \mathbb{E}[X]$  and  $\mu_Y = \mathbb{E}[Y]$ . The *covariance matrix* of  $X$  and  $Y$  is the  $k \times m$  matrix defined by

$$\text{Cov}(X, Y) = \mathbb{E}[(X - \mu_X)(Y - \mu_Y)^\top].$$

The *variance matrix* (or simply variance) of a random vector  $X \in \mathbb{R}^k$  is the  $k \times k$  covariance matrix of  $X$  with itself:

$$\text{Var}(X) = \text{Cov}(X, X) = \mathbb{E}[(X - \mu_X)(X - \mu_X)^\top].$$

For the Euclidean metric, it turns out that minimizing the variance across all unbiased estimators is equivalent to minimizing the expected squared error of the estimator.

**Lemma 2.7** (Bias-Variance Decomposition). *Let  $\delta(X)$  be an estimator of  $\phi(\theta)$  with finite second moments. Then,*

$$\mathbb{E}_\theta \|\delta(X) - \phi(\theta)\|^2 = \|\mathbb{E}_\theta[\delta(X)] - \phi(\theta)\|^2 + \text{Trace}(\text{Var}_\theta(\delta(X))). \quad (2.1)$$

*Proof.* See Exercise 2.4.  $\square$

The first term in (2.1) is called the (squared) bias of the estimator, and the second term is the ‘variance term’. The lemma states that the expected squared error of any estimator is the sum of the squared bias and the variance. For unbiased estimators, (the trace of) the variance effectively measures the average squared Euclidean distance from the true parameter value. This is one of the reasons to compare unbiased estimators based on their variance. This leads us to the concept of a UMVUE.

**Definition 2.8.** An estimator  $\delta$  is a *uniformly minimum variance unbiased estimator (UMVUE)* of  $\phi(\theta)$  if it is unbiased, i.e.,  $\mathbb{E}_\theta[\delta(X)] = \phi(\theta)$  for all  $\theta \in \Theta$ , and if for any other unbiased estimator  $\delta'$ ,

$$\text{Var}_\theta(\delta(X)) \leq \text{Var}_\theta(\delta'(X)) \quad \text{for all } \theta \in \Theta.$$

For a formal definition of the matrix ordering  $\leq$  (the Loewner order), see Definition C.10 in Appendix C. The notation  $\text{Var}_\theta$  denotes the variance operator with respect to the expectation operator  $\mathbb{E}_\theta$ .

Finding a UMVUE is a challenging problem in general. However, for certain models, those where complete sufficient statistics exist, the UMVUE can be found using the following theorem.

**Theorem 2.9** (Lehmann-Scheffé). *Let  $T$  be a complete sufficient statistic for  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ . If  $\delta_0$  is any unbiased estimator of  $\phi(\theta)$  with finite variance, then  $\delta(X) = \mathbb{E}[\delta_0(X) | T(X)]$  is the a.s. unique UMVUE of  $\phi(\theta)$ .*

*Proof.* By sufficiency,  $\delta(X) = \mathbb{E}[\delta_0(X) | T]$  admits a version not depending on  $\theta$ , so it is a valid estimator. By the tower property,  $\mathbb{E}_\theta[\delta(X)] = \mathbb{E}_\theta[\delta_0(X)] = \phi(\theta)$ , so  $\delta$  is unbiased. For any  $v \in \mathbb{R}^k$ , the loss function  $L_v(\delta, \theta) = (v^\top(\delta - \phi(\theta)))^2$  is convex in  $\delta$ . By Rao-Blackwell (Theorem 1.43),

$$\mathbb{E}_\theta[(v^\top(\delta(X) - \phi(\theta)))^2] \leq \mathbb{E}_\theta[(v^\top(\delta_0(X) - \phi(\theta)))^2].$$

Since both estimators are unbiased, this gives

$$v^\top \text{Var}_\theta(\delta) v \leq v^\top \text{Var}_\theta(\delta_0) v \quad \text{for all } v \in \mathbb{R}^k,$$

i.e.,  $\text{Var}_\theta(\delta) \leq \text{Var}_\theta(\delta_0)$  in the positive semidefinite ordering.

Now suppose  $\delta'$  is any other unbiased estimator of  $\phi(\theta)$ . Define  $\psi(T) = \mathbb{E}[\delta'(X) | T] - \delta(X)$ . Then

$$\mathbb{E}_\theta[\psi(T)] = \phi(\theta) - \phi(\theta) = 0 \quad \text{for all } \theta \in \Theta.$$

By completeness,  $\psi(T) = 0$  almost surely, so  $\mathbb{E}[\delta'(X) | T] = \delta(X)$  almost surely. By Rao-Blackwell,  $\text{Var}_\theta(\delta) \leq \text{Var}_\theta(\delta')$ . Since  $\delta'$  was arbitrary,  $\delta$  is UMVUE.  $\square$

The Lehmann-Scheffé theorem provides a strategy for finding a unique, best unbiased estimator:

1. Start with an arbitrary unbiased estimator  $\delta_0$ ;
2. Find a complete sufficient statistic  $T$ ;

3. Apply the Rao-Blackwell theorem to obtain the UMVUE  $\delta(X) = \mathbb{E}[\delta_0(X) | T]$ . This is sometimes called ‘‘Rao-Blackwellization’’.

We illustrate the use of the Lehmann-Scheffé theorem with two examples below: estimating the CDF of a distribution at a fixed point in a parametric setting and in a semiparametric setting.

**Example 2.10** (Normal mean with known variance). Consider the model  $\mathcal{P} = \{N(\theta, \sigma^2)^{\otimes n} : \theta \in \mathbb{R}\}$ , corresponding to observing  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2) =: P_\theta$ , where  $\sigma^2 > 0$  is known. The sample mean  $\bar{X}$  is a complete sufficient statistic for  $\theta$  (see Example 1.16 combined with Proposition 1.29). Suppose we want to estimate the CDF at a point  $t \in \mathbb{R}$ , i.e.,  $\phi(\theta) = P_\theta((-\infty, t])$ . Consider the unbiased estimator  $\delta_0(X) = \mathbb{1}_{\{X_1 \leq t\}}$ . Since  $\bar{X}$  is complete sufficient, the UMVUE is given by  $\delta(X) = \mathbb{E}[\delta_0(X) | \bar{X}]$  by the Lehmann-Scheffé theorem.

We can compute the UMVUE explicitly (Exercise 2.2):

$$\delta(X) = \Phi\left(\sqrt{\frac{n}{n-1}} \frac{t - \bar{X}}{\sigma}\right).$$

◇

**Example 2.11** (Estimating the cumulative distribution function). Consider observing  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} P$ , where  $P$  is any probability distribution on  $\mathbb{R}$ . The corresponding statistical experiment is  $(\mathbb{R}^n, \mathcal{B}(\mathbb{R})^n, \mathcal{P}, \mathcal{P})$  where

$$\mathcal{P} = \{P : P \text{ is a probability distribution on } \mathbb{R}\}.$$

Given  $P \in \mathcal{P}$ , let  $F_P$  be the cumulative distribution function of  $P$ :  $F_P(t) = P((-\infty, t])$ . To estimate  $\phi(P) = F_P(t)$  at a fixed point  $t \in \mathbb{R}$ , a natural estimator is the empirical distribution function:

$$\delta(X) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{X_i \leq t\}}.$$

For a fixed  $t$ , the random variable  $Y_i = \mathbb{1}_{\{X_i \leq t\}}$  is Bernoulli distributed with parameter  $p = P(X_i \leq t) = F_P(t)$ . Thus,

$$\mathbb{E}_P[\delta(X)] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}_P[Y_i] = \frac{1}{n} \cdot n F_P(t) = F_P(t),$$

showing that  $\delta(X)$  is an unbiased estimator for  $F_P(t)$ . Its variance is given by

$$\text{Var}_P(\delta(X)) = \frac{1}{n^2} \sum_{i=1}^n \text{Var}_P(Y_i) = \frac{1}{n} F_P(t)(1 - F_P(t)).$$

By Exercise 1.17, the order statistics  $T(X) = (X_{(1)}, \dots, X_{(n)})$  are a complete sufficient statistic for this model. Furthermore,

$$\mathbb{E}_P \left[ \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{X_i \leq t\}} \mid T(X) \right] = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{X_i \leq t\}}.$$

Hence,  $\delta(X)$  is the UMVUE for  $\phi(P) = F_P(t)$  by the Lehmann-Scheffé theorem.  $\diamond$

Returning briefly to our earlier discussion concerning parametric vs semiparametric estimation problems, a further investigation the above examples reveal an important phenomenon: in both problems, it can be shown that the accuracy of the estimator is of the order  $1/\sqrt{n}$ : the rate as a function of the sample size at which we can expect the estimator to be accurate is the same. However, the (in both cases optimal!) variances differ between the two models (see Exercise 2.2). This is expected: the parametric model is more informative and allows us to estimate the parameter with more precision. In the semiparametric model, we are paying a price for the flexibility of the model; its infinite dimensional nature.

### 2.1.1 The Cramér-Rao lower bound

In some statistical models, a differentiable relationship between  $\Theta$  and  $\mathcal{P}$  allows us to derive fundamental limits on estimation accuracy for smooth functionals of the parameter. The key idea is that if the distribution  $P_\theta$  changes smoothly with  $\theta$ , we can quantify how much information the data carries about the parameter.

Consider a model  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  dominated by a measure  $\mu$  with densities  $p_\theta = dP_\theta/d\mu$ , where  $\Theta$  is an open subset of  $\mathbb{R}^d$ . If the map  $\theta \mapsto p_\theta(x)$  is differentiable for each  $x$ , we can define the *score function*

$$S_\theta(x) = \nabla_\theta \log p_\theta(x).$$

Under regularity conditions that permit interchanging differentiation and integration, the expected score is zero:  $\mathbb{E}_\theta[S_\theta(X)] = 0$ . The *Fisher information matrix* is then defined as the covariance of the score:

$$I(\theta) = \mathbb{E}_\theta[S_\theta(X)S_\theta(X)^\top],$$

which (under regularity conditions) can equivalently be computed as

$$I(\theta) = -\mathbb{E}_\theta[\nabla_\theta^2 \log p_\theta(X)].$$

The Cramér-Rao lower bound states that the variance of any unbiased estimator of  $g(\theta)$

is at least  $\nabla g(\theta)^\top I(\theta)^{-1} \nabla g(\theta)$ . This result is fundamental: it shows that estimation precision is governed by the Fisher information, which quantifies how sensitively the distribution responds to changes in  $\theta$ .

The classical approach requires verifying regularity conditions for each model—conditions that ensure differentiation under the integral sign is valid. It turns out that a weaker notion of differentiability “on average” suffices and leads to a cleaner and much more general theory. This is the concept of *differentiability in quadratic mean*.

**Definition 2.12** (Differentiability in Quadratic Mean). A statistical model  $\{P_\theta : \theta \in \Theta\}$  with densities  $p_\theta$  is *differentiable in quadratic mean (DQM)* at  $\theta$  if there exists a measurable function  $S_\theta : \mathcal{X} \rightarrow \mathbb{R}^d$  such that

$$\int \left( \sqrt{p_{\theta+h}(x)} - \sqrt{p_\theta(x)} - \frac{1}{2} h^\top S_\theta(x) \sqrt{p_\theta(x)} \right)^2 d\mu(x) = o(\|h\|^2) \quad \text{as } h \rightarrow 0.$$

DQM implies that the Fisher information matrix  $I(\theta) = \mathbb{E}_\theta[S_\theta(X)S_\theta(X)^\top]$  exists and roughly speaking allows for exchange of differentiation and integration. It effectively replaces the “standard” regularity conditions that we might be familiar with from e.g. undergraduate textbooks on statistics.

**Lemma 2.13.** *Let the model  $\{P_\theta : \theta \in \Theta\}$  be differentiable in quadratic mean at  $\theta$  with score  $S_\theta$ . Then:*

- (i) *The Fisher information  $I(\theta) = E_\theta[S_\theta S_\theta^\top]$  is well-defined with all entries finite.*
- (ii) *If  $T : \mathcal{X} \rightarrow \mathbb{R}$  is a measurable function with  $T^2$  uniformly integrable under  $\mathbb{E}_{\theta'}$  for all  $\theta'$  in a neighborhood of  $\theta$ , then  $\psi(\theta') = E_{\theta'}[T]$  is differentiable at  $\theta$  with*

$$\nabla \psi(\theta) = E_\theta[T \cdot S_\theta].$$

*Proof.* Exercise 2.8. □

The DQM condition allows us to differentiate expectations of statistics, which is key to establishing a fundamental limit on the variance of any unbiased estimator. This limit is determined by the Fisher information, quantifying the intuition that estimation is harder when the distribution  $P_\theta$  changes slowly with  $\theta$  (low information). This leads us to the famous Cramér-Rao Lower Bound.

**Theorem 2.14** (Cramér-Rao Lower Bound – Biased Case). *Consider a model  $\{P_\theta : \theta \in \Theta\}$  that is DQM at  $\theta \in \Theta$  with positive definite Fisher information matrix  $I(\theta)$ . Let  $\delta(X)$  be an  $\mathbb{R}^k$ -valued estimator that is uniformly square-integrable under  $P_{\theta'}$  for all  $\theta'$  in a neighborhood of  $\theta$  and write  $\psi(\theta) = \mathbb{E}_\theta[\delta(X)]$  for the expectation of the estimator.*

It holds that

$$\text{Var}_\theta(\delta(X)) \geq \nabla\psi(\theta)^\top I(\theta)^{-1} \nabla\psi(\theta).$$

*Proof.* By definition, we have  $\psi(\theta) = \mathbb{E}_\theta[\delta(X)] = \int \delta(x)p_\theta(x) d\mu(x)$ . Using Lemma 2.13, we have

$$\nabla\psi(\theta) = \mathbb{E}_\theta[\delta(X)S_\theta(X)],$$

and

$$\mathbb{E}_\theta[S_\theta(X)] = \mathbb{E}_\theta[1 \cdot S_\theta(X)] = \nabla 1 = 0.$$

Combining these, we obtain

$$\nabla\psi(\theta) = \text{Cov}_\theta(\delta(X), S_\theta(X)).$$

Now, for any constant vector  $a \in \mathbb{R}^d$ , consider the scalar random variable  $Z = a^\top S_\theta(X)$ . The covariance between  $\delta(X)$  and  $Z$  is

$$\text{Cov}_\theta(\delta(X), Z) = \text{Cov}_\theta(\delta(X), a^\top S_\theta(X)) = a^\top \text{Cov}_\theta(\delta(X), S_\theta(X)) = a^\top \nabla\psi(\theta).$$

Applying the Cauchy-Schwarz inequality to the covariance squared, we have

$$(\text{Cov}_\theta(\delta(X), Z))^2 \leq \text{Var}_\theta(\delta(X)) \text{Var}_\theta(Z).$$

Substituting the expressions for covariance and variance, noting that  $\text{Var}_\theta(Z) = \text{Var}_\theta(a^\top S_\theta(X)) = a^\top I(\theta)a$ , we get

$$(a^\top \nabla\psi(\theta))^2 \leq \text{Var}_\theta(\delta(X))(a^\top I(\theta)a).$$

This inequality holds for any vector  $a$ . To obtain the tightest bound, we choose  $a = I(\theta)^{-1} \nabla\psi(\theta)$ . With this choice:

$$a^\top \nabla\psi(\theta) = \nabla\psi(\theta)^\top I(\theta)^{-1} \nabla\psi(\theta)$$

and

$$a^\top I(\theta)a = \nabla\psi(\theta)^\top I(\theta)^{-1} I(\theta) I(\theta)^{-1} \nabla\psi(\theta) = \nabla\psi(\theta)^\top I(\theta)^{-1} \nabla\psi(\theta).$$

The inequality becomes

$$(\nabla\psi(\theta)^\top I(\theta)^{-1} \nabla\psi(\theta))^2 \leq \text{Var}_\theta(\delta(X)) (\nabla\psi(\theta)^\top I(\theta)^{-1} \nabla\psi(\theta)).$$

Assuming  $\nabla\psi(\theta)^\top I(\theta)^{-1} \nabla\psi(\theta) > 0$  (otherwise the bound is trivial), we can multiply

by the inverse on both sides to obtain

$$\text{Var}_\theta(\delta(X)) \geq \nabla\psi(\theta)^\top I(\theta)^{-1} \nabla\psi(\theta).$$

□

The bound in Theorem 2.14 applies to any estimator, regardless of whether it is biased or unbiased. For unbiased estimators, the bound simplifies and takes a particularly interpretable form.

**Corollary 2.15.** *Assume the setting of Theorem 2.14. If  $\delta(X)$  is an unbiased estimator of  $\phi(\theta)$  in a neighborhood of  $\theta$  and  $\phi : \Theta \rightarrow \mathbb{R}^d$  is differentiable, then*

$$\text{Var}_\theta(\delta(X)) \geq \nabla\phi(\theta)^\top I(\theta)^{-1} \nabla\phi(\theta).$$

*If  $\phi$  is the identity function, then this reduces to the familiar inequality:*

$$\text{Var}_\theta(\delta(X)) \geq I(\theta)^{-1}. \quad (2.2)$$

*Proof.* Note that unbiasedness implies  $\psi(\theta) = \phi(\theta)$ . If  $\phi$  is the identity function on  $\mathbb{R}^d$ , it follows that  $\nabla\phi(\theta) = I_d$ . □

The following example shows that the requirement of unbiasedness in a neighborhood of  $\theta_1$  is critical for the result of Corollary 2.15 to hold.

**Example 2.16.** Consider  $X \sim N(\theta, I_d)$ ,  $\theta \in \mathbb{R}^d$  and the estimator

$$\delta(X) = \omega\theta_1 + (1 - \omega)X$$

for some  $\omega \in [0, 1]$  and  $\theta_1 \in \mathbb{R}^d$ . Estimator is unbiased at  $\theta_1$ . However, its variance is

$$\text{Var}_{\theta_1}(\delta(X)) = (1 - \omega)^2 I_d.$$

For  $\omega > 0$ , this is strictly smaller than the right-hand side of (2.2), which evaluates to  $I(\theta_1)^{-1} = I_d$  (check). Indeed, for  $\omega > 0$ , the estimator is not unbiased over any neighborhood of  $\theta_1$ . Setting  $\omega = 0$  gives the UMVUE. ◇

If  $\delta(X)$  is unbiased, the inequalities of Corollary 2.15 hold for all  $\theta \in \Theta$ . For unbiased estimators, the Cramér-Rao lower bound provides a target in terms of what is the best possible variance to achieve. Clearly, if  $\delta(X)$  is unbiased and attains the Cramer-Rao lower bound, it is a UMVUE. The converse is not true in general: in certain problems, the UMVUE might not attain the Cramér-Rao lower bound.

However, in certain problems, attaining the Cramér-Rao lower bound is not only a sufficient condition for the estimator to be UMVUE, but also a necessary condition. The implication goes really far: it also tells us the form that our decision rule should have, given that it is unbiased and attains the Cramér-Rao lower bound. This form is affine function of the score. This insight will prove to be useful later when we study asymptotic properties of maximum likelihood estimators in Part II of the course.

**Proposition 2.17** (Attainment of the Cramér-Rao bound). *Under the conditions of the Cramér-Rao theorem, equality holds if and only if*

$$\delta(X) = \psi(\theta) + \nabla\psi(\theta)^\top I(\theta)^{-1} S_\theta(X) \quad P_\theta\text{-a.s.}$$

*In particular, the bound is attained if and only if  $\delta(X)$  is an affine function of the score.*

*Proof.* Fix  $\theta$  and  $v \in \mathbb{R}^k$ . Consider the scalar estimator  $\delta_v(X) = v^\top \delta(X)$  with mean  $\psi_v(\theta) = v^\top \psi(\theta)$ . Applying the (scalar) Cramér-Rao inequality to  $\delta_v$  gives

$$\text{Var}_\theta(\delta_v(X)) \geq \nabla\psi_v(\theta)^\top I(\theta)^{-1} \nabla\psi_v(\theta) = v^\top \left( \nabla\psi(\theta)^\top I(\theta)^{-1} \nabla\psi(\theta) \right) v.$$

Since this holds for all  $v$ , it is equivalent to the stated matrix inequality.

Moreover, in the scalar proof the inequality comes from Cauchy-Schwarz applied to  $\text{Cov}_\theta(\delta_v(X), a^\top S_\theta(X))$  with the choice  $a = I(\theta)^{-1} \nabla\psi_v(\theta)$ . Equality in Cauchy-Schwarz holds if and only if

$$\delta_v(X) - \psi_v(\theta) = a^\top S_\theta(X) \quad P_\theta\text{-a.s.}$$

With  $a = I(\theta)^{-1} \nabla\psi(\theta) v$ , this becomes

$$v^\top (\delta(X) - \psi(\theta)) = v^\top \nabla\psi(\theta)^\top I(\theta)^{-1} S_\theta(X) \quad P_\theta\text{-a.s.}$$

for every  $v \in \mathbb{R}^k$ , which implies the vector identity in the statement. The converse direction is immediate by substitution.  $\square$

Let us consider what this result implies. For an unbiased estimator with  $\psi(\theta) = \phi(\theta)$ , Proposition 2.17 tells us that attaining the bound requires

$$\delta(X) = \phi(\theta) + \nabla\phi(\theta)^\top I(\theta)^{-1} S_\theta(X) \quad P_\theta\text{-a.s.}$$

At first glance, this seems problematic: the right-hand side depends on the unknown parameter  $\theta$  through  $\phi(\theta)$ ,  $\nabla\phi(\theta)$ ,  $I(\theta)$ , and  $S_\theta(X)$ . For the estimator to be a valid statistic—a function of the data alone—these  $\theta$ -dependent terms must combine in a way that eliminates the dependence on  $\theta$ . This places strong constraints on the model:

only in special cases does such cancellation occur. Exponential families provide the canonical example.

**Example 2.18** (Some exponential families attain the bound naturally). Consider a natural exponential family with density

$$p_{\theta}(x) = h(x) \exp(\theta^{\top} T(x) - A(\theta)),$$

where  $\theta \in \Theta \subseteq \mathbb{R}^d$  is the natural parameter and  $A(\theta)$  is twice differentiable. The score is

$$S_{\theta}(X) = \nabla_{\theta} \log p_{\theta}(X) = T(X) - \nabla A(\theta).$$

Since  $E_{\theta}[S_{\theta}(X)] = 0$ , we have  $E_{\theta}[T(X)] = \nabla A(\theta)$ . The Fisher information is

$$I(\theta) = \text{Cov}_{\theta}(S_{\theta}(X)) = \text{Cov}_{\theta}(T(X)) = \nabla^2 A(\theta).$$

Now consider estimating  $\phi(\theta) = \nabla A(\theta) = E_{\theta}[T(X)]$  by the estimator  $\delta(X) = T(X)$ . This estimator is unbiased, and satisfies the attainment condition:

$$\delta(X) - \psi(\theta) = T(X) - \nabla A(\theta) = S_{\theta}(X) = I(\theta)^{-1} \nabla \psi(\theta)^{\top} S_{\theta}(X),$$

where the last equality uses  $\nabla \psi(\theta) = \nabla^2 A(\theta) = I(\theta)$ . Thus, the sufficient statistic  $T(X)$  achieves the Cramér-Rao lower bound for estimating its own expectation.  $\diamond$

## 2.2 Invariance

In Section 2.1.1, we saw that models with a differentiable structure allow us to derive fundamental limits on estimation accuracy through the Fisher information. Another type of structure that proves useful is that of *symmetry*: if transforming the data in a certain way corresponds to a transformation of the parameter that leaves the model's form unchanged, we say the model is invariant under that transformation.

When the loss function respects the same symmetry, it is often natural to restrict attention to decision rules that also respect it. The word “natural” here has both technical and conceptual interpretations. On the technical side, invariance can simplify the analysis: as we will see, equivariant estimators in invariant problems have constant risk, reducing the comparison of decision rules to a single number. On the conceptual side, invariance captures the intuition that our estimates should not depend on arbitrary choices such as the coordinate system (rotation invariance) or unit of measurement (scale invariance).

This section formalizes these ideas and illustrates them in classical location, location-

scale, and covariance models. There is much more to say on this topic than fits into this section. The interested reader is referred to Chapter 3 of Lehmann and Romano 2005, Chapter 6 of Lehmann and Casella 2006 and Berger 1985.

### 2.2.1 Invariant models

The idea of invariance, or that of symmetries generally, is closely related to the concept of a group.

**Definition 2.19.** A *group* is a set  $G$  with an operation  $\cdot : G \times G \rightarrow G$  such that

1.  $(a \cdot b) \cdot c = a \cdot (b \cdot c)$  for all  $a, b, c \in G$  (associativity);
2. there exists  $e \in G$  with  $e \cdot a = a \cdot e = a$  for all  $a \in G$  (identity);
3. for each  $a \in G$  there exists  $a^{-1} \in G$  with  $a \cdot a^{-1} = a^{-1} \cdot a = e$  (inverse).

Groups are common objects in mathematics, and many of the most important groups in statistics are related to groups in mathematics that we are already familiar with.

**Example 2.20.** •  $(\mathbb{Z}, + : (a, b) \mapsto a + b)$  is a group with identity 0 and inverse  $-a$ .

- $(\mathbb{R}_{>0}, \times : (a, b) \mapsto ab)$  is a group with identity 1 and inverse  $1/a$ .
- $\text{GL}(p)$  (invertible  $p \times p$  matrices) is a group under matrix multiplication.
- The permutation group  $\mathfrak{S}_n$  acts on  $\mathcal{X}^n$  by permuting coordinates.

◇

**Definition 2.21** (Group action). A group  $G$  *acts on* a set  $A$  if there is a map  $G \times A \rightarrow A$ , written  $(g, x) \mapsto gx$ , such that  $ex = x$  and  $g(hx) = (gh)x$  for all  $g, h \in G$  and  $x \in A$ . The action is *transitive* if for all  $x, y \in A$ , there exists  $g \in G$  such that  $gx = y$ .

In statistical models, we sometimes have actions on the sample space  $\mathcal{X}$  and the parameter space  $\Theta$ . Sometimes, actions on the parameter space have an ‘inverse’ action on the sample space that ‘respects’ the data generating process: whether we act on the data, or perform the same corresponding action on the parameter, the data generating process remains the same.

**Definition 2.22** (Equivariance of a model). Consider statistical experiment with  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  defined on a sample space  $(\mathcal{X}, \mathcal{X})$ . Let  $G$  act on  $\mathcal{X}$  and  $\Theta$ , such that its action is measurable. The model  $\mathcal{P}$  is *equivariant* under  $G$  if

$$P_{g\theta}(A) = P_\theta(g^{-1}A) \quad \text{for all } g \in G, \theta \in \Theta, A \in \mathcal{X}.$$

Equivalently: if  $X \sim P_\theta$ , then  $gX \sim P_{g\theta}$ .

One of the most important examples of an equivariant model is the *location family*.

**Example 2.23** (Location family). Consider a statistical experiment  $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d), \mathcal{P}, \Theta)$  with parameter space  $\Theta = \mathbb{R}^d$  where  $\mathcal{P}$  is dominated with respect to the Lebesgue measure, with Lebesgue density  $p(x|\theta)$  a.e. equal to  $f(x - \theta)$  for some measurable function  $f : \mathbb{R}^d \rightarrow [0, \infty)$ .

The model  $\mathcal{P}$  is equivariant under the group  $G = (\mathbb{R}^d, +)$  acting on  $\mathbb{R}^d$  by translation, i.e.  $g_c x = x + c$  for all  $c \in \mathbb{R}^d$  and  $x \in \mathbb{R}^d$ .

Indeed, if  $X \sim P_\theta$ , then  $X + c \sim P_{\theta+c}$ , since

$$P_{\theta+c}(A) = \int_A f(x - (\theta + c)) dx = \int_{x-c \in A} f(x - \theta) dx = P_\theta(A - c).$$

where we used the change of variables  $y = x + c$  and translation invariance of Lebesgue measure.  $\diamond$

Many common distributions are location families, such as the normal distribution, Laplace distribution, Cauchy distribution, etc. Another important example of an equivariant model is the *scale family*.

**Example 2.24** (Scale family). Consider a statistical experiment  $(\mathbb{R}_{>0}, \mathcal{B}(\mathbb{R}_{>0}), \mathcal{P}, \Theta)$  with parameter space  $\Theta = \mathbb{R}_{>0}$ , where  $\mathcal{P}$  is dominated with respect to Lebesgue measure on  $\mathbb{R}_{>0}$ , with density

$$p(x | \sigma) = \frac{1}{\sigma} f\left(\frac{x}{\sigma}\right)$$

for some measurable function  $f : \mathbb{R}_{>0} \rightarrow [0, \infty)$  integrating to one.

The model  $\mathcal{P}$  is equivariant under the multiplicative group  $G = (\mathbb{R}_{>0}, \times)$  acting on  $\mathbb{R}_{>0}$  by scaling:  $g_c x = cx$  for  $c > 0$ . Indeed, if  $X \sim P_\sigma$ , then  $cX \sim P_{c\sigma}$ , since

$$P_{c\sigma}(A) = \int_A \frac{1}{c\sigma} f\left(\frac{x}{c\sigma}\right) dx = \int_{c^{-1}A} \frac{1}{\sigma} f\left(\frac{y}{\sigma}\right) dy = P_\sigma(c^{-1}A).$$

Common examples include the exponential family  $\text{Exp}(1/\sigma)$  and the chi-squared distribution scaled by  $\sigma^2$ .  $\diamond$

Another canonical example of an equivariant model is the multivariate standard normal distribution; which is spherically symmetric, on top of being a location and scale family.

**Example 2.25** (Spherically symmetric normal). Consider observing  $X \sim N_d(\theta, \sigma^2 I_d)$  with  $\theta \in \mathbb{R}^d$  and  $\sigma^2 > 0$  known. The group  $G$  of  $d \times d$  orthonormal matrices under matrix multiplication acts on both  $\mathbb{R}^d$  and  $\Theta = \mathbb{R}^d$  by matrix-vector multiplication:  $g_Q x = Qx$ .

The model is equivariant under this action. If  $X \sim N_d(\theta, \sigma^2 I_d)$ , then

$$QX \sim N_d(Q\theta, \sigma^2 QI_dQ^\top) = N_d(Q\theta, \sigma^2 I_d),$$

using  $QQ^\top = I_d$ . Thus  $QX \sim P_{Q\theta}$ , as required. ◇

### 2.2.2 Invariance and estimation

For models that are equivariant under a group action, it is natural to consider decision rules that respect the same symmetry. The intuition is straightforward: if the statistical problem is unchanged by a transformation, the solution should transform accordingly. Put differently, if two scientists analyze the same data but use different coordinate systems—one rotated relative to the other, or one using meters while the other uses feet—their estimates should be related by the same transformation. An estimator that violates this principle would give answers that depend on arbitrary choices having nothing to do with the data.

Suppose we are interested in estimating  $\theta \in \Theta$ , taking  $\mathcal{D} = \Theta$  (with some suitable  $\sigma$ -algebra). The action of  $G$  on  $\Theta$  induces an action on  $\mathcal{D}$  by  $g_{\mathcal{D}}(d) = gd$  for all  $g \in G$  and  $d \in \mathcal{D}$ . In some applications it would be unnatural for the loss function to depend on the orientation in the parameter space for which the estimation error occurs. For example, for a GPS system, the loss of predicting a certain location should not depend on one's initial orientation relative to the true location. This brings us to the concept of invariant loss.

That is, if we decide  $d$  based on data  $X$  and the true state turns out to be  $\theta$  (for which we incur loss  $L(\theta, d)$ ), this loss should be the same as someone who decides  $g_{\mathcal{D}}(d)$  based on data  $gX$  and the true state turning out to be  $g\theta$  (for which they incur loss  $L(g\theta, g_{\mathcal{D}}(d))$ ). This motivates the following definition.

**Definition 2.26** (Invariant loss). Consider a decision problem  $(\mathcal{X}, \mathcal{X}, \mathcal{P}, \Theta, (\mathcal{D}, \mathcal{D}), L)$ . Suppose  $G$  acts on  $\mathcal{X}$ ,  $\Theta$ , and  $\mathcal{D}$ , and these actions are measurable. Write  $g_{\mathcal{D}}$  for the induced action on  $\mathcal{D}$ .

A loss function  $L(\theta, d)$  is *invariant* under  $G$  if

$$L(g\theta, g_{\mathcal{D}} d) = L(\theta, d) \quad \text{for all } g \in G, \theta \in \Theta, d \in \mathcal{D}.$$

A decision problem is *invariant* under  $G$  if the model is equivariant and loss function are invariant under  $G$ .

**Example 2.27** (Revisiting the normal location model). Recall the equivariant normal location model from Example 2.25:  $X \sim N_d(\theta, \sigma^2 I_d)$  with  $\theta \in \mathbb{R}^d$  and  $\sigma^2 > 0$  known,

with the group  $G$  of  $d \times d$  orthonormal matrices under matrix multiplication acts on both  $\mathbb{R}^d$  and  $\Theta = \mathbb{R}^d$  by matrix-vector multiplication:  $g_Q x = Qx$ .

If we are interested in estimating  $\theta$ , we can consider the loss function  $L(\theta, d) = \|\theta - d\|^2$ , defined on  $\mathbb{R}^d \times \mathbb{R}^d$ . This loss is invariant under  $G$  since  $\|Q\theta - Qd\|^2 = \|\theta - d\|^2$ , turning the corresponding decision problem into an invariant one.  $\diamond$

For an invariant decision problem, it can be natural to restrict attention to estimators that respect the same symmetry. If the data  $X$  lead us to the estimate  $\delta(X)$ , then the transformed data  $gX$  should lead us to the correspondingly transformed estimate  $g_{\mathcal{D}}\delta(X)$ . This motivates the following definition.

**Definition 2.28** (Equivariant decision rule). Consider a decision problem with decision space  $(\mathcal{D}, \mathcal{D})$ . Suppose  $G$  acts on  $\mathcal{X}$ ,  $\Theta$ , and  $\mathcal{D}$ , and these actions are measurable. Write  $g_{\mathcal{D}}$  for the induced action on  $\mathcal{D}$ . A decision rule  $\delta : \mathcal{X} \rightarrow \mathcal{D}$  is *equivariant* if

$$\delta(gx) = g_{\mathcal{D}} \delta(x) \quad \text{for all } g \in G, x \in \mathcal{X}.$$

Equivariant estimators in invariant problems have constant risk, which greatly simplifies the task of finding optimal procedures.

**Theorem 2.29.** *Assume  $G$  acts transitively on  $\Theta$  (i.e. for all  $\theta, \theta' \in \Theta$  there exists  $g \in G$  with  $\theta' = g\theta$ ). If the model  $\mathcal{P}$  is equivariant, the loss is invariant, and  $\delta$  is equivariant, then the risk  $\mathcal{R}(\theta, \delta)$  is constant in  $\theta$ .*

*Proof.* Fix  $\theta_0 \in \Theta$ . For any  $\theta = g\theta_0$ , using model equivariance and then equivariance and invariance,

$$\begin{aligned} \mathcal{R}(\theta, \delta) &= \mathbb{E}_{g\theta_0}[L(g\theta_0, \delta(X))] \\ &= \mathbb{E}_{\theta_0}[L(g\theta_0, \delta(gX))] \\ &= \mathbb{E}_{\theta_0}[L(g\theta_0, \tilde{g} \delta(X))] \\ &= \mathbb{E}_{\theta_0}[L(\theta_0, \delta(X))] = \mathcal{R}(\theta_0, \delta). \end{aligned} \quad \square$$

If we are convinced that equivariant decision rules are the natural ones to consider in an invariant problem, then the goal becomes finding the best among them. This is formalized by the uniformly minimum risk equivariant estimator (UMREE), which plays a role analogous to the UMVUE in the class of unbiased estimators. Theorem 2.29 shows that every equivariant estimator has constant risk, so comparing two equivariant estimators reduces to comparing a single number rather than two functions on  $\Theta$ .

**Definition 2.30** (Uniformly Minimum Risk Equivariant Estimator). Consider an invariant decision problem: a model  $\mathcal{P} = \{P_{\theta} : \theta \in \Theta\}$  that is equivariant under  $G$ , and

a loss function  $L$  that is invariant under  $G$ . An estimator  $\delta^*$  is a *uniformly minimum risk equivariant estimator (UMREE)* if:

- (i)  $\delta^*$  is equivariant:  $\delta^*(gx) = g_{\mathcal{D}} \delta^*(x)$  for all  $g \in G$  and  $x \in \mathcal{X}$ , and
- (ii) for any other equivariant estimator  $\delta$ ,

$$\mathcal{R}(\theta, \delta^*) \leq \mathcal{R}(\theta, \delta) \quad \text{for all } \theta \in \Theta.$$

We now apply the general theory to one of the most important invariant problems: estimation in a location family under squared error loss. This setting illustrates how the UMREE can be characterized explicitly as a Bayesian posterior mean under an improper prior.

Consider observing  $X = (X_1, \dots, X_n)$  with joint density  $\prod_{i=1}^n f(x_i - \theta)$  with respect to Lebesgue measure, where  $\theta \in \mathbb{R}^d$  and  $x_i \in \mathbb{R}^d$ . The translation group  $G = (\mathbb{R}^d, +)$  acts on the sample space  $\mathbb{R}^{nd}$  by  $g_c x = (x_1 + c, \dots, x_n + c)$  and on the parameter space by  $g_c \theta = \theta + c$ . Since Lebesgue measure is translation-invariant, the model is equivariant: if  $X \sim P_\theta$ , then  $X + c\mathbf{1} \sim P_{\theta+c}$ .

For squared error loss  $L(\theta, d) = \|d - \theta\|^2$ , the induced action on decisions is  $g_c d = d + c$ , and the loss is invariant since  $\|(d+c) - (\theta+c)\|^2 = \|d - \theta\|^2$ . An estimator  $\delta$  is equivariant if and only if  $\delta(x + c\mathbf{1}) = \delta(x) + c$  for all  $c \in \mathbb{R}^d$ . This is a substantial restriction: for instance, the constant estimator  $\delta(x) = 0$  is not equivariant, while the sample mean and geometric median are.

Since  $G$  acts transitively on  $\Theta = \mathbb{R}^d$ , Theorem 2.29 implies that every equivariant estimator has constant risk. The UMREE is therefore the equivariant estimator minimizing  $\mathcal{R}(\theta_0, \delta)$  for any fixed  $\theta_0$ ; taking  $\theta_0 = 0$  is conventional. The following theorem identifies this optimal estimator.

**Theorem 2.31** (Pitman estimator in  $\mathbb{R}^d$ ). *Let  $X = (X_1, \dots, X_n)$  with  $X_i \in \mathbb{R}^d$  have joint density  $\prod_{i=1}^n f(x_i - \theta)$  with respect to Lebesgue measure on  $\mathbb{R}^{nd}$ , where  $\theta \in \mathbb{R}^d$ . Under squared error loss  $L(\theta, \delta) = \|\delta - \theta\|^2$ , the ( $P_\theta$ -a.s. unique) UMREE is*

$$\delta^*(x) = \frac{\int_{\mathbb{R}^d} \theta \prod_{i=1}^n f(x_i - \theta) d\theta}{\int_{\mathbb{R}^d} \prod_{i=1}^n f(x_i - \theta) d\theta},$$

*provided the integrals are finite.*

*Proof.* The translation group  $G = (\mathbb{R}^d, +)$  acts on  $\mathbb{R}^{nd}$  by  $g_c x = (x_1 + c, \dots, x_n + c)$  and on  $\Theta = \mathbb{R}^d$  by  $g_c \theta = \theta + c$ . Since Lebesgue measure on  $\mathbb{R}^{nd}$  is translation-invariant, the model is equivariant. The squared error loss is invariant since  $\|\delta + c - (\theta + c)\| = \|\delta - \theta\|$ .

By Theorem 2.29, every translation-equivariant estimator has constant risk, so it suffices to minimize  $\mathcal{R}(0, \delta) = \mathbb{E}_0[\|\delta(X)\|^2]$  over equivariant  $\delta$ .

First,  $\delta^*$  is equivariant: substituting  $\eta = \theta - c$ ,

$$\delta^*(x_1 + c, \dots, x_n + c) = \frac{\int_{\mathbb{R}^d} (\eta + c) \prod_i f(x_i - \eta) d\eta}{\int_{\mathbb{R}^d} \prod_i f(x_i - \eta) d\eta} = \delta^*(x) + c.$$

Let  $\delta$  be any other equivariant estimator and write  $h = \delta - \delta^*$ . Then  $h$  is translation-invariant. We claim  $\mathbb{E}_0[\langle \delta^*(X), h(X) \rangle] = 0$ .

By definition,  $\delta^*(x)$  minimizes  $\int_{\mathbb{R}^d} \|\theta - d\|^2 \prod_i f(x_i - \theta) d\theta$  over  $d \in \mathbb{R}^d$ . The first-order condition gives

$$\int_{\mathbb{R}^d} (\delta^*(x) - \theta) \prod_i f(x_i - \theta) d\theta = 0.$$

Taking the inner product with  $h(x)$ , integrating over  $x$  under  $P_0$ , and applying Fubini's theorem with translation invariance of  $h$  yields  $\mathbb{E}_0[\langle \delta^*(X), h(X) \rangle] = 0$ .

Finally,

$$\begin{aligned} \mathbb{E}_0[\|\delta(X)\|^2] &= \mathbb{E}_0[\|\delta^*(X) + h(X)\|^2] \\ &= \mathbb{E}_0[\|\delta^*(X)\|^2] + 2\mathbb{E}_0[\langle \delta^*(X), h(X) \rangle] + \mathbb{E}_0[\|h(X)\|^2] \\ &\geq \mathbb{E}_0[\|\delta^*(X)\|^2], \end{aligned}$$

with equality if and only if  $h = 0$  a.s., implying  $\delta^*$  is  $P_\theta$ -a.s. unique.  $\square$

The Pitman estimator admits an elegant Bayesian interpretation: it is the ‘posterior mean’ under the ‘uniform prior’  $\pi(\theta) \propto 1$  on  $\mathbb{R}^d$ . Although this prior is improper (it does not integrate to a finite value), the posterior is proper whenever the likelihood is integrable, and the resulting estimator is well-defined. The uniform prior is the *right Haar measure* for the translation group—the unique (up to scale) measure on  $\mathbb{R}^d$  that is invariant under the group action – explored in more generality in Section 2.2.3.

We now illustrate the Pitman estimator in two classical location families.

**Example 2.32** (Normal location). For  $X_i \stackrel{\text{iid}}{\sim} N_d(\theta, \sigma^2 I_d)$  with  $\sigma^2$  known, the joint density is proportional to  $\exp(-\frac{1}{2\sigma^2} \sum_i \|x_i - \theta\|^2)$ . Completing the square in  $\theta$ , the Pitman estimator evaluates to  $\delta^*(X) = \bar{X}$ , which coincides with both the MLE and the UMVUE.  $\diamond$

**Example 2.33** (Uniform location). For  $X_i \stackrel{\text{iid}}{\sim} \text{Uniform}(\theta, \theta + 1)$ , the joint density is  $\prod_i \mathbb{1}_{\{\theta \leq x_i \leq \theta + 1\}} = \mathbb{1}_{\{X_{(n)} - 1 \leq \theta \leq X_{(1)}\}}$ . This is constant (equal to 1) on the interval  $[X_{(n)} - 1, X_{(1)}]$  and zero elsewhere. The Pitman estimator is therefore the midpoint of this interval:

$$\delta^*(X) = \frac{X_{(1)} + X_{(n)} - 1}{2}.$$

This differs from the MLE, which is any point in  $[X_{(n)} - 1, X_{(1)}]$  (conventionally taken as  $\hat{\theta} = X_{(n)} - 1$ ). The Pitman estimator uses information from both extremes, while the MLE uses only one.  $\diamond$

These examples highlight that the Pitman estimator may or may not coincide with other familiar estimators, depending on the model. For the Cauchy location family, the Pitman estimator takes a more complex form; see Exercise 2.11.

*Remark 2.34.* The concept of UMREE differs from the concept of UMVUE in that the latter is defined in the context of unbiased estimators and their variance, whilst the UMREE is defined in the context of equivariant estimators and *a specific loss function*. For different loss functions, we obtain different UMREE's.

### 2.2.3 ♠ Haar measures and the general UMREE construction

The Pitman estimator for location families relied on the fact that Lebesgue measure is translation-invariant. This observation generalizes: for any locally compact group, there exists a canonical “invariant measure” called the Haar measure, which allows us to construct best equivariant estimators via the same ‘Bayesian recipe’.

**Definition 2.35** (Haar measure). Let  $G$  be a locally compact topological group. A *left Haar measure* on  $G$  is a nonzero Borel measure  $\nu_L$  satisfying

$$\nu_L(gA) = \nu_L(A) \quad \text{for all } g \in G \text{ and all Borel sets } A \subseteq G.$$

A *right Haar measure*  $\nu_R$  satisfies  $\nu_R(Ag) = \nu_R(A)$  for all  $g \in G$  and Borel  $A \subseteq G$ .

Equivalently, in terms of integrals:  $\nu_L$  is left-invariant if

$$\int_G f(gh) d\nu_L(h) = \int_G f(h) d\nu_L(h) \quad \text{for all } g \in G \text{ and integrable } f.$$

and similarly for right invariance.

**Theorem 2.36** (Haar, 1933). *Let  $G$  be a locally compact topological group. Then:*

- (i) *A right Haar measure exists.*
- (ii) *Any two right Haar measures differ by a positive multiplicative constant.*

*The analogous statements hold for left Haar measures.*

The proof of existence is nontrivial and relies on techniques from functional analysis; see Folland 2016 for a complete treatment. For our purposes, the key point is that Haar measures exist and are essentially unique, so they provide a canonical choice of “uniform” measure on any group.

- Example 2.37** (Common Haar measures). (i) **Translation group**  $G = (\mathbb{R}^d, +)$ : Lebesgue measure  $d\theta$  is Haar (both left and right as the group is abelian).
- (ii) **Multiplicative group**  $G = (\mathbb{R}_{>0}, \times)$ : The measure  $d\nu(\sigma) = d\sigma/\sigma$  is both left and right Haar.
- (iii) **Location-scale group**  $G = \{(a, b) : a > 0, b \in \mathbb{R}\}$  with operation  $(a_1, b_1) \cdot (a_2, b_2) = (a_1 a_2, a_1 b_2 + b_1)$ : The left Haar measure is  $da db/a^2$ , and the right Haar measure is  $da db/a$ .
- (iv) **Orthogonal group**  $G = O(d)$ : Since  $O(d)$  is compact, the Haar measure is finite and can be normalized to a probability measure (the “uniform distribution” on  $O(d)$ ).
- (v) **General linear group**  $G = GL(p)$ : The left and right Haar measures are  $d\nu(A) = |\det A|^{-p} dA$ , where  $dA$  denotes Lebesgue measure on  $\mathbb{R}^{p \times p}$ .

◇

A group  $G$  is called *unimodular* if its left and right Haar measures coincide. Compact groups and abelian groups are all unimodular. The location-scale group in Example 2.37(iii) is a standard example of a non-unimodular group.

When a group  $G$  acts transitively on a parameter space  $\Theta$ , a Haar measure on  $G$  induces a natural “uniform” measure on  $\Theta$  by *pushing it forward* through the orbit map. Concretely, fix a reference point  $\theta_0 \in \Theta$  and define  $\tau : G \rightarrow \Theta$  by  $\tau(g) = g\theta_0$ ; then the induced measure on  $\Theta$  is the push-forward  $\tau_{\#}\nu$  given by  $\tau_{\#}\nu(A) = \nu(\tau^{-1}(A))$  for measurable  $A \subseteq \Theta$  (and we often denote  $\tau_{\#}\nu$  simply by  $\nu$ ). This measure is invariant under the group action, and different choices of  $\theta_0$  change it only by a multiplicative constant.

We now present the general recipe for constructing best equivariant estimators using Haar measures.

**Theorem 2.38** (UMREE via Haar measure). *Consider an invariant decision problem with model  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  equivariant under a locally compact group  $G$  that acts transitively on  $\Theta$ . Let  $L(\theta, d)$  be an invariant loss function, and let  $\nu$  denote the right Haar measure on  $G$ , and consider the induced measure (also denoted  $\nu$ ) on  $\Theta$  via the group action.*

*Define the generalized Bayes estimator*

$$\delta^*(x) = \operatorname{argmin}_{d \in \mathcal{D}} \int_{\Theta} L(\theta, d) p(x|\theta) d\nu(\theta),$$

*provided the integral is finite. Then  $\delta^*$  is equivariant, and if it exists, it is the UMREE.*

*Proof.* See Berger 1985, Chapter 6. □

To summarize, we could see the estimator  $\delta^*$  of Theorem 2.38 as a ‘recipe’ for constructing the UMREE. Given an invariant decision problem:

1. Identify the group  $G$  under which the model is equivariant and the loss is invariant.
2. Verify transitivity: Check that  $G$  acts transitively on  $\Theta$ .
3. Compute the right Haar measure  $\nu$  on  $G$  (or equivalently, on  $\Theta$  via the action).
4. Form the ‘generalized Bayes’ estimator using  $\nu$  as an improper prior:

$$\delta^*(x) = \operatorname{argmin}_{d \in \mathcal{D}} \int_{\Theta} L(\theta, d) p(x|\theta) d\nu(\theta).$$

If the latter integral is finite,  $\delta^*$  is the UMREE.

## 2.3 Admissibility

The idea behind admissibility is simple: we should not use a decision rule if another rule is strictly better. The idea behind admissibility is simple: we wish to only consider decision rules that are not strictly dominated by some other decision rule.

**Definition 2.39.** A decision rule  $\delta$  is *admissible* if there exists no other estimator  $\delta'$  such that

1.  $\mathcal{R}(\theta, \delta') \leq \mathcal{R}(\theta, \delta)$  for all  $\theta \in \Theta$ , and
2.  $\mathcal{R}(\theta, \delta') < \mathcal{R}(\theta, \delta)$  for at least one  $\theta \in \Theta$ .

If such a  $\delta'$  exists, we say that  $\delta$  is *inadmissible* and that  $\delta'$  *dominates*  $\delta$ .

Admissibility captures a minimal requirement: we should reject any decision rule that is strictly dominated by another. Considering admissibility as a criterion leads to some surprising facts and insights. Perhaps one of the most impactful insights is the so-called *Stein’s shrinkage phenomenon*, which has shaped the way we think about estimation in high-dimensional models.

### 2.3.1 Stein’s shrinkage phenomenon

Consider the normal means model where we observe  $X \sim N_d(\theta, \sigma^2 I_d)$ , for some  $d \in \mathbb{N}$  and  $\sigma > 0$ , and the aim is to estimate the mean  $\theta$ . In the case  $d = 1$  it seems rather clear that if we do not know anything about the parameter  $\theta$ , we can not do much better than estimating it by the observation  $X$ . Proving this rigorously is actually not completely trivial, see Exercise 2.12.

For larger  $d$  it is in fact also not immediately clear whether if we assume no further structure on  $\theta$ , we can do better than simply using the maximum likelihood estimator  $\delta_{\text{MLE}}(X) = X$ . Clearly,  $X$  is a sufficient statistic and moreover a complete one (Example 1.31). It is unbiased over  $\mathbb{R}^d$ , and hence it is the UMVUE. Furthermore, it has invariance properties both in terms of location-shifts and rotations; it is the UMREE for the normal location model with Euclidian loss. It turns out, however, that it is possible to perform strictly better, in the sense of expected quadratic error.

To get a first indication of this fact, note that for any estimator  $\delta$  with a finite covariance we have the bias-variance decomposition (Lemma 2.7)

$$\mathbb{E}_\theta \|\delta(X) - \theta\|^2 = \|\mathbb{E}_\theta \delta(X) - \theta\|^2 + \text{Tr Cov}_\theta \delta(X).$$

If we apply this to  $\delta_c(X) = cX$  we find that  $\mathbb{E}_\theta \|\delta_c(X) - \theta\|^2 = (c-1)^2 \|\theta\|^2 + c^2 \sigma^2 d$ , which, for given  $\theta$ , is minimal for  $c$  equal to

$$c_\theta = \frac{\|\theta\|^2}{\|\theta\|^2 + \sigma^2 d},$$

and the minimal value is

$$\mathbb{E}_\theta \|\delta_{c_\theta}(X) - \theta\|^2 = \frac{\sigma^2 d \|\theta\|^2}{\|\theta\|^2 + \sigma^2 d} = \frac{\|\theta\|^2}{\|\theta\|^2 + \sigma^2 d} \mathbb{E}_\theta \|\delta_{\text{MLE}}(X) - \theta\|^2.$$

Since  $c_\theta < 1$ , this indicates that it might be advantageous to shrink the estimator  $X$  towards 0, that is, to multiply it by a factor strictly smaller than 1. Since  $c_\theta$  depends on the unknown parameter  $\theta$ , one might argue that this is not a sensible estimator. However, it turns out that for  $d \geq 3$ , we can shrink by an appropriate data-dependent constant that leads to an estimator with an expected squared error that is *strictly smaller than that of the MLE for all  $\theta \in \mathbb{R}^d$* .

**Theorem 2.40** (James-Stein). *Define*

$$\delta_{\text{JS}}(X) = \left(1 - \frac{\sigma^2(d-2)}{\|X\|^2}\right) X.$$

*For  $d \geq 3$ , we have  $\mathbb{E}_\theta \|\delta_{\text{JS}}(X) - \theta\|^2 < \mathbb{E}_\theta \|\delta_{\text{MLE}}(X) - \theta\|^2$  for all  $\theta \in \mathbb{R}^d$ .*

*Proof.* For the bias and variance of the  $i$ th component of the JS estimator we have

$$\mathbb{E}_\theta \delta_{\text{JS},i}(X) - \theta_i = -\sigma^2(d-2) \mathbb{E}_\theta \frac{X_i}{\|X\|^2}$$

and

$$\text{Var}_\theta \delta_{\text{JS},i}(X) = \sigma^2 + \sigma^4(d-2)^2 \text{Var}_\theta \frac{X_i}{\|X\|^2} - 2\sigma^2(d-2) \left( \mathbb{E}_\theta \frac{X_i^2}{\|X\|^2} - \mathbb{E}_\theta \frac{\theta_i X_i}{\|X\|^2} \right),$$

respectively. (Note that since  $\mathbb{E}_\theta 1/\|X\|^p$  is finite if and only if  $d > p$ , all expectations here are finite for  $d \geq 3$ . See Exercise 2.13.) It follows that the mean squared error of the estimator is given by

$$\sigma^2 d + \sigma^4(d-2)^2 \mathbb{E}_\theta \frac{1}{\|X\|^2} - 2\sigma^2(d-2) \left( \sum_i \mathbb{E}_\theta \frac{X_i(X_i - \theta_i)}{\|X\|^2} \right)$$

(check!). By Lemma 2.41 below,

$$\mathbb{E}_\theta \frac{X_i(X_i - \theta_i)}{\|X\|^2} = \mathbb{E}_\theta \frac{\sigma^2}{\|X\|^2} - 2\mathbb{E}_\theta \frac{\sigma^2 X_i^2}{\|X\|^4}.$$

Hence, the mean squared error (MSE)  $\mathbb{E}_\theta \|\delta_{\text{JS}}(X) - \theta\|^2$  equals

$$\sigma^2 d - \sigma^4(d-2)^2 \mathbb{E}_\theta \frac{1}{\|X\|^2}.$$

Since the MSE of the MLE  $\delta_{\text{MLE}}(X) = X$  equals  $d\sigma^2$ , this completes the proof.  $\square$

The key tool used in the proof above is Stein's lemma, which provides a useful identity for expectations involving Gaussian random variables.

**Lemma 2.41.** *Let  $X \sim N_d(\theta, I_d)$  and let  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  be an absolutely continuous (in each coordinate a.e.) function such that  $\mathbb{E}_\theta |(\partial f / \partial x_i)(X)| < \infty$  for  $i = 1, \dots, d$ . Then for  $i = 1, \dots, d$ ,*

$$\mathbb{E}_\theta (X_i - \theta_i) f(X) = \mathbb{E}_\theta \frac{\partial f}{\partial x_i}(X).$$

*Proof.* Integration by parts, see Exercise 2.14.  $\square$

The James-Stein theorem gives a number of very interesting insights in statistics for 'high-dimensional' models. It shows that by shrinking the MLE towards zero, thereby reducing the variance at the cost of increasing the bias, we obtain an estimator with a strictly better risk  $\mathbb{E}_\theta \|\delta(X) - \theta\|^2$ . Moreover, although the observed  $X_i$  are independent by assumption, the shrinkage factor depends on all the observations. Hence, to estimate the  $i$ th component  $\theta_i$ , we do not only use the information in  $X_i$ , but we also *borrow strength* from the other observations, even though they are independent coordinate wise.

One argument that Stein (1956) used to intuitively justify the concept of shrinkage is the observation that if  $X \sim N_d(\theta, I_d)$ , then by the law of large numbers it holds for

large  $d$  that  $\|X\|^2 \approx \|\theta\|^2 + d$ . So the norm of the MLE  $X$  is typically substantially larger than the norm of the parameter  $\theta$  it is supposed to estimate. Therefore, it may be beneficial to shrink the vector  $X$  so that the norm is reduced.

Alternatively, we may argue that shrinking reduces the contributions of outliers, i.e. relatively large observations  $X_i$ , on the squared estimation error. This possibly comes at the cost of increasing the error made in the other coordinates, but the net effect is that shrinking improves the total squared error  $\|\delta_{\text{JS}}(X) - \theta\|^2$  of the estimator on average. Observe that this reasoning indicates that it is essential that we assess the quality of the estimator using a norm that simultaneously takes all coordinates of  $\theta$  into account. This allows us to trade off gains in one coordinate with losses in others.

The James-Stein theorem can be generalized in many directions, for instance away from the normal distribution with unit variance, using other norms, other statistical models, et cetera. The precise form of the shrinking is not crucial either. Shrinking towards a fixed point  $v \in \mathbb{R}^d$  other than 0 works just as well for instance (see Exercise 2.15). The general message is always that in high-dimensional settings it is typically advantageous to somehow reduce the variance by shrinking, or otherwise regularizing. We explore this further in the next section.

Theorem 2.40 shows that for  $d \geq 3$ , the MLE  $\delta_{\text{MLE}}(X) = X$  is inadmissible in the model  $X \sim N_d(\theta, I_d)$ , with respect to the squared Euclidean risk. By definition, this means that there exists another estimator  $\delta$  such that  $\mathbb{E}_\theta \|\delta(X) - \theta\|^2 \leq \mathbb{E}_\theta \|\delta_{\text{MLE}}(X) - \theta\|^2$  for all  $\theta \in \mathbb{R}^d$ , with strict inequality for at least one  $\theta \in \mathbb{R}^d$ . The theorem asserts that the James-Stein estimator is such an estimator. It can be shown however that the James-Stein estimator itself is inadmissible as well. For example the positive part Stein estimator

$$\delta_{\text{JS}^+}(X) = \left(1 - \frac{\sigma^2(d-2)}{\|X\|^2}\right)_+ X$$

has strictly smaller risk for all  $\theta \in \mathbb{R}^d$ . See for instance Section 3.4 of Tsybakov (2009). Unfortunately,  $\delta_{\text{JS}^+}$  is not admissible either. It turns out that finding an admissible estimator is easy if we take a Bayesian approach – both in terms of its construction and in terms of verifying its admissibility – we will discuss this in Chapter 4.

### 2.3.2 Bias-variance trade-off

The Stein-shrinkage phenomenon demonstrates that in high-dimensional settings, trading bias for variance can yield strict improvements over the best unbiased estimator. This raises a natural question: how far can we push this trade-off? Can we achieve arbitrarily good performance at a particular parameter value by accepting bias elsewhere?

In Example 2.16, we saw an estimator that achieves variance strictly below the Cramér-Rao bound at a specific point  $\theta_1$  by being unbiased only at that point rather

than in a neighborhood. Taken to the extreme, the ‘guesstimator’  $\delta(X) = \theta_1$  is (quite generally) admissible—it achieves a risk at  $\theta_1$  which no other estimator can beat. Of course, this estimator performs terribly elsewhere in the parameter space. Intuitively, there is a ‘no-free-lunch’ principle at play: exceptional performance at one parameter value must come at the cost of degraded performance elsewhere.

The following example demonstrates this phenomenon concretely: a pretest estimator that achieves dramatically reduced risk at  $\theta = 0$  suffers substantially inflated risk at nearby parameter values.

**Example 2.42** (Test first, then estimate). Let  $X \sim N(\theta, \sigma^2)$  and consider squared error loss. The MLE  $\delta_{\text{MLE}}(X) = X$  has constant risk  $R(\theta, \delta_{\text{MLE}}) = \sigma^2$ .

Fix  $t > 0$  and define the pretest (hard-threshold) estimator

$$\delta_t(X) = \begin{cases} 0, & |X| \leq t, \\ X, & |X| > t. \end{cases}$$

At  $\theta = 0$ , writing  $Z \sim N(0, 1)$  and taking  $\sigma = 1$  for simplicity,

$$R(0, \delta_t) = \mathbb{E}[Z^2 \mathbb{1}\{|Z| > t\}] = 2(t\varphi(t) + \Phi(-t)),$$

so for instance  $t = 3$  gives  $R(0, \delta_3) \approx 0.029$ . We know from the fact that the MLE is admissible in this setting (Exercise 2.12) that there must be some  $\theta$  such that  $R(\theta, \delta_3) > R(\theta, X)$ . This is indeed the case:  $R(2, \delta_3) \approx 3.766 > 1$ . For  $|\theta| \rightarrow \infty$ , the  $R(\theta, \delta_3)$  approaches that of  $R(\theta, X)$ . The cost for performance at  $\theta = 0$  is paid for by a worse performance ‘nearby’  $\theta = 0$ .  $\diamond$

Example 2.42 suggests that dramatic gains at one parameter value force losses nearby. Can we quantify this trade-off? The Cramér-Rao bound provides one such tool, but it requires differentiability of the model and is most informative for unbiased estimators. For biased estimators, or for models lacking smooth structure, we need a more general approach.

Understanding this cost is not merely of theoretical interest. Later in this chapter, we will encounter models where trading bias for variance is not optional but *necessary*—unbiased estimators may not exist, or may perform poorly. To navigate such settings, we need tools to characterize the fundamental limitations on estimation.

The *constraint risk inequality* offers exactly this. The idea is simple: if two distributions  $P_f$  and  $P_g$  are ‘similar’, yet the parameters  $f$  and  $g$  are far apart, then no estimator can perform well at both. An estimator that gets close to  $f$  under  $P_f$  will tend to be far from  $g$  under  $P_g$ , and vice versa.

To make this precise, we need to quantify two notions of distance: distance between parameters and similarity between distributions. For parameters, we use a (semi-)metric  $\mathbf{d}$  on  $\Theta$ . For distributions, we use the *Bhattacharyya coefficient*

$$\rho(P_f, P_g) = \int \sqrt{p_f p_g} d\mu,$$

which measures the overlap between two densities. Geometrically,  $\rho(P_f, P_g)$  is the cosine of the angle between  $\sqrt{p_f}$  and  $\sqrt{p_g}$  viewed as unit vectors in  $L^2(\mu)$ . This geometric viewpoint on the space of densities has (implicitly) already appeared in our discussion of differentiability in quadratic mean.

**Lemma 2.43** (Constraint Risk Inequality). *Let  $(\Theta, \mathbf{d})$  be a (semi-)metric space and let  $P_f, P_g$  be probability measures on  $(\mathcal{X}, \mathcal{X})$  dominated by a common measure  $\mu$ , with densities  $p_f$  and  $p_g$ . For any estimator  $\delta : \mathcal{X} \rightarrow \Theta$  and any  $f, g \in \Theta$ ,*

$$\sqrt{\mathbb{E}_f \mathbf{d}(\delta, f)^2} + \sqrt{\mathbb{E}_g \mathbf{d}(\delta, g)^2} \geq \mathbf{d}(f, g) \cdot \rho(P_f, P_g).$$

*Proof.* By the triangle inequality, for all  $x \in \mathcal{X}$ ,

$$\mathbf{d}(f, \delta(x)) + \mathbf{d}(\delta(x), g) \geq \mathbf{d}(f, g).$$

Multiplying both sides by  $\sqrt{p_f(x)p_g(x)}$  and integrating with respect to  $\mu$  gives

$$\int \mathbf{d}(f, \delta) \sqrt{p_f p_g} d\mu + \int \mathbf{d}(\delta, g) \sqrt{p_f p_g} d\mu \geq \mathbf{d}(f, g) \cdot \rho(P_f, P_g).$$

For the first term, the Cauchy–Schwarz inequality yields

$$\int \mathbf{d}(f, \delta) \sqrt{p_f} \cdot \sqrt{p_g} d\mu \leq \sqrt{\int \mathbf{d}(f, \delta)^2 p_f d\mu} \cdot \sqrt{\int p_g d\mu} = \sqrt{\mathbb{E}_f \mathbf{d}(f, \delta)^2}.$$

The same argument applied to the second term completes the proof.  $\square$

The constraint risk inequality reveals a fundamental tension in estimation. The right-hand side,  $\mathbf{d}(f, g) \cdot \rho(P_f, P_g)$ , captures the difficulty of the estimation problem between  $f$  and  $g$ : it is large when the parameters are far apart (large  $\mathbf{d}(f, g)$ ) yet the distributions are similar (large  $\rho$ ). When this product is large, the sum of the root-MSEs at  $f$  and  $g$  must also be large—no estimator can perform well at both.

The bound is most informative when  $\rho(P_f, P_g)$  is not too small. If  $P_f$  and  $P_g$  are nearly orthogonal ( $\rho \approx 0$ ), the bound becomes vacuous; but this is unsurprising, since very different distributions are easy to distinguish. The interesting regime is when *statistical similarity* coexists with *parameter separation*.

We apply the constraint risk inequality in more complicated settings in Section 2.4.1, but for now let us illustrate it in a model where the Cramér-Rao bound does not apply.

**Example 2.44.** Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Uniform}(0, \theta)$  for  $\theta > 0$ . We use Lemma 2.43 to show that the  $\theta^2/n$  MSE achieved by the unbiased estimator  $\frac{n+1}{n}X_{(n)}$  cannot be generally improved by allowing an estimator to be biased.

For  $\theta_1 < \theta_2$ , the densities  $p_{\theta_1} = \theta_1^{-1}\mathbb{1}_{[0, \theta_1]}$  and  $p_{\theta_2} = \theta_2^{-1}\mathbb{1}_{[0, \theta_2]}$  overlap only on  $[0, \theta_1]$ , so

$$\rho(P_{\theta_1}, P_{\theta_2}) = \int_0^{\theta_1} \sqrt{\frac{1}{\theta_1\theta_2}} dx = \sqrt{\frac{\theta_1}{\theta_2}}.$$

For the product measure of  $n$  observations,  $\rho(P_{\theta_1}^{\otimes n}, P_{\theta_2}^{\otimes n}) = (\theta_1/\theta_2)^{n/2}$ . Lemma 2.43 then gives, for any estimator  $\delta$ ,

$$\sqrt{\mathbb{E}_{\theta_1}|\delta - \theta_1|^2} + \sqrt{\mathbb{E}_{\theta_2}|\delta - \theta_2|^2} \geq (\theta_2 - \theta_1) \left(\frac{\theta_1}{\theta_2}\right)^{n/2}.$$

Writing  $\theta_2 = \theta_1 + \epsilon$  for small  $\epsilon > 0$ , the right-hand side is approximately  $\epsilon \cdot e^{-n\epsilon/(2\theta_1)}$ . For any  $\epsilon \in [\theta_1/n, 3\theta_1/n]$ , this quantity is at least of order  $\theta_1/n$ . In particular, for any estimator  $\delta$  and any  $\theta_2 \in [\theta_1 + \theta_1/n, \theta_1 + 3\theta_1/n]$ , either  $\mathbb{E}_{\theta_1}|\delta - \theta_1|^2$  or  $\mathbb{E}_{\theta_2}|\delta - \theta_2|^2$  must be at least of order  $\theta_1^2/n^2$ .

Since the above recipe works for arbitrary  $\theta_1$ , this rules out estimators that attain MSE's of a smaller order than  $\theta^2/n$  across the parameter space, no matter how large or small  $n$  and  $\theta$  are.

◇

## 2.4 Minimax paradigms

Admissibility is a minimal requirement: it rules out estimators that are uniformly dominated, but little else. The guesstimator  $\delta(X) = \theta_1$  is generally admissible—no estimator can beat it at  $\theta_1$ —yet it is clearly unsatisfactory. Admissibility tells us which estimators to avoid, but does not prescribe how to choose among the many that remain.

The constraint risk inequality shows that trade-offs across the parameter space are unavoidable: exceptional performance at one parameter value must be paid for elsewhere. But how should we navigate these trade-offs?

The *minimax paradigm* takes the pessimist's view: assume the worst and optimize accordingly. Rather than asking “is there any  $\theta$  where this estimator is dominated?” (admissibility), we ask “what is the largest risk this estimator can incur?” and seek to minimize this worst-case risk. Where admissibility is permissive—accepting any estimator that is not uniformly beaten—minimaxity is demanding: it insists on the best possible guarantee against the least favorable parameter value.

**Definition 2.45** (Minimax risk and minimax estimator). Consider a decision problem  $(\mathcal{X}, \mathcal{X}, \mathcal{P}, \Theta, (\mathcal{D}, \mathcal{D}), L)$  and let  $\mathcal{C}$  denote the class of all (possibly randomized) decision rules  $\delta : \mathcal{X} \rightarrow \mathcal{D}$ .

The *minimax risk* is defined as

$$R^* := \inf_{\delta \in \mathcal{C}} \sup_{\theta \in \Theta} R(\theta, \delta).$$

A decision rule  $\delta^*$  is called *minimax* if it achieves the minimax risk:

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

The quantity  $\sup_{\theta \in \Theta} R(\theta, \delta)$  is called the *maximum risk* (or *worst-case risk*) of  $\delta$ .

The minimax criterion can be interpreted as a two-player zero-sum game. In an estimation problem, the statistician chooses an estimator  $\delta$ , and then “nature” (or an adversary) chooses the parameter  $\theta$  to maximize the risk. The minimax estimator is the statistician’s optimal strategy in this game, guaranteeing the best possible worst-case performance.

*Remark 2.46* (Pessimism or robustness?). The minimax approach is sometimes criticized as overly pessimistic (or overly conservative): why should we optimize for the worst case when it may rarely occur? However, this perspective has several compelling justifications:

- (i) *Robustness*: The minimax estimator provides a strong *statistical guarantee*—its risk never exceeds  $R^*$ , regardless of the true  $\theta$ .
- (ii) *Ruling out super-efficiency*: As we saw in Example 2.42, achieving exceptionally low risk at some  $\theta$  values necessarily inflates risk elsewhere (cf. the constraint risk inequality). Minimax estimation explicitly penalizes such greedy trade-offs, forcing estimators that do not sacrifice worst-case performance for gains at favorable parameter values.
- (iii) *Unknown or adversarial settings*: In some applications,  $\theta$  may be chosen by an adversary, or we may be clueless about what are ‘likely’ values of the parameter. The minimax estimator is natural in such settings.
- (iv) *Submodel flexibility*: Nothing prevents us from considering minimax risk over a subset  $\Theta' \subset \Theta$ :

$$\sup_{\theta \in \Theta'} R(\theta, \delta) \leq \sup_{\theta \in \Theta} R(\theta, \delta) \tag{2.3}$$

This allows us to calibrate our pessimism to the problem at hand. By considering various subsets  $\Theta'$ , we can study how the difficulty of estimation depends on the

region of the parameter space. Comparing minimax risks across nested subsets reveals which parts of the parameter space drive the difficulty of the problem. For certain models, the minimax risk is only non-trivial for such restriction – for example the uniform distribution studied in Example 2.44. Indeed, in example shows  $\inf_{\delta} \sup_{\theta \in \Theta} R(\theta, \delta) = \infty$  an iid sample of size  $n$  from  $\text{Uniform}[0, \theta]$ ,  $\theta \in \Theta = (0, \infty)$ . We will explore this idea in more detail in Section 2.4.2.

- (v) *Restriction to estimator classes:* Rather than optimizing over all decision rules  $\mathcal{C}$ , we may restrict to a subclass  $\mathcal{C}' \subset \mathcal{C}$ —for instance, unbiased estimators, equivariant estimators, or linear estimators. This yields

$$\inf_{\delta \in \mathcal{C}} \sup_{\theta \in \Theta} R(\theta, \delta) \leq \inf_{\delta \in \mathcal{C}'} \sup_{\theta \in \Theta} R(\theta, \delta).$$

The UMVUE and UMREE can be viewed through this lens: they are minimax within their respective estimator classes for appropriate loss functions.

Finding minimax estimators and determining the minimax risk is generally difficult: the definition involves an infimum over all estimators and a supremum over the parameter space, neither of which admits a direct computation in most problems. We now present several tools that simplify this task in structured settings.

Our first tool connects back to the theory of equivariant estimation developed in Section 2.2. Recall that in invariant decision problems—where both the model and loss respect a group symmetry—equivariant estimators have constant risk (Theorem 2.29). This dramatically simplifies the minimax problem: among estimators with constant risk, the one with the smallest risk is automatically minimax.

**Theorem 2.47** (Hunt-Stein). *Consider a decision problem where a locally compact abelian group  $G$  acts on  $\mathcal{X}$ ,  $\Theta$ , and  $\mathcal{D} = \Theta$ . Assume:*

- (i) *the action of  $G$  on  $\Theta$  is transitive,*
- (ii) *the model is equivariant under  $G$ ,*
- (iii) *the loss  $L$  is invariant under  $G$  and  $d \mapsto L(\theta, d)$  is convex for all  $\theta$ .*

*Then the UMREE  $\delta^*$  is minimax.*

*Proof* (♠). Let  $\delta^*$  be best equivariant with constant risk  $r^*$ . Let  $\nu$  be the Haar measure on  $G$ , and let  $G_1 \subset G_2 \subset \dots$  be an increasing sequence of compact sets with  $0 < \nu(G_n) < \infty$  and  $\bigcup_n G_n = G$ . For any estimator  $\delta$ , define

$$\bar{\delta}_n(x) = \frac{1}{\nu(G_n)} \int_{G_n} g^{-1} \delta(gx) d\nu(g).$$

Since  $\nu_n := \nu(\cdot \cap G_n)/\nu(G_n)$  is a probability measure, convexity and Jensen's inequality give

$$L(\theta, \bar{\delta}_n(x)) \leq \frac{1}{\nu(G_n)} \int_{G_n} L(\theta, g^{-1}\delta(gx)) d\nu(g).$$

Taking expectations and using invariance of the loss and equivariance of the model,

$$R(\theta, \bar{\delta}_n) \leq \frac{1}{\nu(G_n)} \int_{G_n} R(g\theta, \delta) d\nu(g) \leq \sup_{\theta'} R(\theta', \delta).$$

For abelian  $G$ , the sequence  $\bar{\delta}_n$  converges to an equivariant estimator  $\bar{\delta}$  satisfying the same risk bound (Exercise 2.19). Since  $\bar{\delta}$  is equivariant,  $R(\theta, \bar{\delta}) \geq r^*$ . Hence  $\sup_{\theta} R(\theta, \delta) \geq r^*$  for all  $\delta$ , so  $\delta^*$  is minimax.  $\square$

We now apply the Hunt-Stein theorem to determine the minimax risk in the Gaussian location model, and examine how this interacts with the James-Stein phenomenon from Section 2.3.1.

**Example 2.48.** Consider  $X \sim N_d(\theta, \sigma^2 I_d)$  with  $\theta \in \mathbb{R}^d$  under squared error loss  $L(\theta, \delta) = \|\delta - \theta\|^2$ . This is a location family: the translation group  $G = (\mathbb{R}^d, +)$  acts on  $\mathcal{X} = \mathbb{R}^d$  and  $\Theta = \mathbb{R}^d$  by  $g_c(x) = x + c$ , the model is equivariant, the loss is invariant, and  $G$  is locally compact abelian.

By Example 2.32, the (UMREE) Pitman estimator is  $\delta^*(X) = X$ . It has constant risk  $R(\theta, \delta^*) = \mathbb{E}_{\theta} \|X - \theta\|^2 = d\sigma^2$ . By the Hunt-Stein theorem,  $\delta^*$  is minimax, so the minimax risk for the estimation problem of estimating  $\theta \in \mathbb{R}^d$  is  $d\sigma^2$ .

For  $d \geq 3$ , Theorem 2.40 shows that the James-Stein estimator satisfies

$$R(\theta, \delta_{\text{JS}}) = d\sigma^2 - (d-2)^2\sigma^4 \mathbb{E}_{\theta} [\|X\|^{-2}] < d\sigma^2 \quad \text{for all } \theta \in \mathbb{R}^d.$$

Thus the James-Stein estimator is also minimax. As  $\|\theta\| \rightarrow \infty$ , the correction term vanishes and  $R(\theta, \delta_{\text{JS}}) \rightarrow d\sigma^2$ , so  $\sup_{\theta} R(\theta, \delta_{\text{JS}}) = d\sigma^2$ .

The moral is that minimaxity and admissibility are complementary criteria. We now have two minimax estimators: the UMVUE/UMREE/MLE and the James-Stein estimator. In high dimensions, the minimax criterion alone does not distinguish between  $X$  and  $\delta_{\text{JS}}$ —both achieve the same worst-case risk. Admissibility could break the tie: among minimax estimators, we might prefer those that are not dominated. Moreover, for any bounded subset  $\Theta' \subset \Theta$ ,  $\sup_{\theta \in \Theta'} R(\theta, \delta_{\text{JS}}) < \sup_{\theta \in \Theta} R(\theta, \delta)$ : if we are even slightly more optimistic than worst-case across the entire parameter space, we prefer the James-Stein estimator.  $\diamond$

Despite appearing to be opposing viewpoints, admissibility and minimaxity are not incompatible. In fact, minimaxity can imply admissibility under the right conditions.

**Theorem 2.49** (Unique minimax implies admissible). *If  $\delta^*$  is the (a.s.) unique minimax estimator, then  $\delta^*$  is admissible.*

*Proof.* Suppose  $\delta^*$  is unique minimax, meaning that if  $\delta'$  is any other estimator,

$$\sup_{\theta} R(\theta, \delta^*) < \sup_{\theta} R(\theta, \delta').$$

This implies that for all  $\delta' \neq \delta^*$ , there exists some  $\theta_0 \in \Theta$  such that  $R(\theta_0, \delta^*) < R(\theta_0, \delta')$ , so  $\delta'$  does not dominate  $\delta^*$ . Since  $\delta'$  was arbitrary,  $\delta^*$  is admissible.

Alternatively, suppose for contradiction that  $\delta^*$  is inadmissible, so some  $\delta'$  dominates it:  $R(\theta, \delta') \leq R(\theta, \delta^*)$  for all  $\theta$ , with strict inequality for at least one  $\theta$ . Then

$$\sup_{\theta} R(\theta, \delta') \leq \sup_{\theta} R(\theta, \delta^*) = R^*,$$

so  $\delta'$  is also minimax—contradicting the uniqueness of  $\delta^*$ .  $\square$

As Example 2.48 illustrates, uniqueness often fails in simple settings: both the MLE and James-Stein estimator are minimax for the Gaussian location model when  $d \geq 3$ . When multiple minimax estimators exist, admissibility provides a criterion for choosing among them.

We now turn to another tool for establishing minimaxity: the submodel flexibility noted in (2.3). If we can identify a submodel  $\mathcal{P}_0 \subset \mathcal{P}$  that captures the “hardest” part of the problem, then finding the minimax estimator over  $\mathcal{P}_0$  suffices.

**Lemma 2.50.** *If  $\delta$  is minimax for  $\theta$  under  $P \in \mathcal{P}_0 \subset \mathcal{P}$  and*

$$\sup_{P \in \mathcal{P}_0} R(P, \delta) = \sup_{P \in \mathcal{P}} R(P, \delta),$$

*then  $\delta$  is minimax for  $\theta$  under  $P \in \mathcal{P}$ .*

*Proof.* For any other estimator  $\delta'$ ,

$$\sup_{P \in \mathcal{P}} R(P, \delta') \geq \sup_{P \in \mathcal{P}_0} R(P, \delta') \geq \sup_{P \in \mathcal{P}_0} R(P, \delta) = \sup_{P \in \mathcal{P}} R(P, \delta).$$

$\square$

We illustrate the power of this lemma by reducing a vast nonparametric problem to the Gaussian location model, where the Hunt-Stein theorem applies.

**Example 2.51** (Population mean with bounded variance). Consider the nonparametric model

$$\mathcal{P} = \{P^{\otimes n} : P \text{ probability measure on } (\mathbb{R}, \mathcal{B}(\mathbb{R})) \text{ with } \text{Var}_P(X) \leq M\}$$

for some known  $M > 0$ . We wish to estimate  $\phi(P) = \mathbb{E}_P[X]$  under squared error loss.

The sample mean has risk  $R(P, \bar{X}) = \text{Var}_P(X)/n \leq M/n$ , with equality when  $\text{Var}_P(X) = M$ . To show  $\bar{X}$  is minimax, consider the Gaussian submodel  $\mathcal{P}_0 = \{N(\theta, M)^{\otimes n} : \theta \in \mathbb{R}\}$ . This is a location family, so by the Hunt-Stein theorem,  $\bar{X}$  is minimax over  $\mathcal{P}_0$  with constant risk  $M/n$ .

Since  $\mathcal{P}_0 \subset \mathcal{P}$  and  $\bar{X}$  achieves its maximum risk  $M/n$  on the submodel  $\mathcal{P}_0$ , Lemma 2.50 implies that  $\bar{X}$  is minimax over all of  $\mathcal{P}$ .  $\diamond$

### 2.4.1 Minimax rates

For some models, like the Gaussian location model studied in Example 2.48, the minimax risk is relatively easy to compute exactly in terms of various problem characteristics, such as dimension, variance, or sample size. Let us summarize the findings thus far.

**Example 2.52** (Minimax rate for the Gaussian location model). Consider the family of Gaussian location estimation problems indexed by  $i = (n, d, \sigma^2) \in \mathbb{N} \times \mathbb{N} \times (0, \infty)$ . For each  $i = (n, d, \sigma^2)$ , we observe  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N_d(\theta, \sigma^2 I_d)$  and wish to estimate  $\theta \in \mathbb{R}^d$  under squared error loss  $L_i(\theta, \delta) = \|\delta - \theta\|^2$ .

From Example 2.48, the minimax risk for a single observation ( $n = 1$ ) is  $d\sigma^2$ . For  $n$  i.i.d. observations, it suffices to consider the sufficient statistic  $\bar{X} \sim N_d(\theta, \sigma^2 I_d/n)$  (by Rao-Blackwell, Theorem 1.43), so rescaling gives minimax risk

$$R_{n,d,\sigma^2}^* = \frac{d\sigma^2}{n}.$$

We can extract rate information by examining how the risk scales with each characteristic; how much difficult does the problem become when we increase e.g. dimension, variance or how much easier it becomes when we increase the sample size.  $\diamond$

When the exact minimax risk is difficult to compute, we often settle for characterizing its *rate*—how the minimax risk scales with problem characteristics. This coarser lens is powerful: it allows us to compare the difficulty of different estimation problems and to identify which estimators are “rate-optimal” without pinning down exact constants.

**Definition 2.53.** Consider a collection of decision problems, indexed by  $i \in I$ , given by the tuple  $(\mathcal{X}_i, \mathcal{Y}_i, \mathcal{P}_i, \Theta_i, (\mathcal{D}_i, \mathcal{L}_i), L_i)$  with risk function  $\mathcal{R}_i$ . The *minimax rate* is a function  $r : I \rightarrow \mathbb{R}$  such that

$$c_* r(i) \leq \inf_{\delta} \sup_{\theta \in \Theta_i} \mathcal{R}_i(\theta, \delta) \leq C_* r(i)$$

for some constants  $c_*, C_* > 0$  and for all  $i \in I$ .

Knowledge of the exact minimax risk immediately yields the rate: in Example 2.52, the minimax rate is  $r(n, d, \sigma^2) = d\sigma^2/n$  with constants  $c_* = C_* = 1$ . More often, exact constants are intractable but the rate remains accessible. Proving a minimax rate requires two ingredients: an *upper bound* (exhibiting an estimator achieving risk  $O(r(i))$ ) and a *lower bound* (showing no estimator can do better than  $\Omega(r(i))$ ).

In many nonparametric problems, achieving the optimal rate requires carefully balancing bias and variance—neither the unbiased estimator nor the lowest-variance estimator is rate-optimal. The minimax rate framework helps identify the correct trade-off, even when exact constants remain elusive. We illustrate with a classical nonparametric model where the exact minimax risk is unknown, but the rate can be determined.

Consider observing  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} f$  where  $f$  is an unknown probability density on  $[0, 1]$ . Rather than estimating the entire density, we focus on a simpler target: evaluating  $f$  at a fixed point  $x_0 \in (0, 1)$ .

Without restrictions on  $f$ , this problem is hopeless—the density could have arbitrary local behavior near  $x_0$ . We therefore assume  $f$  belongs to a *Hölder smoothness class*. For  $\beta > 0$  and  $M > 0$ , define

$$\mathcal{F}_\beta(M) = \left\{ f : [0, 1] \rightarrow \mathbb{R}_+ : \int_0^1 f = 1, |f^{(k)}(x) - f^{(k)}(y)| \leq M|x - y|^\alpha \text{ for all } x, y \in [0, 1] \right\},$$

where  $k = \lfloor \beta \rfloor$  is the number of derivatives and  $\alpha = \beta - k \in [0, 1)$  controls the smoothness of the  $k$ th derivative. The case  $\beta = 1$  corresponds to Lipschitz densities;  $\beta = 2$  requires a Lipschitz first derivative; and so on. Larger  $\beta$  means smoother densities, which should make estimation easier.

Formally, the statistical model is  $\mathcal{P} = \{P_f^{\otimes n} : f \in \mathcal{F}_\beta(M)\}$ , where  $P_f$  denotes the distribution on  $[0, 1]$  with Lebesgue density  $f$ .

Consider the family of estimation problems indexed by  $i = (n, \beta) \in \mathbb{N} \times (0, \infty)$ , with parameter space  $\Theta_i = \mathcal{F}_\beta(M)$  for fixed  $M > 0$ , and loss  $L_i(f, \delta) = (\delta - f(x_0))^2$ .

We are interested in determining the minimax rate for the minimax risk

$$R_{n,\beta}^* = \inf_{\delta} \sup_{f \in \mathcal{F}_\beta(M)} \mathbb{E}_f[(\delta - f(x_0))^2].$$

First interesting observation: the problem has no unbiased estimator.

**Proposition 2.54.** *Consider the decision problem corresponding to estimating  $f(x_0)$  for a fixed  $x_0 \in (0, 1)$  on the basis of  $n$  i.i.d. observations  $X_1, \dots, X_n \sim f(x)dx$  from  $f \in \mathcal{F}_\beta(M)$ . For any sample size  $n \geq 1$ , there is no unbiased estimator of  $f(x_0)$ .*

*Proof.* Exercise 2.20. □

Since no unbiased estimator exists, we must navigate the bias-variance trade-off. The minimax rate framework tells us how to do this optimally.

If  $f$  were constant in a neighborhood of  $x_0$ , then the probability that  $X_i$  falls in an interval  $[x_0 - h, x_0 + h]$  would be approximately  $2h \cdot f(x_0)$ . Counting observations in this interval and dividing by  $2nh$  would give an unbiased estimator. Of course,  $f$  is not constant, so this procedure introduces bias—but if  $f$  is smooth and  $h$  is small, the bias should be small.

This reasoning leads to the *kernel density estimator*

$$\hat{f}_h(x_0) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{X_i - x_0}{h}\right),$$

where  $K : \mathbb{R} \rightarrow \mathbb{R}$  is a *kernel function* satisfying  $\int K = 1$ , and  $h > 0$  is the *bandwidth*. The simplest choice is the box kernel  $K(u) = \frac{1}{2} \mathbb{1}_{\{|u| \leq 1\}}$ , which recovers the histogram-style estimator described above. Smoother kernels (e.g., the ‘Gaussian kernel’  $K(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}$ ) yield smoother estimates but the same asymptotic behavior.

The bandwidth  $h$  controls the bias-variance trade-off. A small  $h$  means we average over a narrow window, capturing local behavior but using few observations—low bias, high variance. A large  $h$  averages over many observations but blurs local structure—low variance, high bias.

To quantify this, we analyze the bias and variance separately. For the bias, Taylor expansion of  $f$  around  $x_0$  combined with the Hölder condition yields (see Exercise 2.21)

$$|\mathbb{E}_f[\hat{f}_h(x_0)] - f(x_0)| \leq C_1 h^\beta$$

for a constant  $C_1$  depending on  $M$  and  $K$ . The smoothness  $\beta$  determines how quickly the bias vanishes as  $h \rightarrow 0$ : smoother densities have smaller bias for the same bandwidth.

For the variance, each summand  $\frac{1}{h} K(\frac{X_i - x_0}{h})$  has magnitude of order  $1/h$  and is nonzero with probability of order  $h$ . This gives (see again Exercise 2.21)

$$\text{Var}_f(\hat{f}_h(x_0)) \leq \frac{C_2}{nh}$$

for a constant  $C_2$ . The variance decreases with  $n$  (more observations) and increases as  $h \rightarrow 0$  (narrower window).

By Lemma 2.7, we obtain

$$\mathbb{E}_f[(\hat{f}_h(x_0) - f(x_0))^2] \leq C_1^2 h^{2\beta} + \frac{C_2}{nh}.$$

This expression captures the bias-variance trade-off: as  $h$  decreases, the first term shrinks but the second grows. The optimal bandwidth  $h^*$  minimizes the sum by

balancing the two terms. Setting  $h^{2\beta} \asymp 1/(nh)$  and solving yields

$$h^* \asymp n^{-1/(2\beta+1)}.$$

Substituting back, both the squared bias and the variance are of order  $n^{-2\beta/(2\beta+1)}$ , giving

$$\sup_{f \in \mathcal{F}_\beta(M)} \mathbb{E}_f[(\hat{f}_{h^*}(x_0) - f(x_0))^2] \lesssim n^{-2\beta/(2\beta+1)}.$$

This establishes an upper bound on the minimax risk: there exists an estimator achieving rate  $n^{-2\beta/(2\beta+1)}$ . But is this the best possible? Perhaps a cleverer construction—something other than kernel estimation—could achieve a faster rate. To rule this out, we need a *lower bound* showing that no estimator, however ingenious, can do better.

The constraint risk inequality (Lemma 2.43) is the key tool. Recall the intuition: if two parameter values  $f_0$  and  $f_1$  generate statistically similar distributions yet have well-separated values of the target functional  $f(x_0)$ , then no estimator can perform well at both. The product  $|f_1(x_0) - f_0(x_0)| \cdot \rho(P_{f_0}^{\otimes n}, P_{f_1}^{\otimes n})$  measures this tension, and the constraint risk inequality converts it into a lower bound on the worst-case risk.

We construct a pair of densities that are hard to distinguish. Let  $f_0 \equiv 1$  be the uniform density on  $[0, 1]$ , and let

$$f_h(x) = 1 + c h^\beta \psi\left(\frac{x - x_0}{h}\right),$$

where  $\psi$  is a smooth bump function with  $\int \psi = 0$  (ensuring  $f_h$  integrates to one) and  $c > 0$  is chosen so that  $f_h \in \mathcal{F}_\beta(M)$ . The Hölder constraint dictates this construction: a bump of width  $h$  can have height at most of order  $h^\beta$ , and we saturate this bound. The pointwise separation is therefore

$$|f_h(x_0) - f_0(x_0)| = c h^\beta \psi(0) \asymp h^\beta.$$

How similar are the distributions  $P_{f_0}^{\otimes n}$  and  $P_{f_h}^{\otimes n}$ ? The perturbation  $f_h - f_0 = c h^\beta \psi((\cdot - x_0)/h)$  has

$$\|f_h - f_0\|_2^2 = c^2 h^{2\beta} \int \psi(u)^2 du \cdot h = C' h^{2\beta+1},$$

since the bump has height  $h^\beta$  and width  $h$ . The Bhattacharyya coefficient satisfies (Exercise 2.22)

$$\rho(P_{f_0}^{\otimes n}, P_{f_h}^{\otimes n}) \geq \exp(-C n h^{2\beta+1})$$

for a constant  $C > 0$ . The distributions remain close (Bhattacharyya coefficient

bounded away from zero) provided  $nh^{2\beta+1} \lesssim 1$ ; they become distinguishable when  $nh^{2\beta+1} \gg 1$ . This reflects the intuition that  $n$  observations, each falling in the bump region with probability  $h$ , provide roughly  $nh$  effective observations for detecting a perturbation of size  $h^\beta$ —and the perturbation is detectable when its squared amplitude  $h^{2\beta}$  exceeds the noise level  $(nh)^{-1}$ , i.e., when  $nh^{2\beta+1} \gg 1$ .

Applying Lemma 2.43:

$$\sqrt{\mathbb{E}_{f_0}(\delta - 1)^2} + \sqrt{\mathbb{E}_{f_h}(\delta - f_h(x_0))^2} \geq h^\beta \cdot \exp(-C n h^{2\beta+1}).$$

The left-hand side is bounded by  $2\sqrt{\sup_f \mathbb{E}_f[(\delta - f(x_0))^2]}$ . Consequently, the worst-case risk of any estimator  $\delta$  satisfies

$$\sup_{f \in \mathcal{F}_\beta(M)} \mathbb{E}_f[(\delta - f(x_0))^2] \gtrsim h^{2\beta} \exp(-C n h^{2\beta+1}).$$

This bound holds for any  $h > 0$ . Optimizing over  $h$ —choosing  $h$  to maximize the right-hand side—we need  $nh^{2\beta+1} \lesssim 1$ , which gives  $h \asymp n^{-1/(2\beta+1)}$ . Substituting:

$$\inf_{\delta} \sup_{f \in \mathcal{F}_\beta(M)} \mathbb{E}_f[(\delta - f(x_0))^2] \gtrsim n^{-2\beta/(2\beta+1)}.$$

*Remark 2.55* (CDF vs density estimation). The contrast with CDF estimation (Example 2.11) is instructive. The empirical CDF  $\hat{F}_n(t) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{X_i \leq t\}}$  is unbiased for  $F(t)$  and achieves the parametric rate  $n^{-1/2}$ . Why is density estimation so much harder?

Geometrically, the CDF integrates the density up to  $t$ , averaging over a macroscopic region. This averaging stabilizes estimation: whether or not  $X_i$  falls below  $t$  is informative about  $F(t)$  regardless of the local shape of  $f$ . The density at a point, however, describes infinitesimal behavior—how much probability mass is packed into an arbitrarily small neighborhood of  $x_0$ . No finite sample can resolve infinitesimal structure without assumptions, which is why smoothness (the Hölder condition) is essential and why the rate  $n^{-2\beta/(2\beta+1)}$  is slower than  $n^{-1/2}$  for any finite  $\beta$ .

## 2.4.2 Adaptation

The kernel density estimator  $\hat{f}_{h^*}$  in the previous section achieves the minimax rate  $n^{-2\beta/(2\beta+1)}$  over  $\mathcal{F}_\beta(M)$ —but this requires choosing the bandwidth  $h^* \asymp n^{-1/(2\beta+1)}$ , which depends on the smoothness  $\beta$ . In practice, a statistician would rarely know the smoothness of the underlying density. In the previous section, we merely analyzed the ‘local difficulty’ of each  $\Theta_\beta$  separately, but a more realistic parameter space would be something like  $\Theta = \bigcup_{\beta \in B} \mathcal{F}_\beta(M)$  for a range of possible smoothness parameters  $B \subset (0, \infty)$ .

This raises a fundamental question: can we construct an estimator that achieves the (near) optimal rate *simultaneously for all*  $\beta$ , without knowing  $\beta$  in advance? An estimator that accomplishes this is called *adaptive*. Adaptation is a remarkably demanding requirement: the estimator must implicitly learn the smoothness of  $f$  from the data and calibrate its bias-variance trade-off accordingly.

More generally, suppose a parameter space admits a decomposition  $\Theta = \bigcup_{\beta \in \mathcal{B}} \Theta_\beta$ , where each subclass  $\Theta_\beta$  captures a different notion of complexity (smoothness, sparsity, etc.). The minimax risk over  $\Theta_\beta$  measures the difficulty of estimation when the statistician *knows* that  $\theta \in \Theta_\beta$ . The adaptive minimax rate asks: what is the best achievable rate when this knowledge is unavailable—when can a single estimator perform well across all slices simultaneously?

**Definition 2.56** (Adaptive minimax rate). Consider a collection of decision problems indexed by  $j \in J$ , with risk functions  $\mathcal{R}_j$ . Suppose  $\Theta_j = \bigcup_{\beta \in \mathcal{B}} \Theta_{j,\beta}$  for a set  $\mathcal{B}$ . The *adaptive minimax rate* for  $\{\Theta_j\}$  indexed by  $\mathcal{B}$  is a function  $r : J \times \mathcal{B} \rightarrow \mathbb{R}$  such that

$$c_* \leq \inf_{\delta} \sup_{\beta \in \mathcal{B}} \frac{\sup_{\theta \in \Theta_{j,\beta}} \mathcal{R}_j(\theta, \delta)}{r(j, \beta)} \leq C_*$$

for some constants  $c_*, C_* > 0$  and for all  $j \in J$ , where the infimum is over all decision rules  $\delta$  that may depend on  $j$  but not on  $\beta$ .

The adaptive minimax rate is always at least as large as the ordinary minimax rate for each ‘slice’  $\Theta_{j,\beta}$ , since the infimum is over a smaller class of estimators. The ratio  $r(j, \beta)/r_{\text{minimax}}(j, \beta)$  quantifies the *cost of adaptation*: the price paid for not knowing  $\beta$ . An interesting question is whether this cost is negligible (absorbed into constants), moderate (e.g., a logarithmic factor), or severe (a polynomial penalty).

Let us return to the example of estimating the height of a density at a point  $x_0 \in (0, 1)$ . The parameter space  $\mathcal{F} = \bigcup_{\beta > 0} \mathcal{F}_\beta(M)$  is naturally indexed by smoothness, and the ordinary minimax rate over each slice is  $n^{-2\beta/(2\beta+1)}$  (Section 2.4.1). In the language of Definition 2.56, an estimator  $\hat{\delta}_n$  (not depending on  $\beta$ ) achieves the upper bound in the adaptive minimax rate if there exists  $C > 0$  (independent of  $n$  and  $\beta$ ) such that

$$\sup_{f \in \mathcal{F}_\beta(M)} \mathbb{E}_f[(\hat{\delta}_n - f(x_0))^2] \leq C \cdot r(n, \beta) \quad \text{for all } \beta \in \mathcal{B}.$$

The question is: what is  $r(n, \beta)$ ? Can it equal the ordinary minimax rate  $n^{-2\beta/(2\beta+1)}$ , or does adaptation impose a penalty? To answer this question, we will use a variation of the constraint risk inequality of Lemma 2.43.

**Lemma 2.57** (Constraint risk inequality via likelihood ratio). *Let  $(\Theta, \mathbf{d})$  be a (semi-)metric space and let  $P_f, P_g$  be probability measures on  $(\mathcal{X}, \mathcal{X})$  with  $P_g \ll P_f$ . Write*

$L = dP_g/dP_f$  and assume  $\mathbb{E}_f[L^2] < \infty$ . Then for any estimator  $\delta : \mathcal{X} \rightarrow \Theta$ ,

$$\mathbb{E}_g[\mathbf{d}(\delta, g)^2] \geq \left( \mathbf{d}(f, g) - \sqrt{\mathbb{E}_f[\mathbf{d}(\delta, f)^2]} \sqrt{\mathbb{E}_f[L^2]} \right)_+^2.$$

*Proof.* By the triangle inequality, for every  $x \in \mathcal{X}$ ,

$$\mathbf{d}(\delta(x), g) \geq \mathbf{d}(f, g) - \mathbf{d}(\delta(x), f).$$

Taking expectations under  $P_g$  and using Jensen's inequality,

$$\sqrt{\mathbb{E}_g[\mathbf{d}(\delta, g)^2]} \geq \mathbb{E}_g[\mathbf{d}(\delta, g)] \geq \mathbf{d}(f, g) - \mathbb{E}_g[\mathbf{d}(\delta, f)].$$

Since  $P_g \ll P_f$  with likelihood ratio  $L = dP_g/dP_f$ ,

$$\mathbb{E}_g[\mathbf{d}(\delta, f)] = \mathbb{E}_f[\mathbf{d}(\delta, f) L].$$

By Cauchy–Schwarz,

$$\mathbb{E}_f[\mathbf{d}(\delta, f) L] \leq \sqrt{\mathbb{E}_f[\mathbf{d}(\delta, f)^2]} \sqrt{\mathbb{E}_f[L^2]}.$$

Combining the above inequalities and squaring the positive part yields the claim.  $\square$

We now apply Lemma 2.57 to quantify the cost of adaptation. The key insight is that an estimator achieving the optimal rate on the smoothest class  $\mathcal{F}_{\beta_{\max}}(M)$  cannot simultaneously achieve the optimal rate on rougher classes—it must incur a logarithmic penalty.

**Proposition 2.58** (Cost of adaptation via the CRI). *Fix  $0 < \beta_{\min} < \beta_{\max} < \infty$  and  $M > 0$ , and consider pointwise density estimation at  $x_0 \in (0, 1)$ . Let  $\delta$  be any estimator. Suppose there exists constants  $A, B > 0$  such that*

$$\sup_{f \in \mathcal{F}_{\beta_{\max}}(M)} \mathbb{E}_f[(\delta - f(x_0))^2] \leq A \log^B(n) n^{-\frac{2\beta_{\max}}{2\beta_{\max}+1}} \quad \text{for all large } n. \quad (2.4)$$

*Then for every  $\beta \in [\beta_{\min}, \beta_{\max})$  there exists a constant  $c = c(\beta, \beta_{\min}, \beta_{\max}, M, A) > 0$  such that for all large  $n$ ,*

$$\sup_{g \in \mathcal{F}_{\beta}(M)} \mathbb{E}_g[(\delta - g(x_0))^2] \geq c \left( \frac{\log n}{n} \right)^{\frac{2\beta}{2\beta+1}}.$$

*In particular, any estimator that is rate-optimal on the smoother class  $\mathcal{F}_{\beta_{\max}}(M)$  must pay a logarithmic penalty on every rougher class.*

*Proof.* Exercise 2.23. □

Proposition 2.58 establishes that adaptation is not free: any estimator achieving the optimal rate  $n^{-2\beta_{\max}/(2\beta_{\max}+1)}$  on the smoothest class must suffer a logarithmic penalty on rougher classes. A natural question is whether this penalty is sharp—can we construct an estimator that achieves the rate  $(\log n/n)^{2\beta/(2\beta+1)}$  uniformly over all  $\beta \in [\beta_{\min}, \beta_{\max}]$ ?

The answer is yes, via *Lepski's method*. The idea is to compute kernel estimators at many bandwidths simultaneously and select the largest bandwidth whose estimate is still consistent with all finer-resolution estimates. We now describe this construction concretely.

Let  $K : \mathbb{R} \rightarrow \mathbb{R}$  be a bounded kernel supported on  $[-1, 1]$  with  $\int K(u) du = 1$ . For  $h > 0$ , define the kernel estimator at  $x_0$  by

$$\hat{f}_h(x_0) := \frac{1}{nh} \sum_{i=1}^n K\left(\frac{X_i - x_0}{h}\right). \quad (2.5)$$

We evaluate this estimator over a dyadic grid of bandwidths  $\mathcal{H} := \{h_j = 2^{-j} : j = j_{\min}, \dots, j_{\max}\}$ , where  $j_{\min}$  and  $j_{\max}$  are chosen so that the coarsest bandwidth  $h_{j_{\min}}$  is of order 1 and the finest  $h_{j_{\max}}$  is of order  $n^{-\frac{1}{2\beta_{\min}+1}}$ . The grid therefore has  $|\mathcal{H}| \asymp \log n$  elements.

The selection rule works as follows. Fix a constant  $A > 0$  and define the threshold

$$\tau(h) := A \sqrt{\frac{\log n}{nh}},$$

which is calibrated to the standard deviation of  $\hat{f}_h(x_0)$  up to the logarithmic factor. The selected bandwidth is

$$\hat{h} := \max \left\{ h \in \mathcal{H} : |\hat{f}_h(x_0) - \hat{f}_{h'}(x_0)| \leq \tau(h') \text{ for all } h' \in \mathcal{H} \text{ with } h' \leq h \right\}, \quad (2.6)$$

and the adaptive estimator is  $\hat{\delta}_n := \hat{f}_{\hat{h}}(x_0)$ . The intuition is that as long as  $h$  is not too large, the estimates  $\hat{f}_h(x_0)$  and  $\hat{f}_{h'}(x_0)$  for  $h' \leq h$  should agree up to their sampling variability. When  $h$  exceeds the optimal bandwidth, the bias of  $\hat{f}_h(x_0)$  becomes detectable: it starts to disagree with finer-resolution estimates by more than their noise level. Lepski's rule selects the largest  $h$  at which no such disagreement is detected. In spirit, this resembles an optimal stopping problem: we scan from coarse to fine resolution, enjoying decreasing bias, and stop just before the variance cost outweighs the gain.

**Proposition 2.59** (Adaptive upper bound via Lepski's method). *Fix  $0 < \beta_{\min} <$*

$\beta_{\max} < \infty$  and  $M > 0$ . There exists a choice of kernel  $K$  (of order at least  $\lfloor \beta_{\max} \rfloor$ ) and a constant  $A > 0$  in (2.6) such that the estimator  $\hat{\delta}_n = \hat{f}_h(x_0)$  in (2.5) satisfies, for all large  $n$ ,

$$\sup_{\beta \in [\beta_{\min}, \beta_{\max}]} \sup_{f \in \mathcal{F}_\beta(M)} \mathbb{E}_f [(\hat{\delta}_n - f(x_0))^2] \lesssim \left( \frac{\log n}{n} \right)^{\frac{2\beta}{2\beta+1}}.$$

*Proof.* Exercise 2.24. □

Combining Proposition 2.59 (the upper bound) with Proposition 2.58 (the lower bound) yields a complete characterization of the adaptive minimax rate.

**Theorem 2.60** (Adaptive pointwise rate over Hölder classes). *Fix  $0 < \beta_{\min} < \beta_{\max} < \infty$  and  $M > 0$ . Consider the union model  $\mathcal{F} = \bigcup_{\beta \in [\beta_{\min}, \beta_{\max}]} \mathcal{F}_\beta(M)$  and the loss  $L(f, \delta) = (\delta - f(x_0))^2$  for a fixed  $x_0 \in (0, 1)$ . There exist constants  $0 < c < C < \infty$  (depending only on  $M, \beta_{\min}, \beta_{\max}$  and the kernel) such that for all  $n$  large enough,*

$$c \leq \inf_{\delta} \sup_{\beta \in [\beta_{\min}, \beta_{\max}]} \sup_{f \in \mathcal{F}_\beta(M)} \frac{\mathbb{E}_f [(\delta - f(x_0))^2]}{(\log n/n)^{2\beta/(2\beta+1)}} \leq C.$$

*In particular, the adaptive minimax rate is*

$$r_{\text{adapt}}(n, \beta) \asymp (\log n/n)^{2\beta/(2\beta+1)}.$$

Adaptation problems arise whenever the difficulty of estimation varies across the parameter space according to some unknown structural quantity—smoothness in density estimation, sparsity level in high-dimensional regression, signal strength in detection problems—and the statistician must calibrate a tuning parameter (bandwidth, regularization strength, threshold) without knowing this quantity. Besides Lepski’s method, approaches come in many different flavors: cross-validation, information criteria, and Bayesian methods that place priors over the hyperparameter. The adaptive minimax framework provides a unified lens for studying such problems, and its conclusion is noteworthy: the minimax paradigm, often criticized as pessimistic, naturally leads us to ask not just “what is the cost of not knowing where in the parameter space the difficulty lies?”—a rather more nuanced question.

### 2.4.3 (♠) Ill-posedness

Recall the linear regression model of Example 2.1:

$$Y = X\beta + \epsilon, \quad \epsilon \sim N_n(0, \sigma^2 I_n).$$

Given a full column rank design matrix  $X \in \mathbb{R}^{n \times p}$  with  $n > p$ , we can write the statistical model as

$$\mathcal{P} = \{N_n(X\beta, \sigma^2 I_n) : \beta \in \mathbb{R}^p\} = \{N_n(\mu, \sigma^2 I_n) : \mu \in \text{col}(X)\},$$

where  $\text{col}(X)$  denotes the column space of  $X$ . The two descriptions define the same family of distributions, but the indexing is different. If  $\beta$  is the quantity of interest, the first parameterization is natural: we can define a map  $P \mapsto \beta(P)$  from  $\mathcal{P}$  to  $\mathbb{R}^p$  that inherits the structure of  $\mathcal{P}$ , and the map  $\beta \mapsto P_\beta$  is injective (since  $X$  has full column rank).

However, nothing prevents us from indexing a model by any set of sufficient cardinality. Consider the case where  $X$  does not have full column rank—or more dramatically,  $p > n$ . The collection  $\{N_n(X\beta, \sigma^2 I_n) : \beta \in \mathbb{R}^p\}$  still describes a statistical model, but  $\mathbb{R}^p$  is no longer a parameter space in the sense of Definition 1.3: the map  $\beta \mapsto P_\beta$  is not injective, since  $P_\beta = P_{\beta'}$  whenever  $\beta - \beta' \in \ker(X)$ . Even with perfect knowledge of the distribution, the index  $\beta$  cannot be uniquely recovered.

We may nonetheless wish to estimate  $\beta$ —or a functional of it—and can define a risk function

$$\mathcal{R}(\beta, \delta) = \mathbb{E}_{P_\beta}[L(\beta, \delta(Y))].$$

This is a legitimate object, but it is a risk function on the *index set*  $\mathbb{R}^p$ , not on the model  $\mathcal{P}$ . The distinction has concrete consequences:

- (i) *Unbiased estimators need not exist.* An unbiased estimator of  $\beta$  would need to satisfy  $\mathbb{E}_{P_\beta}[\delta(Y)] = \beta$  for all  $\beta \in \mathbb{R}^p$ . But if  $P_\beta = P_{\beta'}$  for  $\beta \neq \beta'$ , then  $\mathbb{E}_{P_\beta}[\delta(Y)] = \mathbb{E}_{P_{\beta'}}[\delta(Y)]$ , making  $\delta$  unable to distinguish  $\beta$  from  $\beta'$ .
- (ii) *Sufficiency and completeness pertain to the model only, no longer the index.* A sufficient statistic reduces the data without losing information about which distribution  $P \in \mathcal{P}$  generated the data—but it says nothing about which index  $\beta$  corresponds to that distribution. In the regression example, the projection  $\hat{\mu} = X(X^\top X)^{-1}X^\top Y$  is sufficient and complete for the model  $\mathcal{P}$  equipped with the parameter space  $\mathcal{P}$ .
- (iii) *Structure of the index set does not correspond to the structure of the model.* Even if the indexing set has structure allowing for differentiability, the Fisher information matrix is typically no longer invertible. Similarly, the equivariance framework of Section 2.2 breaks down: the translation group on  $\mathbb{R}^p$  does not induce a well-defined action on the model when  $\ker(X) \neq \{0\}$ .

(iv) *The minimax risk is often infinite.* If  $L(\beta, \delta) = \|\beta - \delta\|^2$ , then for any estimator  $\delta$ ,

$$\sup_{\beta \in \mathbb{R}^p} \mathcal{R}(\beta, \delta) = \infty,$$

since  $\beta$  can be chosen with an arbitrarily large component in  $\ker(X)$  that  $\delta$  has no hope of recovering.

Consider a map  $\iota : \mathcal{I} \rightarrow \mathcal{P}$  that sends each index value to its corresponding distribution. In a *well-posed* problem,  $\iota$  is injective and its inverse is ‘continuous’: ‘nearby’ distributions correspond to ‘nearby’ parameters, and estimation amounts to inverting  $\iota$ . In an *ill-posed* problem,  $\iota^{-1}$  is either undefined (non-identifiability) or ‘discontinuous’ (instability): distributions that are statistically indistinguishable can correspond to very different parameter values. The minimax rate then reflects both the complexity of  $\mathcal{I}$  and the severity of this instability.

As a remedy, we may restrict  $\beta$  to a subset  $\mathcal{I} \subset \mathbb{R}^p$  that constrains its complexity. The choice of  $\mathcal{I}$  determines the difficulty of the problem. One route is to restrict the index set until it can be identified through the model: impose constraints on  $\beta \in \mathcal{I}$  strong enough until we can define a map  $P \mapsto \beta(P)$  from  $\mathcal{P}$  to  $\mathcal{I}$ .

**Example 2.61** (The RIP condition). Let  $Y = X\beta + \epsilon$  with  $X \in \mathbb{R}^{n \times p}$ ,  $p > n$ , and  $\epsilon \sim N_n(0, \sigma^2 I_n)$ . Without restrictions,  $\beta$  is not identifiable:  $\ker(X) \neq \{0\}$ , so infinitely many values of  $\beta$  produce the same distribution.

Restricting to sparse parameters— $\Theta_s = \{\beta \in \mathbb{R}^p : \|\beta\|_0 \leq s\}$  for  $s \ll n$ —restores identifiability under conditions on  $X$ . A sufficient condition is the *restricted isometry property* (RIP): for some  $\gamma_s \in (0, 1)$ ,

$$(1 - \gamma_s)\|\beta\|^2 \leq \|X\beta\|^2 \leq (1 + \gamma_s)\|\beta\|^2 \quad \text{for all } s\text{-sparse } \beta.$$

This ensures that  $X$  acts nearly isometrically on sparse vectors, so distinct sparse  $\beta$  produce distinguishable observations.

The minimax rate over  $\Theta_s$  turns out to be  $s \log(p/s)/n$ , which depends on the sparsity  $s$ , the ambient dimension  $p$ , and the sample size  $n$ . The  $\log(p/s)$  factor reflects the cost of not knowing which  $s$  coordinates are active—a search problem layered on top of estimation.  $\diamond$

However, the minimax framework does not require identifiability. To get an informative analysis, it only requires that the worst-case risk is finite.

**Example 2.62** (Prediction loss without identifiability). Consider the same setup as Example 2.61, but now take a loss function that does not penalize distinctions the data

cannot make. The *prediction loss*

$$L(\beta, \delta) = \frac{1}{n} \|X(\delta - \beta)\|^2$$

measures how well we estimate the mean response  $X\beta$ , not  $\beta$  itself. If  $\beta - \beta' \in \ker(X)$ , then  $L(\beta, d) = L(\beta', d)$ : equivalent parameters incur no loss against each other. Under this loss, the minimax rate over  $\Theta_s = \{\beta \in \mathbb{R}^p : \|\beta\|_0 \leq s\}$  is

$$\inf_{\delta} \sup_{\beta \in \Theta_s} \frac{1}{n} \mathbb{E}_{\beta} \|X(\delta - \beta)\|^2 \asymp \frac{s\sigma^2 \log(p/s)}{n},$$

under conditions on  $X$  that are weaker than the RIP—identifiability of  $\beta$  is not required.

The factor  $s\sigma^2/n$  is the parametric rate for estimating  $s$  unknown coordinates. The logarithmic factor  $\log(p/s)$  reflects the combinatorial cost of not knowing which  $s$  coordinates are active—a search problem layered on top of estimation, reminiscent of the adaptation cost encountered in Section 2.4.2.

When  $\sigma_{\min}(X) > 0$ , the prediction loss and the estimation loss  $\|\delta - \beta\|^2$  are comparable up to constants, since

$$\sigma_{\min}(X)^2 \|\beta - \beta'\|^2 \leq \|X(\beta - \beta')\|^2 \leq \sigma_{\max}(X)^2 \|\beta - \beta'\|^2.$$

In this case, the minimax rate under estimation loss is of the same order. When  $\sigma_{\min}(X) = 0$ —as is necessarily the case when  $p > n$ —these two losses decouple: parameters that are far apart in  $\ell_2$  may produce identical distributions, and estimation loss becomes the harder problem. The prediction loss sidesteps this difficulty by measuring performance in the metric that the data actually see.

A natural estimator is the LASSO,

$$\hat{\beta}_{\text{LASSO}} = \operatorname{argmin}_{\beta \in \mathbb{R}^p} \left\{ \frac{1}{2n} \|Y - X\beta\|^2 + \lambda \|\beta\|_1 \right\}, \quad (2.7)$$

which replaces the intractable  $\ell_0$ -constraint with a convex  $\ell_1$ -penalty. The tuning parameter  $\lambda > 0$  plays a role analogous to the bandwidth in kernel density estimation: it controls the bias-variance trade-off, with larger  $\lambda$  producing sparser—and hence more biased but lower variance—estimates. For an appropriate choice of  $\lambda$ , the LASSO achieves the minimax rate over each  $\Theta_s$  simultaneously, showing it attains the adaptive minimax rate for the unknown sparsity  $s$  without requiring it as an input. We refer the interested reader to Geer 2016 for a thorough treatment.  $\diamond$

## Exercises

*Exercise 2.1* (UMVUE for the mean). Consider the (nonparametric) model corresponding to observing  $X_1, \dots, X_n$  i.i.d. from an unknown distribution  $P$  on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$  with finite variance. We wish to estimate the population mean  $\phi(P) = \mathbb{E}_P[X_1]$ .

- Show that the sample mean  $\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i$  is the UMVUE for  $\phi(P) = \mathbb{E}_P[X_1]$ . You may use the result from Exercise 1.17 that the order statistics are a complete sufficient statistic for this model.
- Show that the sample variance  $S^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X}_n)^2$  is the UMVUE for the population variance  $\sigma^2(P) = \text{Var}_P(X_1)$ .

*Exercise 2.2* (UMVUE for the CDF in the normal mean model). Consider a statistical model corresponding to  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$ ,  $\theta \in \mathbb{R}$  unknown, known variance  $\sigma^2 > 0$ . We wish to estimate the CDF at a fixed point  $t$ , i.e.,  $\phi(\theta) = \Phi((t - \theta)/\sigma)$ .

- Show that the UMVUE for  $\phi(\theta)$  is given by

$$\delta(X) = \Phi\left(\frac{t - \bar{X}}{\sigma\sqrt{1 - 1/n}}\right).$$

- Compare the variance of  $\delta(X)$  with the variance of the empirical CDF  $\hat{F}_n(t) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{\{X_i \leq t\}}$  of Example 2.11. Which one is smaller and why?

*Exercise 2.3* (Linear model). Let  $Y \sim N_n(X\beta, \sigma^2 I_n)$  for unknown  $\beta \in \mathbb{R}^p$  and  $\sigma^2 > 0$ , where  $X \in \mathbb{R}^{n \times p}$  has full column rank.

- Show that  $(\hat{\beta}_{\text{OLS}}, s^2)$ , where  $\hat{\beta}_{\text{OLS}} = (X^\top X)^{-1} X^\top Y$  and  $s^2 = \frac{1}{n-p} \|Y - X\hat{\beta}_{\text{OLS}}\|^2$ , is a complete sufficient statistic for  $(\beta, \sigma^2)$ .
- Conclude that  $\hat{\beta}_{\text{OLS}}$  is the UMVUE for  $\beta$ .
- Recall that the Gauss-Markov theorem states that  $\hat{\beta}_{\text{OLS}}$  is the Best Linear Unbiased Estimator (BLUE) regardless of the distribution of  $Y$ , as long as it has mean  $X\beta$  and covariance  $\sigma^2 I_n$ . How does the UMVUE property under normality relate to the BLUE property?

*Exercise 2.4* (Bias-Variance Decomposition). Prove Lemma 2.7.

*Exercise 2.5* (Consistency and Bias). Let  $\hat{\theta}_1, \hat{\theta}_2, \dots$  be i.i.d. random vectors in  $\mathbb{R}^d$  with finite covariance matrix  $\Sigma$  and mean vector  $\mu$ . Consider ‘the estimator’  $\bar{\theta}_m = \frac{1}{m} \sum_{j=1}^m \hat{\theta}_j$  of  $\theta \in \mathbb{R}^d$ . Show that  $\mathbb{E}[\|\bar{\theta}_m - \theta\|^2] \rightarrow 0$  if and only if  $\mathbb{E}[\hat{\theta}_1] = \theta$ .

*Exercise 2.6* (Uncorrelated with 0-unbiased estimators). Let  $\delta(X)$  have finite variance. Show that a necessary and sufficient condition for  $\delta$  to be the UMVUE of its expectation  $g(\theta) = \mathbb{E}_\theta[\delta(X)]$  is that  $\text{Cov}_\theta(\delta(X), U(X)) = 0$  for all  $\theta \in \Theta$  and all statistics  $U$  such that  $\mathbb{E}_\theta[U(X)] = 0$  for all  $\theta \in \Theta$  (i.e.,  $U$  is an unbiased estimator of zero).

*Exercise 2.7* (Cramer-Rao Lower Bounds). (a) Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$  with known variance  $\sigma^2 > 0$ . Compute the Cramer-Rao lower bound for the variance of any unbiased estimator of  $\theta \in \mathbb{R}$ .

(b) Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Bernoulli}(p)$  for  $p \in (0, 1)$ . Derive the Cramer-Rao lower bound for the variance of any unbiased estimator of  $p$ . What is the noticeable difference compared to the normal distribution case? What is the worst-case lower bound (over  $p \in (0, 1)$ )?

*Exercise 2.8* (DQM implications). The aim is to prove Lemma 2.13. Throughout, let  $\mu$  be a dominating measure for the model with densities  $p_\theta = dP_\theta/d\mu$ .

- (a) Show that  $\sqrt{p_\theta}, \sqrt{p_{\theta+h}} \in L^2(\mu)$ , and conclude that  $A_h := \sqrt{p_{\theta+h}} - \sqrt{p_\theta} \in L^2(\mu)$ .
- (b) Using part (a) and the fact that  $L^2(\mu)$  is a vector space, conclude that  $h^\top S_\theta \sqrt{p_\theta} \in L^2(\mu)$  for all sufficiently small  $h$  and hence  $I(\theta) = E_\theta[S_\theta S_\theta^\top]$  has all entries finite.
- (c) Using the algebraic identity  $a - b = (\sqrt{a} - \sqrt{b})(\sqrt{a} + \sqrt{b})$  and the DQM expansion, show that

$$p_{\theta+h} - p_\theta = h^\top S_\theta p_\theta + \tilde{r}_h,$$

where  $\tilde{r}_h$  is a remainder term that you should specify explicitly in terms of  $r_h := \sqrt{p_{\theta+h}} - \sqrt{p_\theta} - \frac{1}{2} h^\top S_\theta \sqrt{p_\theta}$ .

- (d) Let  $T : \mathcal{X} \rightarrow \mathbb{R}$  satisfy  $E_\theta[T^2] < \infty$ . Show that the contribution of the remainder term to  $\psi(\theta + h) - \psi(\theta)$  is negligible:

$$\int T(x) \tilde{r}_h(x) d\mu(x) = o(\|h\|).$$

*Hint:* Use the Cauchy-Schwarz inequality and the bound  $\|r_h\|_{L^2(\mu)} = o(\|h\|)$ .

- (e) Combine the results of parts (c) and (d) to conclude that if  $E_{\theta'}[T^2] < \infty$  for all  $\theta'$  in a neighborhood of  $\theta$ , then  $\psi(\theta') = E_{\theta'}[T]$  is differentiable at  $\theta$  with  $\nabla \psi(\theta) = E_\theta[T \cdot S_\theta]$ .

*Exercise 2.9* (Covariance matrix estimation as an invariant decision problem). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N_p(0, \Sigma)$  with  $\Sigma$  positive definite, so the sufficient statistic is  $S = \sum_{i=1}^n X_i X_i^\top \sim \text{Wishart}_p(n, \Sigma)$ . The parameter space is  $\Theta = \mathcal{S}_p^{++}$ , the set of  $p \times p$  positive definite matrices.

Consider the general linear group  $G = \text{GL}(p)$  acting on data by  $g_A(X_1, \dots, X_n)$  as  $(A, X_i) \mapsto AX_i$  (equivalently,  $g_A S = A S A^\top$ ) and on parameters by  $g_A \Sigma = A \Sigma A^\top$ .

- Show that the model is equivariant under this group action.
- The squared Frobenius loss  $L(\Sigma, \delta) = \|\delta - \Sigma\|_F^2$ , where  $\|M\|_F = \sqrt{\text{Tr}(M^\top M)}$  is the Frobenius norm, is *not* invariant under this action. Verify this by finding matrices  $A$ ,  $\Sigma$ , and  $\delta$  such that  $L(A \Sigma A^\top, A \delta A^\top) \neq L(\Sigma, \delta)$ .
- The *Stein loss* is defined as

$$L_S(\Sigma, \delta) = \text{Tr}(\delta \Sigma^{-1}) - \log |\delta \Sigma^{-1}| - p.$$

Show that Stein loss is invariant under the action of  $\text{GL}(p)$ .

*Exercise 2.10* (Pitman estimator for a scale family). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Exp}(\sigma)$  with density  $f(x | \sigma) = \frac{1}{\sigma} e^{-x/\sigma}$  for  $x > 0$  and  $\sigma > 0$ . We wish to estimate  $\sigma$  under the scale-invariant loss

$$L(\sigma, \delta) = \left( \frac{\delta}{\sigma} - 1 \right)^2.$$

- Verify that this loss is invariant under the multiplicative group  $G = (\mathbb{R}_{>0}, \times)$  acting by  $g_c \sigma = c\sigma$  and  $g_c \delta = c\delta$ .
- Show that an UMREE estimator is of the form  $\delta^*(x) = a \sum_{i=1}^n x_i$  for some constant  $a > 0$ . *Hint:* Consider an equivariant estimator  $\delta(cx) = c\delta(x)$  and its Rao-Blackwellization  $\delta^* = \mathbb{E}_\sigma[\delta(X) | \bar{X}]$ , where  $\bar{X} = n^{-1} \sum_{i=1}^n X_i$ .
- Find the UMREE by minimizing  $\mathcal{R}(1, \delta^*)$  in  $a > 0$ . *Hint:* If  $X_i \stackrel{\text{iid}}{\sim} \text{Exp}(1)$ , then  $\sum_{i=1}^n X_i \sim \text{Gamma}(n, 1)$ .

*Exercise 2.11* (Pitman estimator for the Cauchy location family). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Cauchy}(\theta, 1)$  with density

$$f(x - \theta) = \frac{1}{\pi(1 + (x - \theta)^2)}, \quad x \in \mathbb{R}, \theta \in \mathbb{R}.$$

- Write down the Pitman estimator for  $\theta$  under squared error loss.

(b) For  $n = 2$ , show that the Pitman estimator can be written as

$$\delta^*(X_1, X_2) = \frac{X_1 + X_2}{2} + \frac{1}{2}(X_1 - X_2) \cdot g\left(\frac{X_1 - X_2}{2}\right)$$

for some odd function  $g : \mathbb{R} \rightarrow \mathbb{R}$ , and reason that  $g \equiv 0$ .

*Hint:* Use the substitution  $\eta = \theta - \frac{X_1 + X_2}{2}$  and let  $u = \frac{X_1 - X_2}{2}$ .

(c) For  $n = 3$ , show that as  $x_3 \rightarrow \infty$  with  $x_1, x_2$  fixed, the Pitman estimator satisfies

$$\delta^*(x_1, x_2, x_3) \rightarrow \frac{x_1 + x_2}{2}.$$

Interpret this result.

*Exercise 2.12* (Admissibility of the MLE in the normal mean model for  $d = 1$ ). For  $d = 1$  and  $d = 2$  the MLE  $X$  is admissible in the model  $X \sim N_d(\theta, I)$ . This exercise deals with the case  $d = 1$ . So we assume that  $X \sim N(\theta, 1)$ . The goal is to prove that there exists no other estimator  $\hat{\theta}$  such that  $E_\theta(\hat{\theta} - \theta)^2 \leq E_\theta(X - \theta)^2$  for all  $\theta \in \mathbb{R}$ , with strict inequality for some  $\theta \in \mathbb{R}$ .

For  $\tau > 0$ , consider the  $N(0, \tau)$  prior on the parameter  $\theta$ . Denote the corresponding prior density by  $\pi_\tau$ .

(i) Show that if an estimator  $\hat{\theta}$  as described above would exist, then there would exist an  $\varepsilon > 0$  and  $\theta_0 < \theta_1$  such that

$$1 - \int E_\theta(\hat{\theta} - \theta)^2 \pi_\tau(\theta) d\theta \geq \varepsilon \int_{\theta_0}^{\theta_1} \pi_\tau(\theta) d\theta.$$

(ii) Let  $\tilde{\theta}_\tau$  be the posterior mean corresponding to the prior  $\pi_\tau$ . Compute the corresponding Bayes risk

$$\int E_\theta(\tilde{\theta}_\tau - \theta)^2 \pi_\tau(\theta) d\theta.$$

You may use without proof that the posterior mean minimizes this integrated risk among all estimators.

(iii) Using the results of (i) and (ii), show that if an estimator  $\hat{\theta}$  as described above would exist, then

$$\frac{1 - \int E_\theta(\hat{\theta} - \theta)^2 \pi_\tau(\theta) d\theta}{1 - \int E_\theta(\tilde{\theta}_\tau - \theta)^2 \pi_\tau(\theta) d\theta} \rightarrow \infty$$

as  $\tau \rightarrow \infty$ . Derive a contradiction.

*Remark 2.63.* Admissibility of the MLE in the case  $d = 2$  can also be proved using this approach via the Bayes risk. The analysis is more involved however, since using conjugate Gaussian priors as in the case  $d = 1$  does not work. See Problem 4.5 on p. 398 of Lehmann and Casella (1998).

*Exercise 2.13* (Negative moments of the multivariate Gaussian). Let  $X \sim N_d(0, I)$ . Show that  $E(1/\|X\|^p) < \infty$  if and only if  $d > p$ .

*Exercise 2.14* (Proof of the James-Stein lemma). Prove Lemma 2.41.

*Exercise 2.15* (Shrinking towards another point). Let  $X \sim N_d(\theta, I)$  and  $v \in \mathbb{R}^d$ . Define the estimator

$$\tilde{\theta}_{\text{JS}} = v + \left(1 - \frac{d-2}{\|X-v\|^2}\right)(X-v).$$

Prove that for  $d \geq 3$ , this estimator also satisfies  $E_\theta \|\tilde{\theta}_{\text{JS}} - \theta\|^2 < E_\theta \|\hat{\theta}_{\text{MLE}} - \theta\|^2$  for all  $\theta \in \mathbb{R}^d$ .

*Exercise 2.16* (Oracle version of James-Stein). Use the expression for the risk of the James-Stein estimator to prove that if  $X \sim N(\theta, \sigma^2 I)$ , then for every  $\theta \in \mathbb{R}^d$  and  $d \geq 3$ ,

$$E_\theta \|\hat{\theta}_{\text{JS}} - \theta\|^2 \leq 4\sigma^2 + \inf_{c \in \mathbb{R}} E_\theta \|cX - \theta\|^2.$$

This is a so-called oracle inequality that asserts that up to a constant, the risk of the James-Stein estimator is as good as the risk that could be achieved by an oracle that may use its knowledge of the true parameter  $\theta$  to choose the degree of shrinking.

*Exercise 2.17* ((♠) Estimating the distribution is hard). Let  $\mathcal{P}$  be the set of all probability measures on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$  with variance bounded by  $\sigma^2$ . This exercise shows that estimating the distribution  $P$  itself in total variation distance is impossible with uniform control over  $\mathcal{P}$ .

Let  $P_0 = N(0, 1)$ . For  $M > 1$ , define the mixture distribution

$$P_M = \left(1 - \frac{1}{M}\right) N(0, 1) + \frac{1}{M} N(M^2, 1).$$

(a) Verify that  $P_0, P_M \in \mathcal{P}$  for all  $M > 1$ .

(b) Show that  $d_{\text{TV}}(P_0, P_M) \rightarrow 1$  as  $M \rightarrow \infty$ .

*Hint:* Consider the event  $A_M = \{x : x > M^2/2\}$  and compute  $P_0(A_M)$  and  $P_M(A_M)$ .

- (c) Let  $P^{\otimes n}$  denote the  $n$ -fold product measure corresponding to  $n$  i.i.d. draws from  $P$ . Show that for any fixed  $n$ ,

$$d_{TV}(P_0^{\otimes n}, P_M^{\otimes n}) \rightarrow 0 \quad \text{as } M \rightarrow \infty.$$

*Hint: Let  $N$  be the number of samples from the  $N(M^2, 1)$  component. Show that  $P_M^{\otimes n}(N = 0) \rightarrow 1$  as  $M \rightarrow \infty$ , and that conditionally on  $N = 0$ , the two product measures coincide.*

- (d) Conclude that for any estimator  $\hat{P}_n : \mathbb{R}^n \rightarrow \mathcal{P}$  and any sample size  $n$ ,

$$\sup_{P \in \mathcal{P}} E_P[d_{TV}(\hat{P}_n, P)] \geq \frac{1}{2}.$$

*Hint: Use Le Cam's method: for any estimator and any pair of distributions  $P, Q$ ,*

$$E_P[d_{TV}(\hat{P}_n, P)] + E_Q[d_{TV}(\hat{P}_n, Q)] \geq d_{TV}(P, Q)(1 - d_{TV}(P^{\otimes n}, Q^{\otimes n})).$$

*Exercise 2.18.* Let  $P_\theta = N(\theta, \sigma^2)$  and  $P_{\theta'} = N(\theta', \sigma^2)$  be two univariate normal distributions with the same variance. Show that

$$d_{TV}(P_\theta, P_{\theta'}) \leq \frac{1}{2\sigma} |\theta - \theta'|.$$

Argue that this implies that estimating the mean  $\theta$  is almost equally doable as estimating the distribution  $P_\theta$  itself.

*Hint: Use Pinsker's inequality, which relates total variation distance to Kullback-Leibler divergence:  $d_{TV}(P, Q) \leq \sqrt{\frac{1}{2} D_{KL}(P \| Q)}$ .*

*Exercise 2.19 (♠).* This exercise completes the proof of the Hunt-Stein theorem. Let  $G$  be a locally compact abelian group with Følner sequence  $\{G_n\}$ , and let  $\bar{\delta}_n$  be the partial group averages defined in the proof of Theorem 2.47.

- (a) Show that  $\bar{\delta}_n$  is asymptotically equivariant: for all  $h \in G$ ,

$$\mathbb{E}_\theta \|\bar{\delta}_n(hX) - h\bar{\delta}_n(X)\|^2 \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

*Hint: Express the difference as integrals over  $G_n \triangle hG_n$  and use the Følner property.*

- (b) Let  $r^*$  be the constant risk of the UMREE. Show that  $\liminf_n R(\theta, \bar{\delta}_n) \geq r^*$ .

*Hint: If  $R(\theta, \bar{\delta}_{n_k}) < r^* - \epsilon$  along a subsequence, use a compactness argument to extract a limit that is equivariant with risk strictly below  $r^*$ , contradicting the definition of the UMREE.*

*Exercise 2.20 (Non-existence of unbiased density estimators).* Let  $\mathcal{F}$  be the class of Lipschitz densities on  $[0, 1]$  with a fixed Lipschitz constant  $M > 0$ . We wish to show that for any fixed  $x_0 \in (0, 1)$  and any sample size  $n \geq 1$ , there is no unbiased estimator of  $f(x_0)$ .

We proceed by contradiction.

- (a) Suppose  $\delta(X_1, \dots, X_n)$  is an unbiased estimator, i.e.,  $\mathbb{E}_f[\delta] = f(x_0)$  for all  $f \in \mathcal{F}$ . Show that there exists a symmetric unbiased estimator  $\bar{\delta}$  of  $f(x_0)$ .
- (b) Fix an appropriate  $f_0 \in \mathcal{F}$  with small enough Lipschitz constant, and consider perturbations  $f_\epsilon = f_0 + \epsilon g$  where  $g$  appropriately Lipschitz, supported on an interval  $[a, b] \subset [0, 1]$  not containing  $x_0$ , and satisfies  $\int g = 0$ . Use the binomial expansion a limiting argument or dominated convergence theorem to show that the unbiasedness condition implies

$$\int_0^1 g(t) h_{f_0}(t) dt = 0,$$

where  $h_{f_0}(t) = \int_{[0,1]^{n-1}} \bar{\delta}(t, x_2, \dots, x_n) \prod_{j=2}^n f_0(x_j) dx_j$ .

- (c) Use the result from (a) to show that  $h_{f_0}(t)$  must be constant for almost every  $t \in [0, 1] \setminus \{x_0\}$ . *Hint: for  $\epsilon$  small enough,  $\epsilon g$  can be say  $M/2$  Lipschitz for any Lipschitz  $g$ . Show that part (b) implies  $\int_a^b \psi(t) h_{f_0}(t) dt = \frac{\int_a^b \psi}{b-a} \cdot \int_a^b h_{f_0}(t) dt$  for any Lipschitz function  $\psi$  on  $[a, b]$ . What does this imply if you choose  $\psi$  (approximating) an indicator function of an interval  $[a, s]$  not containing  $x_0$  and differentiate in  $s$  using the Fundamental Theorem of Calculus (see Theorem B.24)?*
- (d) Show that this constant must be  $f_0(x_0)$ .
- (e) Deduce that for any fixed  $t \neq x_0$ , the function  $\bar{\delta}_t(x_2, \dots, x_n) = \bar{\delta}(t, x_2, \dots, x_n)$  is an unbiased at  $f_0$ :  $\mathbb{E}_{f_0} \bar{\delta}_t = f_0(x_0)$  based on  $n - 1$  observations. Explain why this leads to a contradiction. *Hint: Establish that for some  $\delta' : [0, 1] \rightarrow \mathbb{R}_+$ ,  $\int \delta'(x_1) f(x_1) dx_1 = f(x_0)$  holds for any  $M/2$ -Lipschitz density  $f$ , and use part (c) and (d) to show that  $\delta'$  is constant a.e., leading to a contradiction.*

*Exercise 2.21 (Kernel density estimation bounds).* Consider the kernel density estimator  $\hat{f}_h(x_0) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{X_i - x_0}{h}\right)$  for a density  $f \in \mathcal{F}_\beta(M)$  at a point  $x_0$ . Assume the kernel

$K$  satisfies  $\int K(u) du = 1$ ,  $\int |u|^\beta |K(u)| du < \infty$ , and  $\int u^j K(u) du = 0$  for all integers  $1 \leq j < \beta$ .

(a) Show that the bias is bounded by

$$|\mathbb{E}_f[\hat{f}_h(x_0)] - f(x_0)| \leq C_1 h^\beta,$$

where  $C_1$  depends on  $M$  and  $K$ .

*Hint:* Write  $\mathbb{E}_f[\hat{f}_h(x_0)] = \int K(u) f(x_0 + hu) du$  via a change of variables. With  $k = \lfloor \beta \rfloor$ , use Taylor's theorem with integral remainder to order  $k - 1$ :

$$f(x_0 + hu) = \sum_{j=0}^{k-1} \frac{f^{(j)}(x_0)}{j!} (hu)^j + \frac{1}{(k-1)!} \int_0^{hu} (hu-t)^{k-1} f^{(k)}(x_0+t) dt.$$

Extract the  $k$ -th order term by adding and subtracting  $f^{(k)}(x_0)$  inside the integral. The moment conditions on  $K$  eliminate the polynomial terms. For the integral remainder, use the Hölder condition.

(b) Show that the variance is bounded by

$$\text{Var}_f(\hat{f}_h(x_0)) \leq \frac{C_2}{nh},$$

where  $C_2$  depends on  $\|K\|_\infty$  (or  $\|K\|_2^2$ ) and  $f(x_0)$  (or  $\|f\|_\infty$ ).

*Exercise 2.22* (Bhattacharyya affinity for Hölder bumps). Let  $P_{f_0}$  be the uniform distribution on  $[0, 1]$  and let  $P_{f_h}$  have density

$$f_h(x) = 1 + c h^\beta \psi\left(\frac{x - x_0}{h}\right),$$

where  $\psi$  is supported on  $[-1/2, 1/2]$  with  $\int \psi = 0$ ,  $\|\psi\|_\infty < \infty$ , and  $c > 0$  is small enough that  $f_h \geq 1/2$ . This is the Hölder-saturated bump construction from Section 2.4.1.

Show that the Bhattacharyya affinity between the product measures satisfies

$$\rho(P_{f_0}^{\otimes n}, P_{f_h}^{\otimes n}) \geq \exp(-C n h^{2\beta+1})$$

for some constant  $C > 0$  depending on  $c$  and  $\psi$ .

*Exercise 2.23* (Cost of adaptation). This exercise proves Proposition 2.58. Fix  $0 < \beta_{\min} < \beta_{\max} < \infty$  and  $M > 0$ , and consider pointwise density estimation at  $x_0 \in (0, 1)$ .

Let  $\delta$  be any estimator satisfying

$$\sup_{f \in \mathcal{F}_{\beta_{\max}}(M)} \mathbb{E}_f[(\delta - f(x_0))^2] \leq A \log^B(n) n^{-\frac{2\beta_{\max}}{2\beta_{\max}+1}}$$

for some constants  $A, B > 0$ . Fix  $\beta \in [\beta_{\min}, \beta_{\max}]$ .

(a) Let  $f_0 \equiv 1$ . Why is  $R_0 := \mathbb{E}_{f_0}[(\delta - 1)^2] \leq A \log^B(n) n^{-\frac{2\beta_{\max}}{2\beta_{\max}+1}}$ ?

(b) For  $h \in (0, 1)$ , define

$$g_h(x) = 1 + \kappa h^\beta \psi\left(\frac{x - x_0}{h}\right),$$

where  $\psi$  is a smooth bump function with  $\int \psi = 0$  and  $\psi(0) = 1$ , and  $\kappa > 0$  is chosen small enough that  $g_h \in \mathcal{F}_\beta(M)$  and  $g_h \geq 1/2$ . Show that  $|g_h(x_0) - 1| = \kappa h^\beta$ .

(c) Let  $L_h^{(n)} = dP_{g_h}^{\otimes n} / dP_{f_0}^{\otimes n}$ . Using Lemma 2.57 and the second-moment bound  $\mathbb{E}_{f_0}[(L_h^{(n)})^2] \leq \exp(Cnh^{2\beta+1})$ , show that

$$\mathbb{E}_{g_h}[(\delta - g_h(x_0))^2] \geq \left( c_1 h^\beta - \sqrt{A} \log^{B/2}(n) n^{-\frac{\beta_{\max}}{2\beta_{\max}+1}} \exp\left(\frac{1}{2}Cnh^{2\beta+1}\right) \right)_+^2.$$

(d) Choose  $h$  to satisfy

$$\exp\left(\frac{1}{2}Cnh^{2\beta+1}\right) = \frac{c_1 \log^{-B/2}(n)}{2\sqrt{A}} h^\beta n^{\frac{\beta_{\max}}{2\beta_{\max}+1}}.$$

You do not need to solve for  $h$  explicitly, and may assume constants and  $n$  to be appropriately large. Show that with this choice,  $\mathbb{E}_{g_h}[(\delta - g_h(x_0))^2] \geq c_2 h^{2\beta}$  for some constant  $c_2 > 0$ .

(e) Taking logarithms in the equation from (d), show that  $h \asymp (\log n/n)^{1/(2\beta+1)}$  for large  $n$ . Conclude that for any  $\beta \in [\beta_{\min}, \beta_{\max}]$ ,

$$\sup_{g \in \mathcal{F}_\beta(M)} \mathbb{E}_g[(\delta - g(x_0))^2] \gtrsim \left( \frac{\log n}{n} \right)^{\frac{2\beta}{2\beta+1}}.$$

*Exercise 2.24* (Lepski's method: adaptive upper bound). This exercise proves Proposition 2.59. Consider the kernel estimator  $\hat{f}_h(x_0) = \frac{1}{nh} \sum_{i=1}^n K((X_i - x_0)/h)$ , the dyadic bandwidth grid  $\mathcal{H} = \{2^{-j} : j = j_{\min}, \dots, j_{\max}\}$ , such that the coarsest bandwidth  $h_{j_{\min}}$  is of order 1, the finest  $h_{j_{\max}}$  is of order  $n^{-\frac{1}{2\beta_{\min}+1}}$ , and  $|\mathcal{H}| \asymp \log n$ . Define the 'Lepski selector'

$$\hat{h} = \max \left\{ h \in \mathcal{H} : |\hat{f}_h(x_0) - \hat{f}_{h'}(x_0)| \leq \tau(h') \text{ for all } h' \in \mathcal{H} \text{ with } h' \leq h \right\},$$

where  $\tau(h) = A\sqrt{\frac{\log n}{nh}}$  for a constant  $A > 0$ .

(a) (*Variance control*) Show that for each fixed  $h \in \mathcal{H}$ ,

$$\text{Var}_f(\hat{f}_h(x_0)) \leq \frac{C_K}{nh}$$

for a constant  $C_K$  depending on the kernel  $K$  and  $\|f\|_\infty$ .

(b) ( $\spadesuit$ ) Using Bernstein's inequality, show that there exists a constant  $c > 0$  such that for  $A$  large enough,

$$\mathbb{P}_f \left( |\hat{f}_h(x_0) - \mathbb{E}_f[\hat{f}_h(x_0)]| > \frac{\tau(h)}{2} \right) \leq n^{-cA^2}$$

for each  $h \in \mathcal{H}$ . Conclude by a union bound that with probability at least  $1 - n^{-2}$  (for large  $A$ ), we have  $|\hat{f}_h(x_0) - \mathbb{E}_f[\hat{f}_h(x_0)]| \leq \tau(h)/2$  simultaneously for all  $h \in \mathcal{H}$ .

(c) (*Bias control*) Let  $f \in \mathcal{F}_\beta(M)$  and let  $h_\beta^* = (\log(n)/n)^{1/(2\beta+1)}$  be the oracle bandwidth. Show that the bias satisfies

$$|\mathbb{E}_f[\hat{f}_h(x_0)] - f(x_0)| \leq C_1 h^\beta$$

for a constant  $C_1$  depending on  $M$  and  $K$ .

(d) (*Oracle bandwidth is valid*) Define the oracle bandwidth in the grid as  $h^* = \max\{h \in \mathcal{H} : h \leq h_\beta^*\}$ . On the event from (b), show that  $h^*$  satisfies the Lepski criterion, so  $\hat{h} \geq h^*$ .

*Hint:* For  $h', h \in \mathcal{H}$  with  $h' \leq h \leq h^*$ , use the triangle inequality and the concentration bound from (b) to show  $|\hat{f}_h(x_0) - \hat{f}_{h'}(x_0)| \leq \tau(h')$ .

(e) (*Bounding the selected bandwidth*) On the event from (b), show that the selected bandwidth  $\hat{h}$  satisfies

$$|\mathbb{E}_f[\hat{f}_{\hat{h}}(x_0)] - f(x_0)| \lesssim \tau(\hat{h}).$$

*Hint:* By definition of  $\hat{h}$ , there exists  $h' = \hat{h}/2 \in \mathcal{H}$  such that  $|\hat{f}_{\hat{h}}(x_0) - \hat{f}_{h'}(x_0)| \leq \tau(h')$ . Combine with concentration.

(f) (*Conclusion*) Combine parts (b)–(e) to show that for  $f \in \mathcal{F}_\beta(M)$ ,  $\beta \in [\beta_{\min}, \beta_{\max}]$ ,

$$\mathbb{E}_f[(\hat{f}_{\hat{h}}(x_0) - f(x_0))^2] \lesssim \left(\frac{\log n}{n}\right)^{\frac{2\beta}{2\beta+1}}.$$

Conclude that the estimator  $\hat{f}_{\hat{h}}(x_0)$  is adaptive in the sense of Definition 2.56.

*Exercise 2.25* (♠ Smoothness cannot be estimated uniformly). Fix  $0 < \beta_0 < \beta_1 \leq \beta_{\max}$ ,  $M > 0$ , and  $x_0 \in (0, 1)$ . Let  $\mathcal{F}_\beta(M)$  be the Hölder class on  $[0, 1]$  (as defined in Section 2.4.1) and define the smoothness index

$$\beta(f) := \sup \left\{ \alpha \in [\beta_{\min}, \beta_{\max}] : f \in \mathcal{F}_\alpha(M) \right\}.$$

(For simplicity you may assume  $\beta_1 = \beta_{\max}$ ; otherwise replace  $\beta_{\max}$  by  $\beta_1$  in the definition of  $\beta(f)$ .)

Let  $g \equiv 1$  and let  $\psi$  be a  $C^\infty$  bump supported on  $[-1/2, 1/2]$  with  $\int \psi = 0$  and  $\psi(0) = 1$ . For  $h > 0$ , define

$$f_h(x) = 1 + \kappa h^{\beta_0} \psi\left(\frac{x - x_0}{h}\right),$$

where  $\kappa > 0$  is chosen small enough that  $f_h \geq 1/2$  on  $[0, 1]$  (for all sufficiently small  $h$ ).

- (a) Show that  $\beta(g) = \beta_1$ .
- (b) Show that for all sufficiently small  $h$ , we have  $f_h \in \mathcal{F}_{\beta_0}(M)$  but  $f_h \notin \mathcal{F}_{\beta_1}(M)$ . Conclude that  $\beta(f_h) = \beta_0$  for all sufficiently small  $h$ .
- (c) Using Exercise 2.22, show that there exists a constant  $C > 0$  such that

$$\rho(P_g^{\otimes n}, P_{f_h}^{\otimes n}) \geq \exp(-C n h^{2\beta_0+1}).$$

- (d) Choose  $h = h_n \downarrow 0$  such that  $n h_n^{2\beta_0+1} \rightarrow 0$  and conclude that

$$\mathbf{d}_{\text{TV}}(P_g^{\otimes n}, P_{f_{h_n}}^{\otimes n}) \rightarrow 0.$$

- (e) Let  $\hat{\beta}_n$  be any estimator of  $\beta(f)$  based on  $X_1, \dots, X_n$  and define the test

$$\phi_n := \mathbb{1} \left\{ \hat{\beta}_n > (\beta_0 + \beta_1)/2 \right\}.$$

Use Le Cam's two-point method to show

$$\liminf_{n \rightarrow \infty} \max \left\{ P_g(|\hat{\beta}_n - \beta_1| > (\beta_1 - \beta_0)/2), P_{f_{h_n}}(|\hat{\beta}_n - \beta_0| > (\beta_1 - \beta_0)/2) \right\} \geq \frac{1}{2}.$$

Conclude that  $\beta(f)$  is not uniformly consistently estimable on  $\mathcal{F}_{\beta_0}(M) \cup \mathcal{F}_{\beta_1}(M)$ , hence not on  $\bigcup_\beta \mathcal{F}_\beta(M)$ .

### 3 Hypothesis Testing

In this chapter, we study the problem of *hypothesis testing*: deciding on the truth, or falsehood of a statement on the basis of observed data that may provide evidence in support of, or against said statement. Before we formulate hypothesis testing as a decision-theoretic problem, let us reflect on what it is trying to accomplish.

The basic situation is this: we have a conjecture about the world, and we collect data that bears on its truth. The data will rarely settle the matter with certainty—we observe a single realization from a distribution, not the distribution itself. The question is how to quantify the evidence.

The question is how to quantify the evidence. One natural approach, developed by Fisher, is to ask: *how surprising is the observed data if the conjecture is true?* If the answer is “very surprising,” we have grounds for doubt. To make this precise, the conjecture is formalized as a statement about the data-generating distribution—the *null hypothesis*, denoted  $H_0$ . For example:

$H_0$  : “the data is generated by a normal distribution with mean 0 and variance 1”.

To assess whether the data supports  $H_0$ , we compute a *test statistic*  $T : \mathcal{X} \rightarrow \mathbb{R}$  designed so that large values of  $T$  indicate disagreement with  $H_0$ . The *p-value* is then defined as

$$p(x) = P_{H_0}(T(X) \geq T(x)),$$

the probability, assuming  $H_0$  is true, of observing a test statistic at least as extreme as the one observed. A small *p-value* suggests that the observed data would be surprising under  $H_0$ .

To convert this continuous measure of evidence into a binary decision, we fix a threshold  $\alpha \in (0, 1)$ —the *significance level*—and reject  $H_0$  whenever  $p(x) \leq \alpha$ . Equivalently, we reject when  $T(x)$  exceeds a critical value  $c_\alpha$  chosen so that  $P_{H_0}(T(X) > c_\alpha) = \alpha$ . The significance level bounds the probability of a false rejection: if  $H_0$  is true, the probability of mistakenly rejecting it is at most  $\alpha$ .

**Example 3.1** (Fisher’s tea tasting experiment). A subject claims she can distinguish whether milk or tea was poured first into a cup. To test this claim, consider the following experiment: prepare eight cups, four with milk poured first and four with tea poured first, present them in random order, and ask the subject to identify exactly four as “milk-first.”

The null hypothesis is

$H_0$  : the subject has no discriminatory ability and is guessing at random.

Under  $H_0$ , every subset of four cups is equally likely to be labeled “milk-first.” Let  $X$  denote the number of truly milk-first cups among those she labels as such. Then  $X \in \{0, 1, 2, 3, 4\}$  and, under  $H_0$ ,

$$X \sim \text{Hypergeometric}(N = 8, K = 4, n = 4), \quad P_{H_0}(X = k) = \frac{\binom{4}{k} \binom{4}{4-k}}{\binom{8}{4}}.$$

A natural test statistic is  $T(X) = X$  itself: more correct identifications indicate greater evidence against  $H_0$ . The  $p$ -value for observing  $X = x$  is

$$p(x) = P_{H_0}(X \geq x) = \sum_{k=x}^4 \frac{\binom{4}{k} \binom{4}{4-k}}{\binom{8}{4}}.$$

If she identifies all four correctly,  $p(4) = 1/70 \approx 0.014$ . If she identifies three correctly,  $P_{H_0}(X \geq 3) = 17/70 \approx 0.243$ . At significance level  $\alpha = 0.05$ , the rejection rule is: reject  $H_0$  if and only if  $X = 4$ .  $\diamond$

In this example, the test statistic was essentially forced by the structure of the problem: “more correct” is the obvious notion of “more extreme.” The alternative hypothesis—that the subject has discriminatory ability—was left implicit and qualitative. This is characteristic of the Fisherian approach: the null hypothesis is primary, and the  $p$ -value measures how surprising the data is under  $H_0$ .

But what happens when the problem does not dictate a unique notion of extremeness?

**Example 3.2** (Ambiguity without an alternative). Let  $X = (X_1, X_2)^\top$  and consider the simple null hypothesis

$$H_0 : X \sim N_2(0, I_2).$$

In  $\mathbb{R}^2$ , there is no canonical choice of what “extreme under  $H_0$ ” should mean. Here are three equally reasonable test statistics:

- (i) *Radial extremeness*:  $T_1(X) = \|X\|^2 = X_1^2 + X_2^2$ . Under  $H_0$ ,  $T_1 \sim \chi_2^2$ . The rejection region  $\mathcal{R}_1 = \{x : \|x\|^2 > \chi_{2,1-\alpha}^2\}$  consists of points outside a circle centered at the origin.
- (ii) *Coordinatewise extremeness*:  $T_2(X) = \max\{|X_1|, |X_2|\}$ . The rejection region  $\mathcal{R}_2 = \{x : \max(|x_1|, |x_2|) > c_2(\alpha)\}$  consists of points outside an axis-aligned square.

(iii) *Directional extremeness*:  $T_3(X) = |X_1 + X_2|$ . Under  $H_0$ ,  $X_1 + X_2 \sim N(0, 2)$ . The rejection region  $\mathcal{R}_3 = \{x : |x_1 + x_2| > \sqrt{2} z_{1-\alpha/2}\}$  consists of points outside a diagonal strip.

All three tests have exact level  $\alpha$ . Yet they lead to different conclusions on the same data. At  $\alpha = 0.05$ :

$x$	$p_1(x)$	$p_2(x)$	$p_3(x)$	Rejected by
(2.3, 0.1)	0.071	0.042	0.090	$T_2$ only
(1.7, 1.7)	0.056	0.170	0.016	$T_3$ only

The observation (2.3, 0.1) is extreme in the  $\ell_\infty$ -sense but not radially or diagonally; (1.7, 1.7) is extreme along the diagonal but not in the other senses.  $\diamond$

The Fisherian framework provides no guidance for choosing among these tests. Each is a valid level- $\alpha$  test, but they differ in probability of rejecting  $H_0$  when it is false, depending on the alternative. The test  $T_3$  is powerful against alternatives where the mean shifts along the direction (1, 1), but weak against shifts along (1, -1). Without specifying what alternatives we care about, we cannot say which test is better.

One might respond: the test should be specified in advance, before seeing the data, to prevent the analyst from choosing whichever test happens to reject. This is sound practice, but it sidesteps the question rather than answering it. *Which* test should be specified in advance? The injunction to preregister does not tell us whether to use  $T_1$ ,  $T_2$ , or  $T_3$ —only that we must commit to one before looking at the data.

Neyman and Pearson's answer is that the choice of test should be guided by the *alternative hypothesis*: a precise statement about what departures from  $H_0$  we wish to detect. If we are concerned that the mean might be nonzero, we should say so explicitly—and then choose the test that is most powerful against that alternative. The alternative is not merely the logical negation of  $H_0$ ; it encodes our scientific question. A test optimized for detecting a mean shift along (1, 1) is a different test from one optimized for detecting a mean shift along (1, 0), and both are different from one designed to detect an increase in variance. By specifying the alternative, we make this dependence explicit: our test needs to make sense in light of what we are trying to find evidence for.

There is a second, perhaps more fundamental, reason to specify an alternative: it allows us to consider *power*, the probability of rejecting  $H_0$  when a specific alternative is true. Without this, we cannot interpret a failure to reject. Suppose a study finds no significant effect of a drug. Does this mean the drug is ineffective, or merely that the study was too small to detect a real effect? The  $p$ -value cannot answer this question—it only measures surprise under  $H_0$ . But if we have specified the alternative, we can

ask: had the drug effect been  $\mu = \mu_1$ , what was our probability of detecting it? If the answer is 0.95, a failure to reject is informative: we would very likely have detected an effect of size  $\mu_1$  had it existed, so its absence is evidence that the true effect is smaller. If the answer is 0.10, a failure to reject tells us almost nothing: we would have missed an effect of size  $\mu_1$  nine times out of ten even if it were real. Without such a notion, we do not know whether our study had any real chance of detecting a meaningful effect—which could lead to mistaking absence of evidence for evidence of absence.

This discussion points to a classification of errors. A hypothesis test can fail in two ways:

- (i) *Type I error*: rejecting  $H_0$  when it is true (a false positive),
- (ii) *Type II error*: failing to reject  $H_0$  when it is false (a false negative).

The probability of a Type I error is controlled by the significance level  $\alpha$ —this is what it means for a test to have level  $\alpha$ . The probability of a Type II error depends on which alternative is true; we denote it  $\beta(\theta)$  for  $\theta \in H_1$ . Power is simply  $1 - \beta(\theta)$ : the probability of correctly rejecting  $H_0$  when  $\theta$  is the true parameter.

The Fisherian framework controls Type I error but is silent on Type II error: without an alternative, there is no notion of “failing to detect a true effect.” The Neyman-Pearson framework treats both errors explicitly, seeking tests that minimize Type II error (equivalently, maximize power) subject to a constraint on Type I error. This is the natural formulation as a decision problem: the significance level  $\alpha$  bounds the cost of false positives, and power measures the benefit of true positives.

We now formalize hypothesis testing as a decision problem. Recall from Chapter 1 that a decision problem is specified by a statistical experiment, a decision space, and a loss function. In hypothesis testing, the decision is binary—reject  $H_0$  or not—and the parameter space is partitioned according to which hypothesis is true. We allow for a third region, the indifference region  $\Theta_I$ , consisting of parameter values for which we do not specify error requirements. In many problems  $\Theta_I = \emptyset$ , but the three-way partition is useful when there is a gap between what we wish to protect against (Type I error) and what we wish to detect (Type II error). A hypothesis is *simple* if it specifies a single distribution, and *composite* otherwise.

**Definition 3.3.** A *hypothesis testing problem* is a decision problem with decision space  $(\{0, 1\}, 2^{\{0,1\}})$ , in which the parameter space is partitioned into three disjoint subsets  $\Theta_0$ ,  $\Theta_1$ , and  $\Theta_I$ , with  $\Theta_0 \cup \Theta_1 \cup \Theta_I = \Theta$ . The *null hypothesis* is the assertion  $H_0 : \theta \in \Theta_0$ ; the *alternative hypothesis* is  $H_1 : \theta \in \Theta_1$ . The set  $\Theta_I$  is the *indifference region*. A hypothesis is *simple* if the corresponding subset is a singleton, and *composite* otherwise.

A *test* is a (possibly randomized) decision rule  $\delta : \mathcal{X} \times [0, 1] \rightarrow \{0, 1\}$ . By convention, deciding 1 means “reject  $H_0$ ”; deciding 0 means “do not reject  $H_0$ .”

For a non-randomized test  $\delta$ , we call the set  $\{x \in \mathcal{X} : \delta(x) = 1\}$  the *rejection region* of the test: it is the event on which we decide to reject  $H_0$ . A typical testing loss function penalizes incorrect decisions:

$$L(\theta, d) = \begin{cases} a & \text{if } \theta \in \Theta_0 \text{ and } d = 1, \\ b & \text{if } \theta \in \Theta_1 \text{ and } d = 0, \\ 0 & \text{otherwise,} \end{cases} \quad (3.1)$$

where  $a, b > 0$  represent the costs of making a Type I or a Type II error, respectively. The case  $a = b = 1$  corresponds to symmetric 0-1 loss. The risk of a test  $\delta$  is then

$$\mathcal{R}(\theta, \delta) = \mathbb{E}_\theta[L(\theta, \delta(X, U))] = \begin{cases} a \cdot P_\theta(\delta = 1) & \text{if } \theta \in \Theta_0, \\ b \cdot P_\theta(\delta = 0) & \text{if } \theta \in \Theta_1, \\ 0 & \text{if } \theta \in \Theta_I. \end{cases} \quad (3.2)$$

Minimizing the risk on  $\Theta_0$  and on  $\Theta_1$  pulls in opposite directions: a test that rarely rejects has small risk on  $\Theta_0$  but large risk on  $\Theta_1$ , and vice versa. The indifference region  $\Theta_I$  incurs no loss by definition—we do not penalize either decision when  $\theta \in \Theta_I$ . A good test balances these competing demands; the ratio  $a/b$  governs how aggressively the test trades off one type of error against the other.

Another, more common approach is to treat the two error types asymmetrically: constrain the probability of incorrectly rejecting  $H_0$  (the *size*) to be at most some prescribed *level*  $\alpha$ , and maximize the probability of correctly rejecting it when  $H_1$  is true (the *power*). These two formulations are somewhat dual: varying the cost ratio  $a/b$  in the first traces out a family of optimal tests in a similar way – and for simple hypotheses, an identical way – to varying the level in the second.

**Definition 3.4.** The *power function* of a test  $\delta$  is  $\beta_\delta : \Theta \rightarrow [0, 1]$  defined by

$$\beta_\delta(\theta) = \int_0^1 P_\theta(\delta(X, u) = 1) du,$$

the probability of rejecting  $H_0$  when  $\theta$  is the true parameter. In the above display, the integral averages over the randomization; for non-randomized tests, this reduces to  $P_\theta(\delta(X) = 1)$ .

On  $\Theta_0$ , the power function gives the probability of a Type I error; we want it small. On  $\Theta_1$ , it gives the probability of correctly rejecting  $H_0$ ; we want it large. The complementary quantity  $1 - \beta_\delta(\theta)$  for  $\theta \in \Theta_1$  is the probability of a Type II error.

**Definition 3.5.** The *size* of a test  $\delta$  is

$$\alpha(\delta) := \sup_{\theta \in \Theta_0} \beta_\delta(\theta).$$

A test is of *level*  $\alpha \in [0, 1]$  if its size is at most  $\alpha$ . We write  $\mathcal{C}_\alpha$  for the class of all level- $\alpha$  tests.

The size is the worst-case Type I error probability. Note that  $\mathcal{C}_\alpha \subseteq \mathcal{C}_{\alpha'}$  whenever  $\alpha \leq \alpha'$ : a test with smaller size automatically has smaller level.

**Definition 3.6.** A test  $\delta \in \mathcal{C}_\alpha$  is *admissible at level*  $\alpha$  if there is no other test  $\delta' \in \mathcal{C}_\alpha$  with  $\beta_{\delta'}(\theta) \geq \beta_\delta(\theta)$  for all  $\theta \in \Theta_1$  and  $\beta_{\delta'}(\theta) > \beta_\delta(\theta)$  for at least one  $\theta \in \Theta_1$ .

In words: a level- $\alpha$  test is admissible if no other level- $\alpha$  test has uniformly at least as much power, with strictly more power somewhere. This parallels Definition 2.39 for estimators, with the power function playing the role of negative risk.

Inadmissible tests should be avoided: they leave power on the table, failing to detect alternatives that another valid test would catch. But admissibility is a weak requirement—it only rules out dominated tests. Just as with estimation, we would like a stronger criterion: among all level- $\alpha$  tests, find the one with highest power.

**Definition 3.7.** Consider testing  $H_0 : \theta \in \Theta_0$  versus  $H_1 : \theta = \theta_1$  (a simple alternative). A test  $\delta^*$  is *most powerful at level*  $\alpha$  if:

- (i)  $\delta^* \in \mathcal{C}_\alpha$ , and
- (ii)  $\beta_{\delta^*}(\theta_1) \geq \beta_\delta(\theta_1)$  for every  $\delta \in \mathcal{C}_\alpha$ .

Given a simple alternative, a most powerful test is automatically admissible, but the converse need not hold. When the alternative is composite ( $|\Theta_1| > 1$ ), we would like a test that is most powerful against every  $\theta_1 \in \Theta_1$  simultaneously—a *uniformly most powerful* (UMP) test. Such tests rarely exist, and much of the theory of hypothesis testing concerns what can be said when they do not. If we wish to summarize the Type II error of a test in a single number, we can consider its worst case over  $\Theta_1$ .

**Definition 3.8.** The *worst-case Type II error* of a test  $\delta$  is

$$\beta(\delta) := \sup_{\theta \in \Theta_1} (1 - \beta_\delta(\theta)) = 1 - \inf_{\theta \in \Theta_1} \beta_\delta(\theta).$$

This is the largest probability of failing to reject  $H_0$  when some alternative in  $\Theta_1$  is true.

The pair  $(\alpha(\delta), \beta(\delta))$  summarizes the worst-case performance of a test:  $\alpha(\delta)$  is the worst-case Type I error (the size), and  $\beta(\delta)$  is the worst-case Type II error. A good test makes both small, but these goals are in tension.

Rather than committing to a single level  $\alpha$ , we often consider an entire family of tests indexed by the level.

**Definition 3.9.** Given a testing problem, *nested family of tests* is a collection  $\{\delta_\alpha : \alpha \in (0, 1)\}$  such that:

- (i)  $\delta_\alpha \in \mathcal{C}_\alpha$  for each  $\alpha \in (0, 1)$ , and
- (ii)  $\delta_\alpha(x) \leq \delta_{\alpha'}(x)$  whenever  $\alpha \leq \alpha'$ .

The second condition ensures monotonicity: if we reject at level  $\alpha$ , we also reject at any less stringent level  $\alpha'$ .

Given a nested family, we can summarize the evidence against  $H_0$  on a continuous scale.

**Definition 3.10.** The *p-value* associated with a nested family of non-randomized tests  $\{\delta_\alpha\}$  is

$$p(x) = \inf\{\alpha \in (0, 1) : \delta_\alpha(x) = 1\}.$$

For a nested family of randomized tests where  $\alpha \mapsto \delta_\alpha(x, u)$  is right-continuous for each  $(x, u)$ , the p-value is the random variable

$$p(x, u) = \inf\{\alpha \in (0, 1) : \delta_\alpha(x, u) = 1\}.$$

Right-continuity ensures the infimum is attained:  $\delta_\alpha(x, u) = 1$  if and only if  $p(x, u) \leq \alpha$ .

The p-value is the smallest level at which we reject with positive probability. For non-randomized tests, it determines the decision at every level:  $\delta_\alpha(x) = 1$  if and only if  $p(x) \leq \alpha$ .

**Proposition 3.11.** *Let  $\{\delta_\alpha\}$  be a nested family of non-randomized tests with associated p-value  $p(X)$ .*

- (a) *If the tests have exact level— $P_\theta(\delta_\alpha(X) = 1) = \alpha$  for each  $\alpha$  and  $\theta \in \Theta_0$ —then  $p(X)$  is exactly uniform on  $(0, 1)$  under each  $\theta \in \Theta_0$ .*
- (b) *If the tests have level  $\alpha$  but not necessarily exact level, then  $P_\theta(p(X) \leq \alpha) \leq \alpha$  for all  $\theta \in \Theta_0$ .*
- (c) *For a simple null  $H_0 : \theta = \theta_0$ , any valid p-value can be randomized to be exactly uniform.*

*Proof.* Since the tests are non-randomized,  $\{p(X) \leq \alpha\} = \{\delta_\alpha(X) = 1\}$ . Parts (a) and (b) follow immediately.

For (c), define

$$\tilde{p}(x, u) = P_{\theta_0}(p(X) < p(x)) + u \cdot P_{\theta_0}(p(X) = p(x)).$$

Then  $P_{\theta_0}(\tilde{p}(X, U) \leq \alpha) = \alpha$  for all  $\alpha \in (0, 1)$ . Let  $F(t) = P_{\theta_0}(p(X) \leq t)$  and  $F^-(t) = P_{\theta_0}(p(X) < t)$ . Then  $\tilde{p}(X, U) = F^-(p(X)) + U \cdot (F(p(X)) - F^-(p(X)))$ . For any  $\alpha \in (0, 1)$ :

$$P_{\theta_0}(\tilde{p}(X, U) \leq \alpha) = P_{\theta_0}(F^-(p(X)) + U(F(p(X)) - F^-(p(X))) \leq \alpha) = \alpha,$$

where the last equality follows from the generalized probability integral transform.  $\square$

A p-value satisfying (b) is called *valid*: it controls the Type I error when used as a test via  $\delta_\alpha(x) = \mathbb{1}\{p(x) \leq \alpha\}$ . Valid p-values that are not exactly uniform are *conservative*—they reject less often than the level permits. Part (c) shows that we can randomize any valid p-value to be exactly uniform; leaving no power on the table.

The specific Type I and Type II error trade-off achieved by a nested family can be visualized as a curve in (size, worst-case Type II error) space: as  $\alpha$  increases from 0 to 1, the size increases while the worst-case Type II error decreases:

$$\text{ROC}(\{\delta_\alpha\}) = \left\{ (\alpha(\delta_\alpha), 1 - \inf_{\theta \in \Theta_1} \beta_{\delta_\alpha}(\theta)) : \alpha \in (0, 1) \right\}.$$

This is the *receiver operating characteristic (ROC)* of the family. Different nested families yield different curves, and the *efficient frontier* is the lower-left boundary of all achievable pairs—the optimal worst-case trade-off no family can improve upon.

**Definition 3.12** (Efficient frontier). Given a testing problem, the *achievable region* is

$$\mathcal{A} = \{(\alpha, \beta) \in [0, 1]^2 : \text{there exists a test } \delta \text{ with } \alpha(\delta) \leq \alpha \text{ and } \beta(\delta) \leq \beta\}.$$

The *efficient frontier*  $\mathcal{E}$  is the lower-left boundary of  $\mathcal{A}$ : the set of  $(\alpha, \beta) \in \mathcal{A}$  such that no  $(\alpha', \beta') \in \mathcal{A}$  satisfies  $\alpha' \leq \alpha$  and  $\beta' \leq \beta$  with at least one inequality strict.

The efficient frontier characterizes the fundamental limits of testing: how much power can we achieve at a given size? For simple hypotheses, we can provide a complete answer—likelihood ratio tests trace out the frontier, and no other tests can improve upon them. For composite hypotheses, the situation is more complex: as mentioned before, UMP tests exist only under special structural conditions, and even when we can compute the efficient frontier, it is not always easy to find the UMP test.

We begin with the cases where the theory is cleanest: simple hypotheses, and composite hypotheses with monotone likelihood ratio.

### 3.1 Simple and monotone hypotheses

Consider a testing problem where both  $H_0$  and  $H_1$  are simple hypotheses. This setting admits a complete solution and provides the foundation for more complex testing problems. In this setting, where  $\Theta_0$  and  $\Theta_1$  are both singletons, admissible tests at level  $\alpha$  are precisely those that are most powerful. For simplicity, we write  $P_0$  and  $P_1$  for the distributions under  $H_0$  and  $H_1$ , respectively.

Before deriving the optimal test, we ask: what is the best we can hope for? The answer is governed by how distinguishable  $P_0$  and  $P_1$  are. Recall from Definition 2.2 that the total variation distance between two probability measures is

$$\mathbf{d}_{TV}(P_0, P_1) = \sup_{A \in \mathcal{X}} |P_0(A) - P_1(A)|.$$

Total variation measures the maximum difference in probability that any event can witness. It quantifies how distinguishable the two distributions are.

**Lemma 3.13** (Le Cam). *For any test  $\delta$  of  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta = \theta_1$ ,*

$$\beta_\delta(\theta_0) + (1 - \beta_\delta(\theta_1)) \geq 1 - \mathbf{d}_{TV}(P_0, P_1).$$

*When  $P_0$  and  $P_1$  have densities  $p_0$  and  $p_1$  with respect to a common dominating measure, equality is achieved by the test that rejects when  $p_1(x) > p_0(x)$ .*

*Proof.* We can consider a nonrandom test without loss of generality (check). Consider arbitrary test  $\delta$  with rejection region  $R = \{x : \delta(x) = 1\}$ , the sum of error probabilities is

$$\beta_\delta(\theta_0) + (1 - \beta_\delta(\theta_1)) = P_0(R) + P_1(R^c) = 1 - (P_1(R) - P_0(R)) \geq 1 - \mathbf{d}_{TV}(P_0, P_1),$$

since  $P_1(R) - P_0(R) \leq \sup_A |P_1(A) - P_0(A)| = \mathbf{d}_{TV}(P_0, P_1)$ .

When densities exist, taking  $R^* = \{x : p_1(x) > p_0(x)\}$  achieves

$$P_1(R^*) - P_0(R^*) = \int_{p_1 > p_0} (p_1 - p_0) d\mu = \mathbf{d}_{TV}(P_0, P_1),$$

where the last equality follows from the variational representation of total variation (Exercise 3.1). □

Lemma 3.13 relates the sum of error probabilities to the total variation distance between  $P_0$  and  $P_1$ . This is intuitive: if two distributions are close in total variation, the data they produce are nearly indistinguishable, and no test can reliably tell them apart. The lemma also hints at what the optimal test should do: compare how likely the observed data is under each hypothesis.

The existence of densities is not a concern in simple hypothesis testing: the measure  $\mu = P_0 + P_1$  dominates both  $P_0$  and  $P_1$ , so densities  $p_0 = dP_0/d\mu$  and  $p_1 = dP_1/d\mu$  always exist. An appropriate *likelihood ratio* can be defined as

$$\Lambda(x) = \frac{p_1(x)}{p_0(x)},$$

with conventions  $\Lambda(x) = +\infty$  if  $p_0(x) = 0$  and  $p_1(x) > 0$ , and  $\Lambda(x) = 0$  if  $p_1(x) = 0$ . Intuitively, large values of  $\Lambda(x)$  indicate that the observation  $x$  is much more likely under  $P_1$  than under  $P_0$ . Note that  $\Lambda$  may take the value  $+\infty$ , but  $P_0(\Lambda = +\infty) = P_0(p_0 = 0) = 0$ , so this causes no difficulty under the null.

The Neyman-Pearson lemma shows that comparing  $\Lambda(x)$  to a threshold yields the most powerful test at any level  $\alpha$ —a complete solution to the problem of finding optimal tests in  $\mathcal{C}_\alpha$ .

**Theorem 3.14** (Neyman-Pearson). *Consider testing  $H_0 : P = P_0$  versus  $H_1 : P = P_1$ , where  $P_0$  and  $P_1$  have densities  $p_0$  and  $p_1$  with respect to a  $\sigma$ -finite measure  $\mu$ . For any  $\alpha \in (0, 1)$ :*

(a) Existence. *There exists a test  $\delta^*$  and a threshold  $c \geq 0$  such that*

$$\delta^*(x) = \begin{cases} 1 & \text{if } p_1(x) > c \cdot p_0(x), \\ \mathbb{1}\{u \leq \gamma\} & \text{if } p_1(x) = c \cdot p_0(x), \\ 0 & \text{if } p_1(x) < c \cdot p_0(x), \end{cases} \quad (3.3)$$

*with  $\mathbb{E}_{P_0}[\delta^*(X)] = \alpha$ . On the set  $\{p_1 = c \cdot p_0\}$ , the test may randomize to achieve exact level  $\alpha$ .*

(b) Optimality. *The test  $\delta^*$  is most powerful at level  $\alpha$ : for any test  $\delta$  with  $\mathbb{E}_{P_0}[\delta(X)] \leq \alpha$ ,*

$$\mathbb{E}_{P_1}[\delta^*(X)] \geq \mathbb{E}_{P_1}[\delta(X)].$$

(c) Uniqueness. *If  $\delta$  is a most powerful level- $\alpha$  test, then  $\delta = \delta^*$  a.e.  $[\mu]$  on  $\{p_1 \neq c \cdot p_0\}$ , for any combination of  $c \geq 0$  and  $\gamma \in [0, 1]$  such that  $\mathbb{E}_{P_0}[\delta^*(X)] = \alpha$ .*

*Proof.* (a) Existence. Define  $\psi(c) = P_0(p_1(X) > c \cdot p_0(X))$  for  $c \geq 0$ . The function  $\psi$  is right-continuous and non-increasing, with  $\psi(0) \leq 1$  and  $\psi(c) \rightarrow 0$  as  $c \rightarrow \infty$ .

Hence there exists  $c^* \geq 0$  such that  $\psi(c^*) \leq \alpha \leq \lim_{c \uparrow c^*} \psi(c)$ . If  $\psi(c^*) = \alpha$ , the non-randomized test (3.3) has exact level  $\alpha$ . Otherwise, define

$$\gamma = \frac{\alpha - \psi(c^*)}{P_0(p_1(X) = c^* \cdot p_0(X))}$$

and set  $\delta^*(x, u) = \mathbb{1}\{u \leq \gamma\}$  for  $x \in \{p_1 = c^* \cdot p_0\}$ . Then  $\mathbb{E}_{P_0}[\delta^*] = \psi(c^*) + \gamma \cdot P_0(p_1 = c^* \cdot p_0) = \alpha$ .

(b) *Optimality.* Let  $\delta^*$  be a test of the form (3.3) with  $\mathbb{E}_{P_0}[\delta^*] = \alpha$ , and let  $\delta$  be any test with  $\mathbb{E}_{P_0}[\delta] \leq \alpha$ . By construction: on  $\{p_1 > c \cdot p_0\}$  we have  $\delta^* = 1$ , so  $\delta^* - \delta \geq 0$ ; on  $\{p_1 < c \cdot p_0\}$  we have  $\delta^* = 0$ , so  $\delta^* - \delta \leq 0$ . In both cases  $\delta^* - \delta$  and  $p_1 - c \cdot p_0$  share the same sign, hence

$$(\delta^*(x) - \delta(x))(p_1(x) - c \cdot p_0(x)) \geq 0 \quad \text{for all } x.$$

Integrating with respect to  $\mu$ :

$$0 \leq \int (\delta^* - \delta)(p_1 - c \cdot p_0) d\mu = \mathbb{E}_{P_1}[\delta^* - \delta] - c \cdot \mathbb{E}_{P_0}[\delta^* - \delta].$$

Rearranging and using  $\mathbb{E}_{P_0}[\delta^*] = \alpha$ :

$$\mathbb{E}_{P_1}[\delta^*] - \mathbb{E}_{P_1}[\delta] \geq c(\alpha - \mathbb{E}_{P_0}[\delta]) \geq 0,$$

since  $\mathbb{E}_{P_0}[\delta] \leq \alpha$  and  $c \geq 0$ .

(c) *Uniqueness.* Suppose  $\delta$  is also most powerful at level  $\alpha$ , so  $\mathbb{E}_{P_1}[\delta] = \mathbb{E}_{P_1}[\delta^*]$ . Equality in the above argument requires

$$\int (\delta^* - \delta)(p_1 - c \cdot p_0) d\mu = 0.$$

Since the integrand is nonnegative, it must vanish  $\mu$ -a.e. On  $\{p_1 > c \cdot p_0\}$ , we have  $p_1 - c \cdot p_0 > 0$ , so  $\delta^* - \delta = 0$ , i.e.,  $\delta = 1 = \delta^*$ . On  $\{p_1 < c \cdot p_0\}$ , we have  $p_1 - c \cdot p_0 < 0$ , so again  $\delta^* - \delta = 0$ , i.e.,  $\delta = 0 = \delta^*$ . Thus  $\delta = \delta^*$  a.e.  $[\mu]$  on  $\{p_1 \neq c \cdot p_0\}$ .  $\square$

The Neyman-Pearson lemma provides a complete solution to the simple-versus-simple testing problem: the likelihood ratio test is optimal.

**Example 3.15** (Neyman-Pearson Test for Gaussians). Consider testing  $H_0 : \mu = 0$  versus  $H_1 : \mu = 1$  based on  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, 1)$ . The likelihood ratio is

$$\Lambda(x) = \frac{\prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-(x_i-1)^2/2}}{\prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-x_i^2/2}} = \exp\left(\sum_{i=1}^n x_i - \frac{n}{2}\right).$$

Since  $\Lambda(x) > c$  if and only if  $\sum_i x_i > \log c + n/2$ , the Neyman-Pearson test rejects when  $\bar{X} = n^{-1} \sum_i X_i$  exceeds a threshold. Under  $H_0$ ,  $\bar{X} \sim N(0, 1/n)$ , so the level- $\alpha$  test rejects when

$$\bar{X} > \frac{z_{1-\alpha}}{\sqrt{n}},$$

where  $z_{1-\alpha}$  is the  $(1 - \alpha)$ -quantile of  $N(0, 1)$ .  $\diamond$

**Example 3.16** (Uniform scale). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Uniform}(0, \theta)$  with  $\theta > 0$ . For testing  $H_0 : \theta = 1$  versus  $H_1 : \theta = 2$ , the joint density is

$$p_\theta(x) = \theta^{-n} \mathbb{1}\{0 \leq x_{(1)}\} \mathbb{1}\{x_{(n)} \leq \theta\},$$

where  $x_{(1)} \leq \dots \leq x_{(n)}$  are the order statistics. The likelihood ratio is

$$\Lambda(x) = \frac{p_2(x)}{p_1(x)} = \begin{cases} 2^{-n} & \text{if } x_{(n)} \leq 1, \\ +\infty & \text{if } 1 < x_{(n)} \leq 2. \end{cases}$$

When  $x_{(n)} > 1$ , the data is impossible under  $H_0$  but possible under  $H_1$ , so we reject with certainty. When  $x_{(n)} \leq 1$ , the likelihood ratio is constant, so any randomization on this region yields the same power per unit of size. The level-0 most powerful test rejects if and only if  $X_{(n)} > 1$ , achieving power  $P_2(X_{(n)} > 1) = 1 - 2^{-n}$ . For level  $\alpha > 0$ , we can augment the power to  $1 - (1 - \alpha)2^{-n}$  by rejecting with probability  $\alpha$  when  $X_{(n)} \leq 1$ . This constancy may seem counterintuitive: one might expect larger values of  $X_{(n)}$  to favor  $H_1$ . But within  $\{X_{(n)} \leq 1\}$ , both hypotheses predict the same relative distribution of  $X_{(n)}$ —larger values are proportionally more likely under both  $\theta = 1$  and  $\theta = 2$ . The evidence for  $H_1$  comes entirely from observing  $X_{(n)} > 1$ , which is impossible under  $H_0$ .  $\diamond$

**Example 3.17** (Cauchy location). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Cauchy}(\theta, 1)$  with density  $p_\theta(x) = \prod_{i=1}^n \frac{1}{\pi(1+(x_i-\theta)^2)}$ . For testing  $H_0 : \theta = 0$  versus  $H_1 : \theta = 1$ , the likelihood ratio is

$$\Lambda(x) = \prod_{i=1}^n \frac{1 + x_i^2}{1 + (x_i - 1)^2}.$$

This does not simplify to a function of a low-dimensional sufficient statistic—the Cauchy family admits no nontrivial sufficient statistic. The Neyman-Pearson test still applies: reject when  $\Lambda(x) > c$ , though the rejection region  $\{x \in \mathbb{R}^n : \Lambda(x) > c\}$  has a complicated geometry that depends on all  $n$  observations.  $\diamond$

These examples illustrate that the Neyman-Pearson test adapts to the structure of the problem: it reduces to a threshold on a sufficient statistic when one exists

(Gaussian), exploits impossible events when the support depends on the parameter (Uniform), and uses the full likelihood ratio when no reduction is possible (Cauchy). In all cases, varying the threshold  $c$  traces out the efficient frontier (Definition 3.12): the boundary of the achievable region  $\mathcal{A}$  in (size, Type II error) space.

**Proposition 3.18.** *Consider a testing problem of simple hypotheses  $H_0 : P = P_0$  versus  $H_1 : P = P_1$ .*

(a) *The achievable region  $\mathcal{A}$  is convex.*

(b) *The efficient frontier is the graph  $\{(\alpha, \beta(\alpha)) : \alpha \in [0, 1]\}$ , where  $\beta(\alpha) = \mathbb{E}_1[1 - \delta_\alpha]$  is the Type II error achieved by the Neyman-Pearson test  $\delta_\alpha$ .*

(c) *The function  $\beta : [0, 1] \rightarrow [0, 1]$  is convex and non-increasing, with  $\beta(0) = 1$  and  $\beta(1) = 0$ .*

*Proof.* Part (a): Suppose  $\delta_1$  achieves  $(\alpha_1, \beta_1)$  and  $\delta_2$  achieves  $(\alpha_2, \beta_2)$ . Define

$$\delta_\lambda(x, u) = \delta_1\left(x, \frac{u}{\lambda}\right) \mathbb{1}\{u \leq \lambda\} + \delta_2\left(x, \frac{u-\lambda}{1-\lambda}\right) \mathbb{1}\{u > \lambda\}.$$

Since  $U/\lambda \sim \text{Uniform}(0, 1)$  conditionally on  $\{U \leq \lambda\}$  and  $(U-\lambda)/(1-\lambda) \sim \text{Uniform}(0, 1)$  conditionally on  $\{U > \lambda\}$ ,

$$\mathbb{E}_0[\delta_\lambda] = \lambda \alpha_1 + (1 - \lambda) \alpha_2, \quad \mathbb{E}_1[1 - \delta_\lambda] = \lambda \beta_1 + (1 - \lambda) \beta_2.$$

Part (b): By Theorem 3.14, the likelihood ratio test minimizes Type II error among all level- $\alpha$  tests.

Part (c): Monotonicity is immediate: larger  $\alpha$  permits more aggressive rejection. Convexity follows from (a): if  $(\alpha_1, \beta(\alpha_1))$  and  $(\alpha_2, \beta(\alpha_2))$  lie on the frontier, so does any convex combination, hence  $\beta(\lambda\alpha_1 + (1 - \lambda)\alpha_2) \leq \lambda\beta(\alpha_1) + (1 - \lambda)\beta(\alpha_2)$ . The boundary values follow from  $\delta \equiv 0$  achieving  $(0, 1)$  and  $\delta \equiv 1$  achieving  $(1, 0)$ .  $\square$

The Neyman-Pearson lemma solves the testing problem when both hypotheses are simple. In practice, the alternative hypothesis is often composite:  $H_1 : \theta \in \Theta_1$  with  $|\Theta_1| > 1$ . Can a single test be optimal against all alternatives simultaneously? For most problems, the answer is no—the test that is most powerful against one alternative is suboptimal against another. But there is an important class of models corresponding composite testing problems where UMP tests do exist: families with monotone likelihood ratio and monotone hypotheses.

**Definition 3.19** (Uniformly Most Powerful Test). A test  $\delta^*$  is *uniformly most powerful (UMP)* at level  $\alpha$  for testing  $H_0 : \theta \in \Theta_0$  versus  $H_1 : \theta \in \Theta_1$  if:

(i)  $\sup_{\theta \in \Theta_0} \mathbb{E}_\theta[\delta^*(X)] \leq \alpha$  (level constraint), and

(ii) for every test  $\delta$  with  $\sup_{\theta \in \Theta_0} \mathbb{E}_\theta[\delta(X)] \leq \alpha$  and every  $\theta_1 \in \Theta_1$ ,

$$\mathbb{E}_{\theta_1}[\delta(X)] \leq \mathbb{E}_{\theta_1}[\delta^*(X)].$$

UMP tests are the “gold standard” for hypothesis testing: they maximize power uniformly over all alternatives while controlling the Type I error. However, UMP tests often do not exist for general testing problems. The following result provides a sufficient condition for when they do exist.

**Theorem 3.20** (UMP Tests for Monotone Likelihood Ratio). *Let  $\{P_\theta : \theta \in \Theta \subseteq \mathbb{R}\}$  have densities  $p_\theta$  with respect to a  $\sigma$ -finite measure  $\mu$ . Suppose the family has monotone likelihood ratio (MLR) in a statistic  $T(x)$ : for  $\theta < \theta'$ , the ratio  $p_{\theta'}(x)/p_\theta(x)$  is a nondecreasing function of  $T(x)$ .*

*For testing  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta > \theta_0$ , the test*

$$\delta^*(x, u) = \begin{cases} 1 & \text{if } T(x) > c, \\ \mathbb{1}\{u \leq \gamma\} & \text{if } T(x) = c, \\ 0 & \text{if } T(x) < c, \end{cases}$$

*with  $c$  and  $\gamma \in [0, 1]$  chosen so that  $\mathbb{E}_{\theta_0}[\delta^*] = \alpha$ , is UMP at level  $\alpha$ . Any UMP level- $\alpha$  test agrees with  $\delta^*$  a.e. on  $\{T \neq c\}$ .*

*Proof.* We repeat the proof of Theorem 3.14 with some modifications. *Existence:* Define  $\psi(c) = P_{\theta_0}(T(X) > c)$ . The function  $\psi$  is right-continuous and non-increasing with  $\psi(c) \rightarrow 1$  as  $c \rightarrow -\infty$  and  $\psi(c) \rightarrow 0$  as  $c \rightarrow +\infty$ . Hence there exists  $c$  such that  $\psi(c) \leq \alpha \leq \psi(c-)$ . Setting  $\gamma = (\alpha - \psi(c))/P_{\theta_0}(T = c)$  when  $P_{\theta_0}(T = c) > 0$ , and  $\gamma = 0$  otherwise, gives  $\mathbb{E}_{\theta_0}[\delta^*] = \alpha$ .

*Optimality:* Fix any  $\theta_1 > \theta_0$ . We show  $\delta^*$  is most powerful at level  $\alpha$  for testing  $\theta_0$  versus  $\theta_1$ . By MLR,  $p_{\theta_1}(x)/p_{\theta_0}(x)$  is a nondecreasing function of  $T(x)$ ; thus,

$$\frac{p_{\theta_1}(x)}{p_{\theta_0}(x)} = g(T(x)) \quad \text{for some nondecreasing function } g.$$

Set  $g(c) = c'$ . By monotonicity of the likelihood ratio in  $T$ :

- On  $\{T > c\}$ :  $p_{\theta_1}(x) \geq c' p_{\theta_0}(x)$ .
- On  $\{T < c\}$ :  $p_{\theta_1}(x) \leq c' p_{\theta_0}(x)$ .

Let  $\bar{\delta}^*(x) = \mathbb{E}^U[\delta^*(x, U)]$  denote the rejection probability of  $\delta^*$  at  $x$ , so  $\bar{\delta}^*(x) = 1$  on  $\{T > c\}$ ,  $\bar{\delta}^*(x) = \gamma$  on  $\{T = c\}$ , and  $\bar{\delta}^*(x) = 0$  on  $\{T < c\}$ . For any test  $\delta$  with rejection probability  $\bar{\delta}(x) = \mathbb{E}^U[\delta(x, U)]$ :

- On  $\{T > c\}$ :  $\bar{\delta}^* - \bar{\delta} = 1 - \bar{\delta} \geq 0$  and  $p_{\theta_1} - c'p_{\theta_0} \geq 0$ .
- On  $\{T < c\}$ :  $\bar{\delta}^* - \bar{\delta} = -\bar{\delta} \leq 0$  and  $p_{\theta_1} - c'p_{\theta_0} \leq 0$ .
- On  $\{T = c\}$ : since  $p_{\theta_1}(x)/p_{\theta_0}(x) = g(T(x))$ , we have

$$\frac{p_{\theta_1}(x)}{p_{\theta_0}(x)} = g(c) = c',$$

and therefore  $p_{\theta_1}(x) = c'p_{\theta_0}(x)$  on this event.

In all cases:

$$(\bar{\delta}^*(x) - \bar{\delta}(x))(p_{\theta_1}(x) - c'p_{\theta_0}(x)) \geq 0 \quad \text{for all } x.$$

Integrating with respect to  $\mu$ :

$$\mathbb{E}_{\theta_1}[\delta^*] - \mathbb{E}_{\theta_1}[\delta] \geq c'(\mathbb{E}_{\theta_0}[\delta^*] - \mathbb{E}_{\theta_0}[\delta]).$$

If  $\mathbb{E}_{\theta_0}[\delta] \leq \alpha = \mathbb{E}_{\theta_0}[\delta^*]$ , then  $\mathbb{E}_{\theta_1}[\delta^*] \geq \mathbb{E}_{\theta_1}[\delta]$ . Since  $\theta_1 > \theta_0$  was arbitrary,  $\delta^*$  is most powerful against every  $\theta_1 > \theta_0$ .

*Level:* We show  $\mathbb{E}_{\theta}[\delta^*] \leq \alpha$  for all  $\theta < \theta_0$ . Fix  $\theta < \theta_0$ . Applying the optimality argument to test  $\theta$  versus  $\theta_0$ , the test  $\delta^*$  is most powerful at level  $\mathbb{E}_{\theta}[\delta^*]$ . Comparing to the constant test  $\tilde{\delta} \equiv \mathbb{E}_{\theta}[\delta^*]$ :

$$\mathbb{E}_{\theta_0}[\delta^*] \geq \mathbb{E}_{\theta_0}[\tilde{\delta}] = \mathbb{E}_{\theta}[\delta^*].$$

Thus  $\mathbb{E}_{\theta}[\delta^*] \leq \alpha$  for all  $\theta < \theta_0$ , and  $\sup_{\theta \leq \theta_0} \mathbb{E}_{\theta}[\delta^*] = \alpha$ .

*Uniqueness:* If  $\delta$  is also UMP at level  $\alpha$ , then for each  $\theta_1 > \theta_0$ , both tests are most powerful for  $\theta_0$  versus  $\theta_1$ . Equality in the above forces  $(\bar{\delta}^* - \bar{\delta})(p_{\theta_1} - c'p_{\theta_0}) = 0$  a.e. On  $\{T > c\}$ , we have  $p_{\theta_1} > c'p_{\theta_0}$ , so  $\bar{\delta} = 1 = \bar{\delta}^*$ . On  $\{T < c\}$ , we have  $p_{\theta_1} < c'p_{\theta_0}$ , so  $\bar{\delta} = 0 = \bar{\delta}^*$ . Thus  $\delta = \delta^*$  a.e. on  $\{T \neq c\}$ .  $\square$

The monotone likelihood ratio property may seem like a restrictive condition, but it is satisfied by many of the most commonly encountered statistical models. The key structural requirement is that larger values of the statistic  $T$  correspond to stronger evidence in favor of larger parameter values—a natural ordering that arises whenever the data “points in the direction” of the parameter.

**Example 3.21** (Exponential Families). One-parameter exponential families with density  $p_{\theta}(x) = h(x) \exp(\eta(\theta)T(x) - A(\theta))$  have monotone likelihood ratio in  $T$  whenever the natural parameter  $\eta(\theta)$  is strictly monotone in  $\theta$ . Indeed, for  $\theta < \theta'$ :

$$\frac{p_{\theta'}(x)}{p_{\theta}(x)} = \exp((\eta(\theta') - \eta(\theta))T(x) - (A(\theta') - A(\theta))),$$

which is increasing in  $T(x)$  when  $\eta(\theta') > \eta(\theta)$ .

Revisiting the exponential families from Example 1.31:

- *Normal location family:* For  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$  with known  $\sigma^2$ , the natural parameter is  $\eta(\mu) = \mu/\sigma^2$ , strictly increasing in  $\mu$ . The family has MLR in  $T = \bar{X}$ . The UMP test for  $H_0 : \mu \leq \mu_0$  versus  $H_1 : \mu > \mu_0$  rejects for large  $\bar{X}$ .
- *Poisson:* For  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Poisson}(\theta)$ , the natural parameter is  $\eta(\theta) = \log \theta$ , strictly increasing. The family has MLR in  $T = \sum_i X_i$ . The UMP test for  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta > \theta_0$  rejects for large  $\sum_i X_i$ .
- *Binomial:* For  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Bernoulli}(p)$ , the natural parameter is  $\eta(p) = \log(p/(1-p))$ , strictly increasing in  $p$ . The family has MLR in  $T = \sum_i X_i$ . The UMP test for  $H_0 : p \leq p_0$  versus  $H_1 : p > p_0$  rejects for large  $\sum_i X_i$ .
- *Exponential:* For  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Exp}(\theta)$  with rate  $\theta > 0$ , the natural parameter is  $\eta(\theta) = -\theta$ , strictly decreasing. The family has MLR in  $T = -\sum_i X_i$ , equivalently decreasing likelihood ratio in  $\sum_i X_i$ . The UMP test for  $H_0 : \theta \geq \theta_0$  versus  $H_1 : \theta < \theta_0$  rejects for large  $\sum_i X_i$ .

◇

Having established when UMP tests exist, we now characterize the efficient frontier for MLR families. A subtlety arises: for testing  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta > \theta_0$  without an indifference region, the worst-case Type II error over  $\Theta_1$  is achieved as  $\theta \downarrow \theta_0$ . The efficient frontier degenerates to the line  $\alpha + \beta = 1$  — no better than random guessing.

To obtain a meaningful frontier, we introduce an indifference region separating the hypotheses: values of  $\theta$  for which we do not require error control. With  $H_0 : \theta \leq \theta_0$  and  $H_1 : \theta \geq \theta_1$  for some  $\theta_1 > \theta_0$ , the worst-case Type II error is now  $P_{\theta_1}(\delta = 0)$

**Proposition 3.22.** *Let  $\{P_\theta\}$  have MLR in  $T$ . For testing  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta \geq \theta_1$  with  $\theta_0 < \theta_1$ :*

(a) *The achievable region  $\mathcal{A}$  is convex.*

(b) *The efficient frontier is the curve  $\{(\alpha(c), \beta(c)) : c \in \mathbb{R}\}$ , where*

$$\alpha(c) = P_{\theta_0}(T > c), \quad \beta(c) = P_{\theta_1}(T \leq c).$$

(c) *The frontier satisfies  $\alpha + \beta \geq 1 - \mathbf{d}_{TV}(P_{\theta_0}, P_{\theta_1})$ , with equality achieved by the likelihood ratio test for  $\theta_0$  versus  $\theta_1$ .*

*Proof.* Exercise 3.6. □

The gap  $\theta_1 - \theta_0$  governs how much the frontier improves over random guessing. In practice, this gap reflects the smallest effect size we wish to detect: in clinical trials,  $\theta_0$  represents no treatment effect and  $\theta_1$  the minimum clinically meaningful effect; in quality control,  $\theta_0$  is the acceptable defect rate and  $\theta_1$  the rate triggering intervention.

*Remark 3.23.* The same test in Theorem 3.20 is UMP when an indifference region separates the hypotheses: for  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta \geq \theta_1$  with  $\theta_1 > \theta_0$ , the threshold test calibrated at  $\theta_0$  remains optimal. The indifference region  $(\theta_0, \theta_1)$  does not change the test, only the interpretation of its performance (see Proposition 3.22).

*Remark 3.24* (Non-existence of UMP for two-sided alternatives). When the family has MLR in  $T$ , no UMP test exists for two-sided alternatives  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$ . By Neyman-Pearson, the most powerful test against any  $\theta_1 > \theta_0$  rejects for large  $T$ , while the most powerful test against any  $\theta_1 < \theta_0$  rejects for small  $T$ . A test that rejects for large  $T$  has power against  $\theta_1 < \theta_0$  strictly less than  $\alpha$ —it is biased toward the null in that direction. No single test can be simultaneously optimal against alternatives on both sides (see Exercise 3.3). This motivates other optimality criteria.

## 3.2 Tests of composite hypotheses

The Neyman-Pearson lemma provides a complete solution for simple hypotheses, and the MLR theory extends this to one-sided composite alternatives. But many of the most important testing problems are composite on both sides. In practice, we are frequently interested in *goodness-of-fit tests* —  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$  or testing whether data follows a certain class of distributions. These types of problems are composite: we test against families of distributions. This type of testing is also central to uncertainty quantification, as we will see in the next section.

But for general composite hypotheses—including two-sided alternatives, where UMP tests do not exist—we lack a canonical choice of test. The difficulty is fundamental: different alternatives call for different tests, and no single test can be optimal against all of them simultaneously. Using additional principles, we could narrow the class of tests under consideration, in the hopes of finding principled testing strategies.

The principles we consider parallel those from the estimation theory of Chapter 2, and carry the same names, though they take on different meanings in the testing context. *Unbiasedness* no longer means  $\mathbb{E}_\theta[\delta] = \theta$ ; instead, it requires that the test is at least as likely to reject under any alternative as under the null—a coherence condition ensuring the test is not “biased” toward the wrong hypothesis. *Invariance* restricts attention to tests that respect the symmetries of the problem: if the testing problem is unchanged by a group of transformations, the test should be too. *Admissibility* retains its usual meaning—do not use a test when another has at least as much power

everywhere and strictly more somewhere. Finally, the *minimax paradigm* takes an adversarial view, seeking tests that optimize the worst-case trade-off between Type I and Type II error. Each approach leads to a different class of optimal tests.

### 3.2.1 Unbiased tests

A different approach to composite testing restricts the class of tests by imposing a coherence condition: the test should be at least as likely to reject under any alternative as under the null. This rules out tests that are “aimed in the wrong direction”—powerful against some alternatives but worse than random guessing against others.

**Definition 3.25.** A test  $\delta$  for  $H_0 : \theta \in \Theta_0$  versus  $H_1 : \theta \in \Theta_1$  is *unbiased at level  $\alpha$*  if:

- (i)  $\sup_{\theta \in \Theta_0} \mathbb{E}_\theta[\delta] \leq \alpha$ , and
- (ii)  $\inf_{\theta \in \Theta_1} \mathbb{E}_\theta[\delta] \geq \alpha$ .

A test is *uniformly most powerful unbiased (UMPU)* at level  $\alpha$  if it is unbiased at level  $\alpha$  and has power at least as large as any other unbiased level- $\alpha$  test at every  $\theta_1 \in \Theta_1$ .

Condition (i) is the usual level constraint. Condition (ii) requires that power exceed the size everywhere in  $\Theta_1$ : the test is more likely to reject under any alternative than under the null. Equivalently, the power function  $\beta_\delta(\theta)$  is minimized on  $\Theta_0$ , not on  $\Theta_1$ —the test is not “biased” toward failing to detect true alternatives.

Unbiasedness rules out pathological tests. For example, when testing  $H_0 : \mu = 0$  versus  $H_1 : \mu \neq 0$  in a normal location family, the one-sided test that rejects for large  $\bar{X}$  is biased: it has power less than  $\alpha$  for  $\mu < 0$ . Requiring unbiasedness forces the rejection region to be symmetric, leading to the two-sided test that rejects for  $|\bar{X}|$  large. We will see that this test is in fact UMPU.

*Remark 3.26.* If  $\Theta_I = \emptyset$  and the power function  $\theta \mapsto \beta_\delta(\theta)$  is continuous—which holds, for instance, in exponential families—then conditions (i) and (ii) together imply  $\beta_\delta(\theta) = \alpha$  on the common boundary of  $\Theta_0$  and  $\Theta_1$ . Indeed, if  $\theta^*$  lies on this boundary, there exist sequences  $\theta_n \in \Theta_0$  and  $\theta'_n \in \Theta_1$  with  $\theta_n, \theta'_n \rightarrow \theta^*$ , giving  $\beta_\delta(\theta^*) \leq \alpha$  from (i) and  $\beta_\delta(\theta^*) \geq \alpha$  from (ii). This is a strong constraint: it pins the power function at the boundary, leaving only the behavior away from the boundary to be optimized. Much of the theory of UMPU tests exploits this boundary condition.

The key to finding UMPU tests is the Neyman-Pearson lemma applied with additional constraints. For exponential families, the boundary condition translates into a system of equations that pins the rejection region.

**Theorem 3.27** (UMPU tests for exponential families). *Let  $\{P_\theta\}$  be a one-parameter exponential family with density  $p_\theta(x) = h(x) \exp(\eta(\theta)T(x) - A(\theta))$ , where  $\eta$  is strictly increasing and  $\theta_0$  is interior to  $\Theta \subset \mathbb{R}$ .*

For testing  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$  at level  $\alpha$ , the UMPU test rejects when  $T(x) < c_1$  or  $T(x) > c_2$ , where  $c_1, c_2$  (and randomization probabilities at the boundaries) are determined by

$$\mathbb{E}_{\theta_0}[\delta^*] = \alpha, \quad (3.4)$$

$$\mathbb{E}_{\theta_0}[T \delta^*] = \alpha \mathbb{E}_{\theta_0}[T]. \quad (3.5)$$

*Sketch.* The boundary conditions (3.4)–(3.5) follow from differentiating the power function at  $\theta_0$  (Exercise 3.8) and using the fact that unbiasedness forces a minimum there (Exercise 3.9(a)). The form of the rejection region and its independence from  $\theta_1$  are established in Exercise 3.9(c)–(e).  $\square$

**Example 3.28** (Two-sided normal test). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$  with  $\sigma^2$  known. For testing  $H_0 : \mu = \mu_0$  versus  $H_1 : \mu \neq \mu_0$ , the sufficient statistic is  $T = \bar{X}$ . The UMPU test rejects when  $|\bar{X} - \mu_0| > c$  where  $c = \sigma z_{1-\alpha/2}/\sqrt{n}$ . This is the familiar two-sided  $z$ -test.

The power function is

$$\beta_{\delta^*}(\mu) = \Phi\left(\frac{\mu - \mu_0}{\sigma/\sqrt{n}} - z_{1-\alpha/2}\right) + \Phi\left(-\frac{\mu - \mu_0}{\sigma/\sqrt{n}} - z_{1-\alpha/2}\right),$$

which is symmetric about  $\mu_0$ , achieves its minimum  $\alpha$  at  $\mu = \mu_0$ , and increases toward 1 as  $|\mu - \mu_0| \rightarrow \infty$ .

The one-sided test rejecting for  $\bar{X} > \mu_0 + \sigma z_{1-\alpha}/\sqrt{n}$  is more powerful for  $\mu > \mu_0$  but has power less than  $\alpha$  for  $\mu < \mu_0$ . Unbiasedness excludes it, and the UMPU test distributes its rejection probability equally in both tails.  $\diamond$

**Example 3.29** (Testing a Poisson rate). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} \text{Poisson}(\theta)$ . For testing  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$ , the UMPU test rejects when  $\sum_i X_i < c_1$  or  $\sum_i X_i > c_2$ , with  $c_1, c_2$  determined by (3.4)–(3.5). Since  $\sum_i X_i$  is discrete, randomization at the boundaries may be needed for exact level  $\alpha$ .  $\diamond$

When the null hypothesis is composite—for instance,  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta > \theta_0$ —the UMPU test coincides with the UMP test from Theorem 3.20, since the one-sided threshold test is already unbiased. The unbiasedness machinery adds genuine content only when the UMP test fails to exist, most notably for two-sided alternatives.

**Example 3.30** (Non-existence of UMPU in multiple dimensions). Let  $X \sim N_d(\theta, I_d)$  with  $d \geq 2$ . Consider testing  $H_0 : \theta = 0$  versus  $H_1 : \theta \neq 0$  at level  $\alpha$ . The unbiasedness constraints now impose  $d + 1$  conditions, and the most powerful unbiased test against a fixed  $\theta_1 \neq 0$  has a rejection region whose shape depends on the direction of  $\theta_1$ . Since different directions yield different tests, no UMPU test exists (Exercise 3.11).

The natural test—reject when  $\|X\|^2 > \chi_{d,1-\alpha}^2$ —is unbiased but not UMPU. It is instead justified by *invariance* under orthogonal transformations (Example 3.36). In  $d = 1$ , the UMPU and invariant tests coincide; for  $d \geq 2$ , invariance provides the principled resolution that unbiasedness cannot.  $\diamond$

*Remark 3.31* (Limitations of unbiasedness). Unbiasedness is a useful restriction, but it has limitations. First, it is primarily effective for one-parameter problems: with nuisance parameters, finding UMPU tests requires conditioning on sufficient statistics for the nuisance parameters, which is tractable mainly within exponential families. Second, unbiasedness is a pointwise condition on  $\Theta_1$ —it says nothing about worst-case power. A UMPU test may have excellent power on average but poor power at specific alternatives near the boundary of  $\Theta_0$ . The minimax paradigm (Section 3.2.3) addresses this concern directly.

### 3.2.2 Invariant tests

When a testing problem possesses symmetry—meaning its structure is unchanged under a group of transformations—it is natural to restrict attention to tests that respect this symmetry. This parallels the invariance theory for estimation (Section 2.2), but with an important simplification: in testing, invariance often reduces a composite problem to a simple one, making the Neyman-Pearson lemma directly applicable.

**Definition 3.32.** A testing problem is *invariant* under a group  $G$  acting on  $\mathcal{X}$  if:

- (i) the model is equivariant:  $X \sim P_\theta$  implies  $gX \sim P_{\bar{g}\theta}$  for some induced action  $\bar{g}$  on  $\Theta$ , for all  $g \in G$ ,
- (ii) the hypotheses are preserved:  $\bar{g}\Theta_0 = \Theta_0$  and  $\bar{g}\Theta_1 = \Theta_1$  for all  $g \in G$ .

A test  $\delta$  is *invariant* under  $G$  if  $\delta(gx) = \delta(x)$  for all  $g \in G$  and  $x \in \mathcal{X}$ .

The goal is to find the *uniformly most powerful invariant (UMPI)* test under a group: a test that is invariant under a group  $G$ , whilst maximizing power against every alternative simultaneously. That is, we want to find a test  $\delta^*$  such that  $\delta^*(gx) = \delta^*(x)$ , whilst for every other level- $\alpha$  test  $\delta$  that satisfies invariance under the same group,

$$\mathbb{E}_\theta[\delta^*(X)] \geq \mathbb{E}_\theta[\delta(X)] \quad \text{for all } \theta \in \Theta_1.$$

The key insight is that finding it reduces to finding a special type of test statistic—one that captures exactly the information that is not washed away by the symmetry.

**Definition 3.33.** A statistic  $M : \mathcal{X} \rightarrow \mathcal{M}$  is a *maximal invariant* under  $G$  if:

- (i)  $M(gx) = M(x)$  for all  $g \in G$  (invariance), and

(ii)  $M(x) = M(x')$  implies  $x' = gx$  for some  $g \in G$  (maximality).

The maximal invariant retains all information not destroyed by the group action: two observations yield the same value of  $M$  if and only if they lie in the same orbit. When the group acts transitively on  $\Theta_0$  and on  $\Theta_1$ —collapsing each to a single orbit—the distribution of  $M(X)$  is completely determined by which hypothesis holds. This reduces the composite testing problem to a simple one, and the Neyman-Pearson lemma gives the optimal invariant test.

**Proposition 3.34.** *Suppose the testing problem is invariant under  $G$  with maximal invariant  $M(X)$ , and  $G$  acts transitively on both  $\Theta_0$  and  $\Theta_1$ .*

(a) *Every invariant test is a function of  $M(X)$ .*

(b) *The distribution of  $M(X)$  is constant on  $\Theta_0$  and constant on  $\Theta_1$ . Denote these distributions  $Q_0$  and  $Q_1$ .*

(c) *The most powerful invariant level- $\alpha$  test is the Neyman-Pearson test of  $Q_0$  versus  $Q_1$ : reject when  $dQ_1/dQ_0(M(X)) > c$ , with  $c$  chosen so that  $Q_0(dQ_1/dQ_0 > c) = \alpha$ .*

*Proof.* (a) If  $\delta$  is invariant and  $M(x) = M(x')$ , then  $x' = gx$  for some  $g$  by maximality, so  $\delta(x') = \delta(gx) = \delta(x)$ . Hence,  $\delta$  is constant on the level sets of  $M$ , i.e.,  $\delta(x) = \phi(M(x))$  for some  $\phi$ .

(b) Let  $\theta, \theta' \in \Theta_0$ . Transitivity gives  $\theta' = g\theta$  for some  $g \in G$ . For any measurable  $B \subset \mathcal{M}$ :

$$P_{\theta'}(M(X) \in B) = P_{g\theta}(M(X) \in B) = P_{\theta}(M(gX) \in B) = P_{\theta}(M(X) \in B),$$

where the last equality uses  $M(gX) = M(X)$ . So  $M(X)$  has the same distribution under every  $\theta \in \Theta_0$ . The same argument applies to  $\Theta_1$ .

(c) By (a), any invariant (possibly random) test  $\delta(x, \cdot)$  can be represented as  $\phi(M(x))$  for some  $\phi : \mathcal{M} \rightarrow [0, 1]$ . The size of  $\delta$  is

$$\mathbb{E}_{\theta}[\delta(X, U)] = \mathbb{E}_{\theta}[\phi(M(X))] = \int \phi dQ_{\theta} \quad \text{for any } \theta \in \Theta_0,$$

using (b). Its power under any  $\theta_1 \in \Theta_1$  is

$$\mathbb{E}_{\theta_1}[\delta(X)] = \int \phi dQ_1.$$

The problem of finding the invariant test maximizing  $\int \phi dQ_1$  subject to  $\int \phi dQ_0 \leq \alpha$  is exactly a simple-versus-simple testing problem with observation  $M(X) \sim Q_i$  under  $H_i$ . By the Neyman-Pearson lemma, the solution rejects when  $dQ_1/dQ_0(M(X)) > c$ .  $\square$

**Example 3.35** (Testing at known signal strength). Let  $X \sim N_d(\theta, I_d)$  with  $d \geq 2$ . For a known  $r_0 > 0$ , test  $H_0 : \theta = 0$  versus  $H_1 : \|\theta\| = r_0$ .

The problem is invariant under rotation, i.e.,  $G = O(d)$ . The null  $\Theta_0 = \{0\}$  is a single orbit, and the alternative  $\Theta_1 = \{\theta : \|\theta\| = r_0\}$  is also a single orbit (any two vectors of the same norm are related by an orthogonal transformation). The maximal invariant is  $M(X) = \|X\|^2$ , with distributions

$$Q_0 = \chi_d^2, \quad Q_1 = \chi_d^2(r_0^2).$$

By Proposition 3.34, the most powerful invariant test is the Neyman-Pearson test of  $Q_0$  versus  $Q_1$ : reject when  $dQ_1/dQ_0(\|X\|^2) > c$ . Since the noncentral  $\chi^2$  likelihood ratio is increasing in  $\|X\|^2$ , this reduces to rejecting when  $\|X\|^2 > c$ , with  $c$  chosen so that  $P(\chi_d^2 > c) = \alpha$ .  $\diamond$

The maximal invariant retains all information not destroyed by the group action: two observations yield the same value of  $M$  if and only if they lie in the same orbit. In most applications,  $G$  acts transitively on  $\Theta_0$ —collapsing the null to a single orbit—so that the distribution of  $M(X)$  under  $H_0$  is unique by Proposition 3.34(b). The alternative  $\Theta_1$ , however, typically splits into multiple orbits, each yielding a different distribution for  $M(X)$ . If these orbits can be indexed by a real-valued parameter  $\tau > 0$  and the resulting family of distributions has monotone likelihood ratio in  $M$ , the UMP invariant test follows from Theorem 3.20.

**Example 3.36** (The  $\chi^2$ -test). Let  $X \sim N_d(\theta, I_d)$ ,  $d \geq 2$ . Test  $H_0 : \theta = 0$  versus  $H_1 : \theta \neq 0$ .

The problem is invariant under the orthogonal group  $G = O(d)$  acting by  $gX = OX$ ,  $\bar{g}\theta = O\theta$ . Both  $\Theta_0 = \{0\}$  and  $\Theta_1 = \mathbb{R}^d \setminus \{0\}$  are preserved. The maximal invariant is  $M(X) = \|X\|^2$ , and the maximal invariant in the parameter space is  $\|\theta\|^2$ .

Under  $H_0$ ,  $\|X\|^2 \sim \chi_d^2$ . Under  $\theta \neq 0$ ,  $\|X\|^2 \sim \chi_d^2(\|\theta\|^2)$  (noncentral  $\chi^2$  with noncentrality  $\|\theta\|^2$ ). The noncentral  $\chi^2$  family has MLR in  $\|X\|^2$  as a function of  $\|\theta\|^2$ : larger values of  $\|X\|^2$  provide stronger evidence for larger  $\|\theta\|^2$ . By Theorem 3.20 applied to the maximal invariant, the UMP invariant test rejects when

$$\|X\|^2 > \chi_{d,1-\alpha}^2.$$

This is the  $\chi^2$ -test from Exercise 3.11, now justified by invariance rather than unbiasedness.  $\diamond$

### 3.2.3 Minimax testing

For general composite hypotheses—including two-sided alternatives, where UMPU/UMPI tests do not exist—we lack a canonical choice of test. The minimax paradigm offers a resolution. The testing loss (3.1) assigns cost  $a$  to Type I errors and  $b$  to Type II errors. By (3.2), the minimax risk is

$$\mathcal{R}_{a,b}(\delta) := \sup_{\theta \in \Theta} \mathcal{R}(\theta, \delta) = \max(a \cdot \alpha(\delta), b \cdot \beta(\delta)), \quad (3.6)$$

where  $\alpha(\delta) = \sup_{\theta \in \Theta_0} \beta_\delta(\theta)$  is the size and  $\beta(\delta) = \sup_{\theta \in \Theta_1} (1 - \beta_\delta(\theta))$  is the worst-case Type II error. Thus, the minimax risk depends on  $\delta$  only through the pair  $(\alpha(\delta), \beta(\delta))$ .

A test attaining the minimax risk, provided it exists, selects the point on the efficient frontier where  $a \cdot \alpha = b \cdot \beta$ . Varying the cost ratio  $a/b$  over  $(0, \infty)$  traces out the frontier: the minimax paradigm does not yield a single test, but a family of tests representing the optimal trade-off between worst-case Type I and worst-case Type II error. This is a complete answer to the composite testing problem: rather than seeking a single test that dominates all others—which generally does not exist—we characterize the set of tests that cannot be improved upon from the minimax point of view.

The existence of a minimax test is provided by the following theorem.

**Theorem 3.37** (Optimal tests for composite hypotheses). *Let  $\Theta_0$  and  $\Theta_1$  be disjoint compact subsets of  $\Theta$ , consider a model dominated by a  $\sigma$ -finite measure  $\mu$  and suppose  $\theta \mapsto p_\theta$  is continuous as a map from  $\Theta$  to  $L_1(\mu)$ .*

*For testing  $H_0 : \theta \in \Theta_0$  versus  $H_1 : \theta \in \Theta_1$ , consider the risk criterion (3.6) for some  $a, b > 0$ .*

*Then, there exists a test  $\delta^* \equiv \delta_{a,b}^*$  minimizing  $\mathcal{R}_{a,b}(\delta)$  over all tests.*

*Proof.* The result is a corollary to the minimax theorem of Chapter 4. □

As  $a/b$  varies, the minimax tests  $\delta_{a,b}^*$  trace out the efficient frontier—the boundary of the achievable (size, worst-case Type II error) region. The next proposition makes this precise.

**Proposition 3.38.** *Assume a testing problem with hypotheses such that neither  $H_0$  nor  $H_1$  can be tested perfectly (i.e., no test achieves both  $\alpha(\delta) = 0$  and  $\beta(\delta) = 0$ ). Then:*

(a) *The achievable region  $\mathcal{A} = \{(\alpha, \beta) \in [0, 1]^2 : \text{there exists a test } \delta \text{ with } \alpha(\delta) \leq \alpha, \beta(\delta) \leq \beta\}$  is convex.*

(b) *Every minimizer of  $R_\lambda(\delta) = \lambda \alpha(\delta) + (1 - \lambda) \beta(\delta)$  for  $\lambda \in (0, 1)$  lies on the efficient*

*frontier*

$$\mathcal{E} = \{(\alpha, \beta) \in \partial\mathcal{A} : \text{no } (\alpha', \beta') \in \mathcal{A} \text{ satisfies } \alpha' \leq \alpha, \beta' \leq \beta \\ \text{with strict inequality in at least one coordinate}\}.$$

(c) Conversely, every point on  $\mathcal{E}$  is achieved by a minimizer of  $R_\lambda$  for some  $\lambda \in (0, 1)$ .

*Proof.* See Exercise 3.14. □

### 3.3 Confidence Sets

Often we want more than a single best guess or a binary decision: we want to quantify uncertainty by reporting a set of parameter values consistent with the observed data. A confidence set does exactly this—it is a data-dependent subset of the parameter space that contains the true parameter with high probability.

**Definition 3.39.** A  $(1 - \alpha)$ -confidence set for  $\theta$  is a set-valued function  $C : \mathcal{X} \rightarrow 2^\Theta$  such that for each  $\theta \in \Theta$ , the event  $\{x : \theta \in C(x)\}$  is measurable and

$$\inf_{\theta \in \Theta} P_\theta(\theta \in C(X)) \geq 1 - \alpha.$$

The quantity  $1 - \alpha$  is the *confidence level*. When  $\Theta \subseteq \mathbb{R}$  and  $C(X)$  is an interval for all  $x$ , we call it a *confidence interval*.

There is a fundamental duality between hypothesis testing and confidence sets: a family of tests can be inverted to produce a confidence set, and conversely, any confidence set determines a family of tests. This connection provides both a constructive method for building confidence sets and a principled way to understand their properties.

For each  $\theta_0 \in \Theta$ , suppose we have a level- $\alpha$  test  $\delta_{\theta_0}$  for the null hypothesis  $H_0 : \theta = \theta_0$ .

**Proposition 3.40** (Test inversion). *The random set*

$$C(X) = \{\theta_0 \in \Theta : \delta_{\theta_0}(X) = 0\},$$

*consisting of all parameter values not rejected by their respective tests, is a  $(1 - \alpha)$ -confidence set for  $\theta$ .*

*Proof.* For coverage, fix any  $\theta \in \Theta$  and set  $\theta_0 = \theta$ . Then

$$P_\theta(\theta \in C(X)) = P_\theta(\delta_\theta(X) = 0) = 1 - P_\theta(\delta_\theta(X) = 1) \geq 1 - \alpha,$$

since  $\delta_\theta$  has level  $\alpha$  for testing  $H_0 : \theta = \theta$ . □

The set  $C(X)$  contains exactly those parameter values that are “compatible” with the observed data according to the tests  $\{\delta_\theta : \theta \in \Theta_0\}$ , in the sense that the data does not provide sufficient evidence to reject them at level  $\alpha$ . The duality runs in both directions.

**Proposition 3.41.** *Let  $C(X)$  be a  $(1 - \alpha)$ -confidence set for  $\theta$ . For each  $\theta_0 \in \Theta$ , define  $\delta_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C(X)\}$ . Then  $\delta_{\theta_0}$  is a level- $\alpha$  test of  $H_0 : \theta = \theta_0$  against  $H_1 : \theta \neq \theta_0$ .*

*Proof.*  $P_{\theta_0}(\delta_{\theta_0}(X) = 1) = P_{\theta_0}(\theta_0 \notin C(X)) \leq \alpha$  by the coverage guarantee.  $\square$

A family of confidence sets  $\{C_\alpha(X) : \alpha \in (0, 1)\}$  is *nested* if  $C_\alpha(x) \supseteq C_{\alpha'}(x)$  whenever  $\alpha < \alpha'$ : higher confidence requires larger sets. Given a nested family, the tests  $\delta_{\theta_0, \alpha}(X) = \mathbb{1}\{\theta_0 \notin C_\alpha(X)\}$  form a nested family in the sense of Definition 3.9, and there is a corresponding  $p$ -value.

**Proposition 3.42** (Confidence sets and  $p$ -values). *Let  $\{C_\alpha(X) : \alpha \in (0, 1)\}$  be a nested family of  $(1 - \alpha)$ -confidence sets for  $\theta$ . Define*

$$p(X; \theta_0) = \inf\{\alpha \in (0, 1) : \theta_0 \notin C_\alpha(X)\}.$$

*Then:*

(a) *The  $p$ -value is valid:  $P_{\theta_0}(p(X; \theta_0) \leq \alpha) \leq \alpha$  for all  $\theta_0 \in \Theta$ .*

(b) *The confidence sets are recovered:  $C_\alpha(X) = \{\theta_0 \in \Theta : p(X; \theta_0) > \alpha\}$ .*

*Proof.* Part (a):  $p(X; \theta_0) \leq \alpha$  if and only if  $\theta_0 \notin C_\alpha(X)$ , so  $P_{\theta_0}(p(X; \theta_0) \leq \alpha) = P_{\theta_0}(\theta_0 \notin C_\alpha(X)) \leq \alpha$ . Part (b):  $\theta_0 \in C_\alpha(X)$  if and only if  $\theta_0 \in C_{\alpha'}(X)$  for all  $\alpha' \leq \alpha$  (by nesting), which is equivalent to  $p(X; \theta_0) > \alpha$ .  $\square$

In hypothesis testing, the level constraint bounds the probability of false rejection, and power measures the probability of correct rejection. For confidence sets, the coverage constraint bounds the probability of non-coverage, and *precision*—measured by the size of the set—plays the role of power: smaller sets are more informative.

**Definition 3.43.** For confidence sets taking values in  $\Theta \subseteq \mathbb{R}^d$ , the *expected volume* of a confidence set  $C(X)$  is  $S_\theta(C) = \mathbb{E}_\theta[|C(X)|]$ , where  $|C|$  denotes Lebesgue measure. For confidence intervals ( $d = 1$ ), this is the expected length.

*Remark 3.44* (Functionals and nuisance parameters). In practice, we often want a confidence set not for the full parameter  $\theta$  but for a functional  $\phi(\theta)$ , where  $\phi : \Theta \rightarrow \Phi$ . A  $(1 - \alpha)$ -confidence set for  $\phi(\theta)$  is a set-valued function  $C : \mathcal{X} \rightarrow 2^\Phi$  satisfying  $\inf_{\theta \in \Theta} P_\theta(\phi(\theta) \in C(X)) \geq 1 - \alpha$ . Everything in this section extends to this setting by replacing  $\theta$  with  $\phi(\theta)$  and  $\Theta$  with  $\Phi$  throughout. When  $\phi$  is injective, testing

$H_0 : \phi(\theta) = \phi_0$  is equivalent to testing a simple null. When  $\phi$  is not injective, the components of  $\theta$  not determined by the constraint  $\phi(\theta) = \phi_0$  act as nuisance parameters, and  $H_0 : \phi(\theta) = \phi_0$  becomes a composite null hypothesis.

### 3.3.1 Uncertainty quantification

Constructing confidence sets of any level  $\alpha$  is always possible: take  $C(x) = \Theta$  for all  $x$ . However, we prefer ones that are “as tight as possible” while still maintaining coverage. Among all  $(1 - \alpha)$ -confidence sets, we prefer those with smaller expected volume—they localize  $\theta$  more precisely. This parallels maximizing power subject to a level constraint. The following notion makes this precise.

**Definition 3.45.** A  $(1 - \alpha)$ -confidence set  $C^*(X)$  for  $\theta$  is *uniformly most accurate (UMA)* if for every other  $(1 - \alpha)$ -confidence set  $C(X)$  and every  $\theta \in \Theta$ ,

$$P_\theta(\theta_0 \in C^*(X)) \leq P_\theta(\theta_0 \in C(X)) \quad \text{for all } \theta_0 \neq \theta.$$

A UMA confidence set includes false values  $\theta_0 \neq \theta$  with minimal probability—it is as “tight” as possible while maintaining coverage. The parallel to UMP tests is exact.

**Proposition 3.46.** Let  $\{\delta_{\theta_0} : \theta_0 \in \Theta\}$  be a family of tests of  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$ . Define  $C(X) = \{\theta_0 : \delta_{\theta_0}(X) = 0\}$ .

(a) If each  $\delta_{\theta_0}$  is UMP at level  $\alpha$ , then  $C(X)$  is UMA at level  $1 - \alpha$ .

(b) If  $C(X)$  is UMA at level  $1 - \alpha$ , then each  $\delta_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C(X)\}$  is UMP at level  $\alpha$ .

*Proof.* Part (a): Let  $C'(X)$  be any other  $(1 - \alpha)$ -confidence set, and let  $\delta'_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C'(X)\}$ . By Proposition 3.41,  $\delta'_{\theta_0}$  has level  $\alpha$ . For any  $\theta \neq \theta_0$ ,

$$P_\theta(\theta_0 \in C(X)) = 1 - P_\theta(\delta_{\theta_0}(X) = 1) \leq 1 - P_\theta(\delta'_{\theta_0}(X) = 1) = P_\theta(\theta_0 \in C'(X)),$$

since  $\delta_{\theta_0}$  is UMP.

Part (b): Let  $\delta'_{\theta_0}$  be any level- $\alpha$  test. Define

$$C'(X) = (C(X) \setminus \{\theta_0\}) \cup \{\theta_0 \in \{\theta_0\} : \delta'_{\theta_0}(X) = 0\}.$$

This is a  $(1 - \alpha)$ -confidence set. Since  $C$  is UMA, for  $\theta \neq \theta_0$ :

$$P_\theta(\delta_{\theta_0}(X) = 1) = 1 - P_\theta(\theta_0 \in C(X)) \geq 1 - P_\theta(\theta_0 \in C'(X)) = P_\theta(\delta'_{\theta_0}(X) = 1). \quad \square$$

Just as UMP tests rarely exist for two-sided alternatives, UMA confidence sets are rare. A common relaxation is to restrict attention to *unbiased* confidence sets: those

satisfying  $P_\theta(\theta_0 \in C(X)) \leq 1 - \alpha$  for all  $\theta_0 \neq \theta$ . An unbiased confidence set includes any false value  $\theta_0$  with probability at most  $1 - \alpha$ —the coverage probability for the true value. The parallel to unbiased tests is exact: the inverted tests  $\delta_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C(X)\}$  satisfy  $\mathbb{E}_\theta[\delta_{\theta_0}] \geq \alpha$  whenever  $\theta \neq \theta_0$ , so power exceeds level throughout the alternative.

**Definition 3.47.** A  $(1 - \alpha)$ -confidence set  $C^*(X)$  for  $\theta$  is *uniformly most accurate unbiased (UMAU)* if it is unbiased and for every other unbiased  $(1 - \alpha)$ -confidence set  $C(X)$ ,

$$P_\theta(\theta_0 \in C^*(X)) \leq P_\theta(\theta_0 \in C(X)) \quad \text{for all } \theta \in \Theta \text{ and } \theta_0 \neq \theta.$$

The duality of Proposition 3.46 extends to the unbiased setting: inverting a family of UMPU tests yields a UMAU confidence set, and conversely.

**Proposition 3.48.** Let  $\{\delta_{\theta_0} : \theta_0 \in \Theta\}$  be a family of tests of  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$ . Define  $C(X) = \{\theta_0 : \delta_{\theta_0}(X) = 0\}$ .

(a) If each  $\delta_{\theta_0}$  is UMPU at level  $\alpha$ , then  $C(X)$  is UMAU at level  $1 - \alpha$ .

(b) If  $C(X)$  is UMAU at level  $1 - \alpha$ , then each  $\delta_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C(X)\}$  is UMPU at level  $\alpha$ .

*Proof.* See Exercise 3.15. □

**Example 3.49** (Normal mean, known variance). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$  with  $\sigma^2$  known. The UMPU test of  $H_0 : \mu = \mu_0$  versus  $H_1 : \mu \neq \mu_0$  rejects when  $|\bar{X} - \mu_0| > z_{1-\alpha/2} \cdot \sigma/\sqrt{n}$  (Example 3.28). Inverting over all  $\mu_0$  gives the UMAU confidence interval

$$C(X) = \left[ \bar{X} - z_{1-\alpha/2} \cdot \frac{\sigma}{\sqrt{n}}, \bar{X} + z_{1-\alpha/2} \cdot \frac{\sigma}{\sqrt{n}} \right].$$

This interval has the shortest expected length among all unbiased  $(1 - \alpha)$ -confidence intervals for  $\mu$ . ◇

Invariance provides another route to optimal confidence sets. When a group  $G$  acts on both the sample space and parameter space, restricting to equivariant confidence sets can yield unique optimal solutions.

**Definition 3.50.** Let  $G$  be a group acting on  $\mathcal{X}$  via  $x \mapsto gx$  and on  $\Theta$  via  $\theta \mapsto \bar{g}\theta$ . A confidence set  $C(X)$  for  $\theta$  is *equivariant* if

$$C(gX) = \bar{g}C(X) := \{\bar{g}\theta : \theta \in C(X)\} \quad \text{for all } g \in G.$$

Equivariance is the natural analog of invariance for set-valued procedures: if the data are transformed by  $g$ , the confidence set transforms accordingly.

**Definition 3.51.** An equivariant  $(1 - \alpha)$ -confidence set  $C^*(X)$  for  $\theta$  is *uniformly most accurate equivariant (UMAE)* if for every other equivariant  $(1 - \alpha)$ -confidence set  $C(X)$ ,

$$P_\theta(\theta_0 \in C^*(X)) \leq P_\theta(\theta_0 \in C(X)) \quad \text{for all } \theta \in \Theta \text{ and } \theta_0 \neq \theta.$$

Inverting a family of UMPI tests yields a UMAE confidence set, and conversely.

**Proposition 3.52.** Consider a model that is equivariant under a group  $G$  that acts transitively on  $\Theta$ . Fix  $\theta^* \in \Theta$  and write  $G_{\theta^*} = \{g \in G : \bar{g}\theta^* = \theta^*\}$ .

- (a) Let  $\delta_{\theta^*}$  be UMPI under  $G_{\theta^*}$  at level  $\alpha$  for testing  $H_0 : \theta = \theta^*$  versus  $H_1 : \theta \neq \theta^*$ , and define the family  $\delta_{\bar{g}\theta^*}(x) = \delta_{\theta^*}(g^{-1}x)$ . Then,  $C(X) = \{\theta_0 : \delta_{\theta_0}(X) = 0\}$  is UMAE at level  $1 - \alpha$ .
- (b) If  $C(X)$  is UMAE at level  $1 - \alpha$ , then each  $\delta_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C(X)\}$  is UMPI for the group  $\{g \in G : \bar{g}\theta_0 = \theta_0\}$  at level  $\alpha$ .

*Proof.* See Exercise 3.16. □

**Example 3.53** (Normal mean, unknown variance). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$  with both parameters unknown. The location-scale group  $G = \{x \mapsto ax + b : a > 0, b \in \mathbb{R}\}$  acts on the data, and equivariance requires  $C(aX + b) = aC(X) + b$ . The UMAE confidence interval for  $\mu$  is

$$C(X) = \left[ \bar{X} - t_{n-1, 1-\alpha/2} \cdot \frac{S}{\sqrt{n}}, \bar{X} + t_{n-1, 1-\alpha/2} \cdot \frac{S}{\sqrt{n}} \right],$$

obtained by inverting the UMPI  $t$ -test. ◇

The UMA, UMAU, and UMAE criteria all measure accuracy by the probability of including false values, pointwise over all  $\theta_0 \neq \theta$ . This is a strong requirement—it implies, for instance, minimization of expected volume.

**Proposition 3.54.** Let  $\Theta \subseteq \mathbb{R}^d$  and let  $C^*(X)$  be a UMA  $(1 - \alpha)$ -confidence set for  $\theta$ . Then  $C^*$  minimizes expected volume among all  $(1 - \alpha)$ -confidence sets: for every  $(1 - \alpha)$ -confidence set  $C(X)$  and every  $\theta \in \Theta$ ,

$$\mathbb{E}_\theta[|C^*(X)|] \leq \mathbb{E}_\theta[|C(X)|],$$

where  $|\cdot|$  denotes Lebesgue measure.

*Proof.* By the UMA property,  $P_\theta(\theta_0 \in C^*(X)) \leq P_\theta(\theta_0 \in C(X))$  for all  $\theta_0 \neq \theta$ . Exchanging integral and expectation over  $\theta_0$ :

$$\mathbb{E}_\theta[|C^*(X)|] = \int_{\mathbb{R}^d} P_\theta(\theta_0 \in C^*(X)) d\theta_0 \leq \int_{\mathbb{R}^d} P_\theta(\theta_0 \in C(X)) d\theta_0 = \mathbb{E}_\theta[|C(X)|]. \quad \square$$

When no UMA (or UMAU, or UMAE) set exists, one can instead minimize a scalar loss such as expected volume, expected diameter, or expected length directly, subject to the coverage constraint. Different losses lead to different optimal procedures, and the choice among them is a decision-theoretic question.

Depending on the task at hand, it may make sense to minimize a scalar loss such as expected volume, expected diameter, or expected length directly, subject to the coverage constraint. Different losses lead to different optimal procedures, and the choice among them is a decision-theoretic question. For  $\Theta \subseteq \mathbb{R}^d$ , natural choices include:

<i>Criterion</i>	<i>Loss</i> $L(\theta, C)$
Volume	$ C $
Diameter	$\sup_{\theta_1, \theta_2 \in C} \ \theta_1 - \theta_2\ $
Excess volume	$ C \setminus B(\theta, r) $ (penalty for mass far from $\theta$ )
Squared radius	$\sup_{\theta_0 \in C} \ \theta_0 - \theta\ ^2$

Different losses lead to different optimal procedures. For instance, minimizing expected length of a confidence interval for the normal variance yields a different interval than inverting the UMPU test (see Exercise 3.18). The choice among these criteria depends on the application at hand.

The expected size of a confidence set cannot be made arbitrarily small: the precision of any confidence procedure is ultimately limited by the distinguishability of the underlying distributions, or a related estimation problem. If e.g. the estimation problem has a lower bound on a related risk, then the confidence set diameter cannot be made arbitrarily small either. The following result makes this precise by connecting confidence set diameter to the total variation distance from Lemma 3.13.

**Proposition 3.55.** *Let  $C(X)$  be a  $(1 - \alpha)$ -confidence set for  $\theta \in \Theta \subseteq \mathbb{R}^d$ , and define the diameter  $\text{diam}(C) = \sup_{\theta, \theta' \in C} \|\theta - \theta'\|$ . For any  $\theta_0, \theta_1 \in \Theta$ ,*

$$\max\{\mathbb{E}_{\theta_0}[\text{diam}(C(X))], \mathbb{E}_{\theta_1}[\text{diam}(C(X))]\} \geq \|\theta_1 - \theta_0\| \cdot (1 - 2\alpha - \mathbf{d}_{TV}(P_{\theta_0}, P_{\theta_1}))_+.$$

*In particular,*

$$\inf_C \sup_{\theta \in \Theta} \mathbb{E}_{\theta}[\text{diam}(C(X))] \geq \sup_{\theta_0, \theta_1 \in \Theta} \|\theta_1 - \theta_0\| \cdot (1 - 2\alpha - \mathbf{d}_{TV}(P_{\theta_0}, P_{\theta_1}))_+,$$

*where the infimum is over all  $(1 - \alpha)$ -confidence sets.*

*Proof.* Fix  $\theta_0, \theta_1 \in \Theta$ . On the event  $E = \{\theta_0 \in C(X)\} \cap \{\theta_1 \in C(X)\}$ , we have  $\text{diam}(C(X)) \geq \|\theta_1 - \theta_0\|$ , so it suffices to bound  $P_{\theta_1}(E)$  from below.

By coverage,  $P_{\theta_1}(\theta_1 \notin C(X)) \leq \alpha$ . For the other term, define the test  $\delta(X) = \mathbb{1}\{\theta_0 \notin C(X)\}$ . By Proposition 3.41,  $\delta$  has level  $\alpha$  for testing  $H_0 : \theta = \theta_0$ . By Lemma 3.13,

$$P_{\theta_0}(\delta = 1) + P_{\theta_1}(\delta = 0) \geq 1 - \mathbf{d}_{TV}(P_{\theta_0}, P_{\theta_1}),$$

so  $P_{\theta_1}(\theta_0 \in C(X)) = P_{\theta_1}(\delta = 0) \geq 1 - \alpha - \mathbf{d}_{TV}(P_{\theta_0}, P_{\theta_1})$ . By a union bound,

$$P_{\theta_1}(E) \geq 1 - P_{\theta_1}(\theta_0 \notin C(X)) - P_{\theta_1}(\theta_1 \notin C(X)) \geq 1 - 2\alpha - \mathbf{d}_{TV}(P_{\theta_0}, P_{\theta_1}).$$

Hence  $\mathbb{E}_{\theta_1}[\text{diam}(C(X))] \geq \|\theta_1 - \theta_0\| \cdot P_{\theta_1}(E) \geq \|\theta_1 - \theta_0\|(1 - 2\alpha - \mathbf{d}_{TV}(P_{\theta_0}, P_{\theta_1}))_+$ . The same argument with the roles of  $\theta_0$  and  $\theta_1$  reversed gives the bound for  $\mathbb{E}_{\theta_0}$ .  $\square$

The bound has a direct parallel to the constraint risk inequality for estimation lower bounds (Lemma 2.43). Both bounds are governed by the same trade-off: the separation  $\|\theta_1 - \theta_0\|$  between two parameter values and a distance/divergence measure for  $P_{\theta_0}, P_{\theta_1}$ , quantifying how distinguishable the corresponding distributions are. Pairs  $(\theta_0, \theta_1)$  that yield tight estimation lower bounds typically also yield tight lower bounds on confidence set diameter, up to constants depending on  $\alpha$ . In particular, the minimax rate for estimation and the minimax expected diameter of confidence sets are of the same order.

## Exercises

*Exercise 3.1* (Variational representation of total variation). Let  $P_0$  and  $P_1$  be probability measures on  $(\mathcal{X}, \mathcal{X})$  dominated by a common  $\sigma$ -finite measure  $\mu$ , with densities  $p_0 = dP_0/d\mu$  and  $p_1 = dP_1/d\mu$ . Recall that the total variation distance is defined as

$$d_{TV}(P_0, P_1) = \sup_{A \in \mathcal{X}} |P_0(A) - P_1(A)|.$$

(a) Show that

$$d_{TV}(P_0, P_1) = \sup_{A \in \mathcal{X}} (P_1(A) - P_0(A)).$$

*Hint: Use the fact that  $P_1(A) - P_0(A) = -(P_1(A^c) - P_0(A^c))$ .*

(b) Show that the supremum in (a) is achieved by  $A^* = \{x : p_1(x) > p_0(x)\}$ , and conclude that

$$d_{TV}(P_0, P_1) = \int_{p_1 > p_0} (p_1 - p_0) d\mu.$$

(c) Prove the symmetric representation

$$d_{TV}(P_0, P_1) = \frac{1}{2} \int |p_1 - p_0| d\mu.$$

*Exercise 3.2* (Efficient frontiers). Consider testing  $H_0 : \theta = 0$  versus  $H_1 : \theta = 1$  based on a single observation  $X$ .

- Let  $X \sim N(\theta, 1)$ . Show that the Neyman-Pearson test rejects for large  $X$ , and compute the efficient frontier  $\{(\alpha, \beta(\alpha)) : \alpha \in [0, 1]\}$ .
- Let  $X \sim \text{Laplace}(\theta, 1)$  with density  $\frac{1}{2}e^{-|x-\theta|}$ . Derive the likelihood ratio test and compute the efficient frontier.
- Plot (sketch) both frontiers on the same axes. Which model allows for better discrimination between the hypotheses?

*Exercise 3.3* (Non-existence of UMP for two-sided alternatives). Suppose that a model  $\{P_\theta : \theta \in \Theta \subseteq \mathbb{R}\}$  is dominated by a common  $\sigma$ -finite measure  $\mu$ , with MLR in a real valued statistic  $T$ , and that if  $\theta_1 \neq \theta_0$ , then  $P_{\theta_0}$  and  $P_{\theta_1}$  differ on  $\{T > c\}$  for all  $c \in \mathbb{R}$ .

Consider testing  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$  at level  $\alpha \in (0, 1)$ .

- Let  $\delta_+$  be the UMP level- $\alpha$  test of  $H_0$  versus  $H_1^+ : \theta > \theta_0$ . Show that  $E_{\theta_1}[\delta_+] < \alpha$  for all  $\theta_1 < \theta_0$ . *Hint: consider what the MP test of  $H_0' : \theta = \theta_1$  vs  $H_1' : \theta = \theta_0$*

of level  $\mathbb{E}_{\theta_0}[\delta_+]$  would be. Alternatively, try changing measures (mimic the NP lemma proof) and apply monotonicity.

- (b) Let  $\delta_-$  be the UMP level- $\alpha$  test of  $H_0$  versus  $H_1^- : \theta < \theta_0$ . Show that  $\delta_-$  rejects for small  $T$ , and that  $E_{\theta_1}[\delta_-] < \alpha$  for all  $\theta_1 > \theta_0$ .
- (c) Conclude that no UMP level- $\alpha$  test exists for the two-sided problem. *Hint: If  $\delta^*$  were UMP, compare its power to  $\delta_+$  and  $\delta_-$ .*

*Exercise 3.4 (Normal variance).* Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(0, \sigma^2)$ . For testing  $H_0 : \sigma^2 = \sigma_0^2$  versus  $H_1 : \sigma^2 = \sigma_1^2$  with  $\sigma_1^2 > \sigma_0^2$ :

- (a) Show the Neyman-Pearson test rejects for large  $\sum_i X_i^2$ .
- (b) Determine the critical value using the distribution of  $\sum_i X_i^2$  under  $H_0$ .
- (c) Does this family have MLR? Is there a UMP test for  $H_0 : \sigma^2 \leq \sigma_0^2$  versus  $H_1 : \sigma^2 > \sigma_0^2$ ?

*Exercise 3.5 (Weighted error loss and Neyman-Pearson).* Consider testing  $H_0 : P = P_0$  versus  $H_1 : P = P_1$  with loss

$$L(P, d) = a \cdot \mathbb{1}\{P = P_0, d = 1\} + b \cdot \mathbb{1}\{P = P_1, d = 0\},$$

where  $a, b > 0$  are the costs of Type I and Type II errors.

- (a) Show that the risk of a test  $\delta$  under  $P_0$  and  $P_1$  is

$$R(P_0, \delta) = a \cdot E_0[\delta], \quad R(P_1, \delta) = b \cdot (1 - E_1[\delta]).$$

- (b) For  $\lambda \in (0, 1)$ , consider minimizing the weighted risk  $\lambda R(P_0, \delta) + (1 - \lambda) R(P_1, \delta)$ . Show the optimal test rejects when

$$\frac{p_1(x)}{p_0(x)} > \frac{\lambda a}{(1 - \lambda) b}.$$

- (c) Conclude that every test minimizing a weighted combination of Type I and Type II error probabilities is a likelihood ratio test.
- (d) Conversely, show that every Neyman-Pearson test with threshold  $c > 0$  minimizes  $\lambda R(P_0, \delta) + (1 - \lambda) R(P_1, \delta)$  for some  $\lambda \in (0, 1)$ .
- (e) As  $\lambda$  varies from 0 to 1, how does the threshold change? Relate this to the Neyman-Pearson trade-off between Type I and Type II errors.

*Exercise 3.6.* Let  $\{P_\theta : \theta \in \mathbb{R}\}$  have MLR in  $T$  with continuous power functions.

- (a) Consider testing  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta > \theta_0$  (no indifference region). Show that for the threshold test  $\delta_c = \mathbb{1}\{T > c\}$ , the worst-case Type II error satisfies

$$\sup_{\theta > \theta_0} P_\theta(\delta_c = 0) = 1 - P_{\theta_0}(T > c) = 1 - \alpha(c).$$

Conclude that  $\alpha + \beta = 1$  for every threshold test, and the efficient frontier is the diagonal—no better than random guessing.

- (b) Now consider testing  $H_0 : \theta \leq \theta_0$  versus  $H_1 : \theta \geq \theta_1$  with  $\theta_1 > \theta_0$ . Show that the worst-case Type II error is  $\beta(c) = P_{\theta_1}(T \leq c)$ , achieved at the boundary of  $\Theta_1$ .
- (c) Show that every point on the efficient frontier is achieved by some threshold test  $\delta_c$ , and that the frontier satisfies  $\alpha + \beta \geq 1 - d_{TV}(P_{\theta_0}, P_{\theta_1})$ .
- (d) The achievable region  $\mathcal{A}$  is convex. Why?

*Exercise 3.7* (Detection boundary in high-dimensional normal model). Let  $X \sim N(\theta, \sigma^2 I_d)$  be a single observation from the  $d$ -dimensional normal model. Consider testing

$$H_0 : \theta = 0 \quad \text{versus} \quad H_1 : \|\theta\|_2^2 \geq \rho^2.$$

- (a) Show that under  $H_0$ ,  $\|X\|_2^2/\sigma^2 \sim \chi_d^2$  (chi-squared with  $d$  degrees of freedom), and under  $H_1$  with  $\|\theta\|_2 = \rho$ ,  $\|X\|_2^2/\sigma^2 \sim \chi_d'^2(\rho^2/\sigma^2)$  (noncentral chi-squared with noncentrality  $\lambda = \rho^2/\sigma^2$ ).
- (b) Recall that  $\chi_d^2$  has mean  $d$  and variance  $2d$ , while  $\chi_d'^2(\lambda)$  has mean  $d + \lambda$  and variance  $2(d + 2\lambda)$ . Show that for the test  $\delta = \mathbb{1}\{\|X\|_2^2 > c\}$ , reliable detection (both errors bounded away from  $1/2$ ) requires the separation condition

$$\rho^2 \gtrsim \sigma^2 \sqrt{d}.$$

*Hint:* Compare the means under  $H_0$  and  $H_1$  to the standard deviations.

- (c) For the normal mean estimation problem, the minimax risk satisfies

$$\inf_{\hat{\theta}} \sup_{\theta \in \mathbb{R}^d} \mathbb{E}_\theta \|\hat{\theta} - \theta\|_2^2 = d\sigma^2,$$

achieved by the MLE  $\hat{\theta} = X$ . Compare the detection boundary  $\rho^2 \asymp \sigma^2 \sqrt{d}$  to the estimation rate  $d\sigma^2$ . For  $d = 100$ , how much smaller is the detection boundary?

- (d) Interpret: why is testing “easier” than estimation in high dimensions? What does this say about detecting the presence of a signal versus locating it?

*Exercise 3.8* (♠ Differentiability of the power function). Let  $\{P_\theta : \theta \in \Theta\}$  be a one-parameter exponential family with density

$$p_\theta(x) = h(x) \exp(\eta(\theta)T(x) - A(\theta))$$

with respect to a  $\sigma$ -finite measure  $\mu$ , where  $\eta : \Theta \rightarrow \mathbb{R}$  is continuously differentiable with  $\eta'(\theta) > 0$ , and  $\theta_0$  lies in the interior of  $\Theta$ . Let  $\delta : \mathcal{X} \rightarrow [0, 1]$  be any (possibly randomized) test.

- (a) Show that  $\mathbb{E}_\theta[|T(X)|] < \infty$  for all  $\theta$  in the interior of  $\Theta$ .

*Hint: Without loss of generality work in the natural parametrization  $\eta = \theta$ . What is  $A(\theta)$ ?*

- (b) Show that the power function  $\beta_\delta(\theta) = \mathbb{E}_\theta[\delta(X)]$  is differentiable at  $\theta_0$ , with

$$\beta'_\delta(\theta_0) = \eta'(\theta_0) (\mathbb{E}_{\theta_0}[T(X) \delta(X)] - \mathbb{E}_{\theta_0}[T(X)] \cdot \mathbb{E}_{\theta_0}[\delta(X)]).$$

*Hint: The derivative of the density is  $\frac{\partial}{\partial \theta} p_\theta(x) = (\eta'(\theta)T(x) - A'(\theta)) p_\theta(x)$ . To apply the dominated convergence theorem, show that there exists an integrable function  $g(x)$  such that  $|(\eta'(\theta)T(x) - A'(\theta)) p_\theta(x)| \leq g(x)$  for all  $\theta$  in a neighborhood of  $\theta_0$ . Then use part (a).*

*Exercise 3.9.* Let  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  with  $\Theta \subseteq \mathbb{R}$  be a one-parameter exponential family on  $(\mathcal{X}, \mathcal{X})$  dominated by a  $\sigma$ -finite measure  $\mu$ , with densities

$$p_\theta(x) = h(x) \exp(\eta(\theta)T(x) - A(\theta)),$$

where the natural parameter  $\eta : \Theta \rightarrow \mathbb{R}$  is strictly increasing and twice differentiable. Consider testing  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$  at level  $\alpha \in (0, 1)$ .

- (a) Show that if  $\delta$  is unbiased at level  $\alpha$  and  $\beta_\delta(\theta) = \mathbb{E}_\theta[\delta(X)]$  is differentiable at  $\theta_0$ , then

$$\mathbb{E}_{\theta_0}[\delta(X)] = \alpha \quad \text{and} \quad \mathbb{E}_{\theta_0}[T(X) \delta(X)] = \alpha \mathbb{E}_{\theta_0}[T(X)].$$

- (b) (Generalized Neyman-Pearson.) Let  $\phi_0, \phi_1 : \mathcal{X} \rightarrow \mathbb{R}$  be measurable functions with  $\mathbb{E}_{\theta_0}[\phi_i(X)^2] < \infty$ . Show that, among all tests  $\delta$  satisfying

$$\mathbb{E}_{\theta_0}[\delta(X) \phi_i(X)] = c_i, \quad i = 0, 1,$$

the test maximizing  $\mathbb{E}_{\theta_1}[\delta(X)]$  for a given  $\theta_1 \neq \theta_0$  rejects when

$$p_{\theta_1}(x) > a_0 \phi_0(x) p_{\theta_0}(x) + a_1 \phi_1(x) p_{\theta_0}(x)$$

for constants  $a_0, a_1$  determined by the constraints.

*Hint: Mimic the proof of the Neyman-Pearson lemma with  $f(x) = a_0 \phi_0(x) p_{\theta_0}(x) + a_1 \phi_1(x) p_{\theta_0}(x)$  playing the role of  $c p_0(x)$ .*

- (c) Apply (b) with  $\phi_0 = 1$  and  $\phi_1 = T$  to show that the UMPU test rejects when

$$\exp((\eta(\theta_1) - \eta(\theta_0)) T(x)) > a_0 + a_1 T(x).$$

Conclude that the rejection region has the form  $\{T < c_1\} \cup \{T > c_2\}$ .

- (d) Show that the constants  $c_1, c_2$  (and randomization probabilities  $\gamma_1, \gamma_2$  at the boundaries) are determined by the system

$$\begin{aligned} \mathbb{E}_{\theta_0}[\delta^*(X)] &= \alpha, \\ \mathbb{E}_{\theta_0}[T(X) \delta^*(X)] &= \alpha \mathbb{E}_{\theta_0}[T(X)], \end{aligned}$$

and that a solution exists.

- (e) Show that the test from (c)–(d) does not depend on the choice of  $\theta_1 \neq \theta_0$ , and conclude that  $\delta^*$  is UMPU.

*Exercise 3.10* (The  $t$ -test as a UMPU test). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$  with both  $\mu$  and  $\sigma^2$  unknown. Consider testing  $H_0 : \mu = \mu_0$  versus  $H_1 : \mu \neq \mu_0$  at level  $\alpha$ .

- (a) Show that the joint density of  $(X_1, \dots, X_n)$  forms a two-parameter exponential family with sufficient statistics  $T_1 = \bar{X}$  and  $T_2 = \sum_{i=1}^n (X_i - \bar{X})^2$  and natural parameters  $\eta_1 = \mu/\sigma^2$  and  $\eta_2 = -1/(2\sigma^2)$ .
- (b) Argue that for testing  $H_0 : \mu = \mu_0$  (with  $\sigma^2$  as a nuisance parameter), the UMPU approach conditions on  $T_2$ . Show that the conditional distribution of  $\bar{X} \mid T_2 = s^2$  is

$$\bar{X} \mid T_2 = s^2 \sim N\left(\mu, \frac{\sigma^2}{n}\right),$$

which still depends on the nuisance parameter  $\sigma^2$ .

- (c) The dependence on  $\sigma^2$  in (b) seems problematic. Resolve this by showing that the distribution of

$$T = \frac{\bar{X} - \mu_0}{S/\sqrt{n}}, \quad S^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2$$

is  $t_{n-1}$ , free of  $\sigma^2$  under  $H_0$ . Show more generally that the distribution of  $T$  depends on  $(\mu, \sigma^2)$  only through the noncentrality parameter  $\gamma = \sqrt{n}(\mu - \mu_0)/\sigma$ ,

and that  $T$  follows a noncentral  $t_{n-1}(\gamma)$  distribution.

*Hint:* Write  $T = Z/\sqrt{V/(n-1)}$  where  $Z = (\bar{X} - \mu_0)/(\sigma/\sqrt{n}) \sim N(\gamma, 1)$  and  $V = T_2/\sigma^2 \sim \chi_{n-1}^2$ , and use the independence of  $\bar{X}$  and  $T_2$  in normal samples.

- (d) Show that the noncentral  $t_{n-1}(\gamma)$  family has monotone likelihood ratio in  $T$  as a function of  $\gamma$ . Since  $H_0 : \mu = \mu_0$  is equivalent to  $\gamma = 0$  regardless of  $\sigma^2$ , conclude by the one-dimensional theory (Exercise 3.9) that the UMPU test of  $\gamma = 0$  versus  $\gamma \neq 0$  rejects when  $|T| > t_{n-1, 1-\alpha/2}$ .
- (e) Verify that this test has size exactly  $\alpha$  for all  $\sigma^2 > 0$  (since  $T \sim t_{n-1}$  under  $H_0$  for every  $\sigma^2$ ), and that it is UMPU for testing  $H_0 : \mu = \mu_0$  versus  $H_1 : \mu \neq \mu_0$ . This is the two-sided  $t$ -test.

*Exercise 3.11* ( $\spadesuit$  Non-existence of UMPU in multiple dimensions). Let  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  with  $\Theta = \mathbb{R}^d$ ,  $d \geq 2$ , be the multivariate normal location model:  $X \sim N_d(\theta, I_d)$ . Consider testing  $H_0 : \theta = 0$  versus  $H_1 : \theta \neq 0$  at level  $\alpha \in (0, 1)$ .

- (a) Show that  $\mathcal{P}$  is a  $d$ -parameter exponential family with sufficient statistic  $T(X) = X$  and natural parameter  $\eta = \theta$ . Conclude that  $\mathbb{E}_0[X_j] = 0$  for all  $j = 1, \dots, d$ .
- (b) Show that if  $\delta$  is unbiased at level  $\alpha$  with differentiable power function  $\beta_\delta(\theta) = \mathbb{E}_\theta[\delta(X)]$ , then

$$\mathbb{E}_0[\delta(X)] = \alpha \quad \text{and} \quad \mathbb{E}_0[X_j \delta(X)] = 0, \quad j = 1, \dots, d.$$

*Hint:* Unbiasedness forces  $\beta_\delta$  to attain its minimum at  $\theta = 0$ , so  $\nabla \beta_\delta(0) = 0$ . Differentiate under the integral sign.

- (c) Fix  $\theta_1 \neq 0$ . Using the generalized Neyman-Pearson lemma (Exercise 3.9(b)) with the  $d+1$  constraints from (b), show that the most powerful unbiased test against  $\theta_1$  rejects when

$$\exp(\theta_1^\top x) > a_0 + a^\top x$$

for constants  $a_0 \in \mathbb{R}$  and  $a \in \mathbb{R}^d$  determined by the constraints.

- (d) Show that the rejection region in (c) depends on the direction of  $\theta_1$ . Conclude that no UMPU test exists for  $d \geq 2$ .

*Hint:* Consider  $\theta_1 = e_1$  and  $\theta_1 = e_2$  separately and argue that the resulting rejection regions differ.

- (e) The  $\chi^2$ -test rejects when  $\|X\|^2 > \chi_{d, 1-\alpha}^2$ . Show that this test is unbiased. Is it UMPU? Compare its power against  $\theta_1$  with the power of the one-dimensional test  $\mathbb{1}\{|\theta_1^\top X / \|\theta_1\| > z_{1-\alpha/2}\}$ .

*Exercise 3.12* ( Hunt-Stein for testing). Let  $G$  be a compact abelian group acting on a testing problem with  $\bar{g}\Theta_0 = \Theta_0$  and  $\bar{g}\Theta_1 = \Theta_1$  for all  $g \in G$ , and let  $\nu$  denote the normalized Haar measure on  $G$  (recall Definition 2.35). Given any test  $\delta$ , define the averaged test

$$\bar{\delta}(x) = \int_G \delta(gx) d\nu(g).$$

- (a) Show that  $\bar{\delta}$  is invariant under  $G$ .  
 (b) Show that  $\alpha(\bar{\delta}) \leq \alpha(\delta)$ . In particular,  $\delta \in \mathcal{C}_\alpha$  implies  $\bar{\delta} \in \mathcal{C}_\alpha$ .

*Hint:* Use  $\bar{g}\Theta_0 = \Theta_0$  to keep  $\bar{g}\theta_0 \in \Theta_0$  for all  $g$ .

- (c) Show that  $\beta(\bar{\delta}) \leq \beta(\delta)$ .  
 (d) Conclude that restricting to invariant tests loses nothing:

$$\inf_{\delta \in \mathcal{C}_\alpha} \beta(\delta) = \inf_{\delta \in \mathcal{C}_\alpha^G} \beta(\delta),$$

where  $\mathcal{C}_\alpha^G$  denotes the class of invariant level- $\alpha$  tests. Show the same holds for the linear scalarization:  $\inf_\delta R_\lambda(\delta) = \inf_{\delta \in \mathcal{C}_\alpha^G} R_\lambda(\delta)$  for any  $\lambda \in (0, 1)$ .

*Exercise 3.13* (Minimax optimality of the  $\chi^2$ -test). Consider testing  $H_0 : \theta = 0$  versus  $H_1 : \|\theta\| = \rho$  based on  $X \sim N_d(\theta, \sigma^2 I_d)$ , with  $d \geq 2$  and  $\rho > 0$  fixed.

- (a) Show that this testing problem is invariant under the orthogonal group  $G = O(d)$  acting by  $gX = OX$ ,  $\bar{g}\theta = O\theta$ . Verify that  $\Theta_0 = \{0\}$  and  $\Theta_1 = \{\theta : \|\theta\| = \rho\}$  are both preserved.  
 (b) The group  $O(d)$  is compact. Apply Exercise 3.12 to conclude that for every test  $\delta$ , there exists an invariant test  $\bar{\delta}$  with  $\alpha(\bar{\delta}) \leq \alpha(\delta)$  and  $\beta(\bar{\delta}) \leq \beta(\delta)$ . Conclude that restricting to invariant tests loses nothing.  
 (c) Show that the maximal invariant is  $M(X) = \|X\|^2$  and that  $O(d)$  acts transitively on both  $\Theta_0 = \{0\}$  and  $\Theta_1 = \{\theta : \|\theta\| = \rho\}$ . Conclude that under  $H_0$ ,  $\|X\|^2/\sigma^2 \sim \chi_d^2$ , and under any  $\theta \in \Theta_1$ ,  $\|X\|^2/\sigma^2 \sim \chi_d^2(\rho^2/\sigma^2)$ .  
 (d) By (b) and (c), the minimax testing problem reduces to a simple-versus-simple problem in  $\|X\|^2$ :

$$\inf_{\delta \in \mathcal{C}_\alpha} \beta(\delta) = \inf_{\phi} P_\rho(\phi(\|X\|^2) = 0), \quad \text{subject to } P_0(\phi(\|X\|^2) = 1) \leq \alpha.$$

Apply the Neyman-Pearson lemma to conclude that the  $\chi^2$ -test  $\delta^*(X) = \mathbb{1}\{\|X\|^2 > \sigma^2 \chi_{d,1-\alpha}^2\}$  is minimax.

- (e) Explain why the same test is also minimax for the harder problem  $H_1 : \|\theta\| \geq \rho$ .  
*Hint: The power of the  $\chi^2$ -test is nondecreasing in  $\|\theta\|$ .*

*Exercise 3.14* (Efficient frontier and linear scalarization). Consider a testing problem with size  $\alpha(\delta) = \sup_{\theta \in \Theta_0} \mathbb{E}_\theta[\delta(X)]$  and worst-case Type II error  $\beta(\delta) = \sup_{\theta \in \Theta_1} (1 - \mathbb{E}_\theta[\delta(X)])$ . Define the achievable region

$$\mathcal{A} = \{(\alpha, \beta) \in [0, 1]^2 : \text{there exists a test } \delta \text{ with } \alpha(\delta) \leq \alpha \text{ and } \beta(\delta) \leq \beta\},$$

the efficient frontier

$$\mathcal{E} = \{(\alpha, \beta) \in \partial\mathcal{A} : \text{no } (\alpha', \beta') \in \mathcal{A} \text{ satisfies } \alpha' \leq \alpha, \beta' \leq \beta \\ \text{with strict inequality in at least one coordinate}\},$$

and the linear scalarization  $R_\lambda(\delta) = \lambda \alpha(\delta) + (1 - \lambda) \beta(\delta)$  for  $\lambda \in (0, 1)$ . Assume the hypotheses are non-degenerate: no test achieves both  $\alpha = 0$  and  $\beta = 0$ .

- (a) Show that  $\mathcal{A}$  is convex. *Hint: Given tests  $\delta_1, \delta_2$  and  $t \in [0, 1]$ , construct a randomized test.*
- (b) Show that if  $\delta_\lambda^*$  minimizes  $R_\lambda$  over all tests, then  $(\alpha(\delta_\lambda^*), \beta(\delta_\lambda^*)) \in \mathcal{E}$ .
- (c) Conversely, show that every  $(\alpha^*, \beta^*) \in \mathcal{E}$  is achieved by a minimizer of  $R_\lambda$  for some  $\lambda \in (0, 1)$ . *Hint: Apply the supporting hyperplane theorem to the convex set  $\mathcal{A}$  at the boundary point  $(\alpha^*, \beta^*)$ , then rule out  $\lambda \in \{0, 1\}$  using the non-degeneracy assumption.*

*Exercise 3.15* (UMPU–UMAU duality). Let  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  be a statistical model, and let  $\alpha \in (0, 1)$ .

- (a) Let  $\{\delta_{\theta_0} : \theta_0 \in \Theta\}$  be a family of UMPU level- $\alpha$  tests of  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$ . Define  $C(X) = \{\theta_0 \in \Theta : \delta_{\theta_0}(X) = 0\}$ . Show that  $C(X)$  is an unbiased  $(1 - \alpha)$ -confidence set and that it is UMAU (Definition 3.47).

*Hint: For unbiasedness of  $C$ , use that each  $\delta_{\theta_0}$  is unbiased. For UMAU optimality, let  $C'$  be any other unbiased  $(1 - \alpha)$ -confidence set and consider the tests  $\delta'_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C'(X)\}$ .*

- (b) Conversely, let  $C^*(X)$  be a UMAU  $(1 - \alpha)$ -confidence set. Show that for each  $\theta_0 \in \Theta$ , the test  $\delta_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C^*(X)\}$  is UMPU at level  $\alpha$ .

*Hint: Show  $\delta_{\theta_0}$  is unbiased and level- $\alpha$  using the properties of  $C^*$ . Then argue that any unbiased test with higher power would yield a competing unbiased confidence set with smaller inclusion probability, contradicting UMAU.*

*Exercise 3.16* (UMPI–UMAE duality). Let  $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$  be a statistical model equivariant under a group  $G$  acting transitively on  $\Theta$ , and let  $\alpha \in (0, 1)$ .

- (a) Let  $\delta_{\theta^*}$  be a UMPI level- $\alpha$  test of  $H_0 : \theta = \theta^*$  versus  $H_1 : \theta \neq \theta^*$  under the (sub)group  $G_{\theta^*} = \{g : \bar{g}\theta^* = \theta^*\}$ , and define the family of tests  $\{\delta_{\theta_0} : \theta_0 \in \Theta\}$  for  $H_0 : \theta = \theta_0$  versus  $H_1 : \theta \neq \theta_0$  by  $\delta_{\bar{g}\theta^*}(x) = \delta_{\theta^*}(g^{-1}x)$ . Show that  $C(X) = \{\theta_0 \in \Theta : \delta_{\theta_0}(X) = 0\}$  is an equivariant  $(1 - \alpha)$ -confidence set and that it is UMAE.
- (b) Conversely, let  $C^*(X)$  be a UMAE  $(1 - \alpha)$ -confidence set. Show that for each  $\theta_0 \in \Theta$ , the test  $\delta_{\theta_0}(X) = \mathbb{1}\{\theta_0 \notin C^*(X)\}$  is UMPI for the group  $G_{\theta_0} = \{g : \bar{g}\theta_0 = \theta_0\}$  at level  $\alpha$ .

*Exercise 3.17* (Minimax estimation bounds imply confidence set bounds). Let  $C(X)$  be a  $(1 - \alpha)$ -confidence set for  $\theta \in \Theta \subseteq \mathbb{R}^d$  with  $\alpha < 1/2$ .

- (a) Show that any  $\hat{\theta}(X) \in C(X)$  satisfies

$$P_\theta(\|\hat{\theta}(X) - \theta\| \leq \text{diam}(C(X))) \geq 1 - \alpha \quad \text{for all } \theta \in \Theta.$$

Conclude that if  $\text{diam}(C(x)) \leq \ell$  for all  $x$ , then  $\hat{\theta}$  satisfies  $\sup_\theta P_\theta(\|\hat{\theta} - \theta\| > \ell) \leq \alpha$ .

- (b) (Contrapositive.) Suppose it is known that for every estimator  $\hat{\theta}$ ,

$$\sup_{\theta \in \Theta} P_\theta(\|\hat{\theta}(X) - \theta\| > r_n) > \alpha.$$

Show that no  $(1 - \alpha)$ -confidence set for  $\theta$  can have diameter bounded by  $r_n$ .

- (c) Suppose  $\Theta$  is bounded with  $\text{diam}(\Theta) = D$ , and  $\text{diam}(C(x)) \leq \ell$  for all  $x$ . Show that any  $\hat{\theta}(X) \in C(X)$  satisfies

$$\sup_{\theta \in \Theta} \mathbb{E}_\theta[\|\hat{\theta}(X) - \theta\|^2] \leq \ell^2 + \alpha D^2.$$

Conclude that if the minimax risk satisfies  $\inf_{\hat{\theta}} \sup_\theta \mathbb{E}_\theta[\|\hat{\theta} - \theta\|^2] \geq R_n^*$ , then

$$\ell \geq \sqrt{R_n^* - \alpha D^2}.$$

*Exercise 3.18* (Confidence intervals for the normal variance). Let  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} N(\mu, \sigma^2)$  with  $\mu$  known. Write  $T = \sum_{i=1}^n (X_i - \mu)^2$  and  $V = T/\sigma^2 \sim \chi_n^2$ .

- (a) Show that any  $(1 - \alpha)$ -confidence interval for  $\sigma^2$  of the form  $C(X) = [T/b, T/a]$  requires  $P(a \leq \chi_n^2 \leq b) \geq 1 - \alpha$ , and that its expected length is  $n\sigma^2(1/a - 1/b)$ .

- (b) Show that the UMPU test of  $H_0 : \sigma^2 = \sigma_0^2$  versus  $H_1 : \sigma^2 \neq \sigma_0^2$  rejects when  $V < a$  or  $V > b$ , where  $(a, b)$  are determined by

$$P(V < a) + P(V > b) = \alpha \quad \text{and} \quad \mathbb{E}[V \mathbb{1}\{V < a\}] + \mathbb{E}[V \mathbb{1}\{V > b\}] = \alpha n.$$

- (c) Show that the confidence interval minimizing expected length subject to  $P(a \leq \chi_n^2 \leq b) = 1 - \alpha$  requires

$$\frac{f_n(a)}{a^2} = \frac{f_n(b)}{b^2},$$

where  $f_n$  is the  $\chi_n^2$  density.

*Hint:* Use Lagrange multipliers to minimize  $1/a - 1/b$  subject to the coverage constraint.

- (d) Take  $n = 10$  and  $\alpha = 0.05$ . Compute both intervals numerically and verify that they differ: the shortest-length interval shifts both endpoints to the left relative to the UMAU interval, reflecting the right-skewness of the  $\chi^2$  distribution.

# 4 Bayesian Decision Theory

There are many reasons to adopt a Bayesian approach to statistics. Loosely speaking; Bayesian inference is built on a simple idea: place a probability distribution on the parameter space, called a *prior*. After observing data  $X = x$ , the prior is updated to a *posterior distribution* via Bayes' theorem, which combines the prior with the likelihood of the observed data.

There are many philosophical cases to make for taking a Bayesian approach. Some argue that priors provide a natural way to incorporate expert knowledge into the analysis. Others appeal to Savage's axioms, which show that any 'rational' agent whose preferences satisfy certain coherence conditions must act as if maximizing expected utility with respect to some prior. Dutch book arguments demonstrate that beliefs violating the axioms of probability are inherently incoherent. Subjectivists may appeal to de Finetti's representation theorem, which concludes that there exists a 'random parameter' that governs the data-generating process under mild exchangeability assumptions. For a thorough account of these and other foundational arguments, see Berger 1985.

In this chapter, we take the decision-theoretic lens. Rather than debating whether priors represent "true beliefs," we study what happens when one *chooses* to minimize average risk with respect to a prior distribution on  $\Theta$ . This leads to Bayes decision rules, and—perhaps surprisingly—reveals that Bayesian procedures occupy a privileged position in the decision-theoretic landscape as well: they are admissible, and under mild conditions, they are the *only* admissible procedures.

## 4.1 Bayes' Decision Procedures and Bayes' Risk

In order to study Bayesian procedures, we first need to equip  $\Theta$  with a  $\sigma$ -algebra  $\mathcal{T}$ , so that we can place a prior distribution on it, and ensure that our loss function is appropriately measurable with respect to this structure. For the remainder of this chapter, we will assume that  $(\Theta, \mathcal{T})$  is a measurable space and recast the definition of a loss function to be bi-measurable. Similarly, we will need some measurability assumptions on our model.

**Definition 4.1.** A *loss function* is a  $(\mathcal{T} \otimes \mathcal{D})/\mathcal{B}(\mathbb{R})$ -measurable function  $L : \Theta \times \mathcal{D} \rightarrow [0, \infty)$ , and we will assume that the model is such that  $\theta \mapsto P_\theta(A)$  is  $\mathcal{T}$ -measurable for each  $A \in \mathcal{X}$ .

With this measurability in place, we can integrate the risk function against a prior distribution on  $\Theta$ . The idea is simple: rather than evaluating a decision rule by its worst-case risk, we take a weighted average of the risk over  $\Theta$  with respect to a prior. The weights could reflect parameter values we deem most plausible (i.e. expert knowledge), or, more pessimistically, they could emphasize parameter values we want our decision rule to perform well on—making the procedure robust in regions of the parameter space we worry about.

**Definition 4.2.** A *prior distribution* is a probability measure  $\pi$  on  $(\Theta, \mathcal{F})$ . The *Bayes' risk* of a decision rule  $\delta$  with respect to a prior  $\pi$  is defined as

$$\mathcal{R}_\pi(\delta) := \int_{\Theta} \mathcal{R}(\theta, \delta) d\pi(\theta).$$

A natural question is: which decision rule minimizes the Bayes' risk?

**Definition 4.3.** A *Bayes' decision rule* for a prior  $\pi$  is a decision rule  $\delta_\pi$  that minimizes the Bayes' risk:

$$\delta_\pi \in \operatorname{argmin}_\delta \int_{\Theta} \mathcal{R}(\theta, \delta) d\pi(\theta).$$

We call a decision rule  $\delta$  a *Bayes' rule* if it minimizes the Bayes' risk for some prior  $\pi$ .

Since  $L \geq 0$ , the infimum  $\inf_\delta \mathcal{R}_\pi(\delta)$  is always well-defined. However, no measurable decision rule may attain it. Lemma 4.7, at the end of this section, provides sufficient conditions for existence of a measurable Bayes rule; under further mild conditions, the Bayes rule is unique.

There is a powerful consequence of uniqueness: if a Bayes' rule is the unique minimizer of the Bayes risk, then it is admissible. To make “unique” precise, we need to specify which sets of data are negligible. The natural choice is the *prior predictive distribution*

$$P_\pi(A) = \int_{\Theta} P_\theta(A) d\pi(\theta),$$

the marginal distribution of the data after integrating out the parameter under the prior.

**Theorem 4.4.** Let  $\delta_\pi$  be a Bayes rule with respect to a prior  $\pi$  with finite Bayes risk  $\mathcal{R}_\pi(\delta_\pi) < \infty$ . If the Bayes rule is unique (up to  $P_\theta$ -null sets), then  $\delta_\pi$  is admissible.

*Proof.* Suppose  $\delta_\pi$  is inadmissible. Then there exists  $\delta'$  with  $\mathcal{R}(\theta, \delta') \leq \mathcal{R}(\theta, \delta_\pi)$  for all  $\theta$  and strict inequality on a set  $A \subseteq \Theta$ . If  $\pi(A) > 0$ , then

$$\mathcal{R}_\pi(\delta') = \int_{\Theta} \mathcal{R}(\theta, \delta') d\pi(\theta) < \int_{\Theta} \mathcal{R}(\theta, \delta_\pi) d\pi(\theta) = \mathcal{R}_\pi(\delta_\pi),$$

contradicting that  $\delta_\pi$  minimizes Bayes risk. If  $\pi(A) = 0$ , then  $\delta'$  also minimizes Bayes risk, contradicting uniqueness.  $\square$

Admissibility of Bayes' decision rules comes at the cost of them typically being biased. We already got a hint of this studying Stein's phenomenon in Section 2.3.1. Indeed, we showed that the unbiased estimator  $X$  is normal many means setting is inadmissible. Exercise 4.5 shows that Bayes' estimators are typically biased.

Bayes' decision rules are closely connected to *posterior distributions*. These are the probability distributions of the parameter  $\theta$ , conditional on the observed data  $x$ . That is, we have a joint distribution on  $(\mathcal{X} \times \Theta, \mathcal{X} \otimes \mathcal{T})$  defined by

$$(A, B) \mapsto \int \mathbf{1}_B(\theta) \mathbf{1}_A(x) dP_\theta(x) d\pi(\theta),$$

and we are interested in whether for every  $x \in \mathcal{X}$  there exist a probability measure  $B \mapsto \pi(B | x)$  on  $(\Theta, \mathcal{T})$  such that 'Bayes rule' holds:

$$dP_\theta(x) d\pi(\theta) = dP_\pi(x) d\pi(\theta | x).$$

This motivates the following formal definition.

**Definition 4.5** (Posterior distribution). Let  $(P_\theta : \theta \in \Theta)$  be a statistical model such that  $\theta \mapsto P_\theta(A)$  is  $\mathcal{T}$ -measurable for each  $A \in \mathcal{X}$ , and let  $\pi$  be a prior on  $(\Theta, \mathcal{T})$ . A *posterior distribution* is a map  $(x, B) \mapsto \pi(B | x)$  such that  $B \mapsto \pi(B | x)$  is a probability measure on  $(\Theta, \mathcal{T})$  for each  $x$ , the map  $x \mapsto \pi(B | x)$  is measurable for each  $B$ , and

$$\int_A \pi(B | x) dP_\pi(x) = \int_B P_\theta(A) d\pi(\theta), \quad \text{for every } A \in \mathcal{X} \text{ and } B \in \mathcal{T}.$$

Posterior distributions exist under the usual conditions guaranteeing the existence of regular conditional distributions; see Theorem B.39 in Appendix B.

When a posterior distribution exists, the Bayes risk decomposes into a pointwise optimization problem: Bayes rules minimize the posterior expected loss for each observed  $x$ .

**Proposition 4.6.** *Let  $\pi$  be a prior on  $(\Theta, \mathcal{T})$  and suppose the posterior distribution  $\pi(\cdot | x)$  exists. Then the Bayes risk of any decision rule  $\delta$  can be written as*

$$\mathcal{R}_\pi(\delta) = \int_{\mathcal{X}} \int_{\Theta} L(\theta, \delta(x)) d\pi(\theta | x) dP_\pi(x).$$

*In particular, a decision rule  $\delta^*$  is Bayes' with respect to  $\pi$  if and only if, for  $P_\pi$ -almost*

every  $x$ ,

$$\delta^*(x) \in \operatorname{argmin}_{d \in \mathcal{D}} \int_{\Theta} L(\theta, d) d\pi(\theta | x),$$

provided  $\delta^*$  can be chosen to be measurable.

*Proof.* By the definition of the posterior distribution (Definition 4.5), for every  $A \in \mathcal{X}$  and  $B \in \mathcal{T}$ ,

$$\int_{\Theta} \int_{\mathcal{X}} \mathbf{1}_B(\theta) \mathbf{1}_A(x) dP_{\theta}(x) d\pi(\theta) = \int_{\mathcal{X}} \int_{\Theta} \mathbf{1}_B(\theta) \mathbf{1}_A(x) d\pi(\theta | x) dP_{\pi}(x),$$

which is often called ‘Bayes rule’. By linearity and the monotone convergence theorem this extends to all nonnegative measurable functions on  $(\Theta \times \mathcal{X}, \mathcal{T} \otimes \mathcal{X})$  (see Appendix B.2.1). Applying this to  $(\theta, x) \mapsto L(\theta, \delta(x))$  gives

$$\mathcal{R}_{\pi}(\delta) = \int_{\Theta} \int_{\mathcal{X}} L(\theta, \delta(x)) dP_{\theta}(x) d\pi(\theta) = \int_{\mathcal{X}} \int_{\Theta} L(\theta, \delta(x)) d\pi(\theta | x) dP_{\pi}(x).$$

Since  $P_{\pi}$  is a probability measure (and thus non-negative), the integral is minimized by minimizing the integrand pointwise. That is, for  $P_{\pi}$ -almost every  $x$ , we should choose  $\delta(x)$  to minimize the posterior expected loss:

$$\int_{\Theta} L(\theta, \delta(x)) d\pi(\theta | x).$$

If  $\delta^*$  can be chosen to be measurable, both directions of the implication hold.  $\square$

Note that the pointwise minimization in Proposition 4.6 produces a deterministic function of  $x$ —so Bayes rules are never randomized. It remains to verify that this pointwise minimizer can be chosen to be measurable. Many sufficient conditions are possible. We present one below.

**Lemma 4.7.** *Suppose the decision space  $(\mathcal{D}, \mathcal{D})$  is a Polish space equipped with its Borel  $\sigma$ -algebra, and that the posterior expected loss  $(x, d) \mapsto \int L(\theta, d) d\pi(\theta | x)$  is jointly measurable and lower semicontinuous in  $d$  for each  $x$ . Then there exists a measurable minimizer  $x \mapsto \delta^*(x)$ , i.e., a Bayes rule that is a (non-randomized) decision rule.*

*Proof* ( $\spadesuit$ ). See e.g. Brown and Purves 1973.  $\square$

Theorem 4.4 shows that unique Bayes rules are admissible. To show uniqueness of Bayes rules, the following lemma is useful.

**Lemma 4.8.** *Suppose that the decision space  $\mathcal{D}$  is a convex subset of a vector space, and that for every  $\theta \in \Theta$ , the loss function  $d \mapsto L(\theta, d)$  is strictly convex. If a Bayes rule  $\delta_{\pi}$  exists and has finite Bayes risk, then it is unique  $P_{\pi}$ -almost everywhere. If the model is dominated by  $P_{\pi}$ , then the Bayes rule is unique up to  $P_{\theta}$ -null sets.*

*Proof.* Suppose  $\delta_1$  and  $\delta_2$  are two Bayes rules with respect to  $\pi$ . Since the Bayes risk is finite and minimized by both, we have  $\mathcal{R}_\pi(\delta_1) = \mathcal{R}_\pi(\delta_2) = \inf_\delta \mathcal{R}_\pi(\delta) < \infty$ .

Consider the decision rule  $\delta' = \frac{1}{2}\delta_1 + \frac{1}{2}\delta_2$ . Since  $\mathcal{D}$  is convex,  $\delta'$  is a valid decision rule. By strict convexity of the loss function, for any  $x$  where  $\delta_1(x) \neq \delta_2(x)$ , we have

$$L(\theta, \delta'(x)) < \frac{1}{2}L(\theta, \delta_1(x)) + \frac{1}{2}L(\theta, \delta_2(x)).$$

Taking expectations with respect to the joint distribution of  $(X, \theta)$  (i.e., integrating against  $dP_\theta(x)d\pi(\theta)$ ), we obtain

$$\mathcal{R}_\pi(\delta') \leq \frac{1}{2}\mathcal{R}_\pi(\delta_1) + \frac{1}{2}\mathcal{R}_\pi(\delta_2) = \mathcal{R}_\pi(\delta_1).$$

The inequality is strict unless  $\delta_1(X) = \delta_2(X)$  with probability 1 under the marginal distribution  $P_\pi$ . If they differed with positive probability,  $\delta'$  would have strictly smaller Bayes risk than the minimum, a contradiction. Thus,  $\delta_1 = \delta_2$   $P_\pi$ -a.e. If the model is dominated by  $P_\pi$ , then  $\delta_1 \neq \delta_2$  being a  $P_\pi$ -null set implies that it is a  $P_\theta$ -null set for all  $\theta \in \Theta$ .  $\square$

## 4.2 Complete Class Theorem

Theorem 4.4 showed that unique Bayes rules are admissible. The complete class theorem establishes a converse: under regularity conditions, every admissible decision rule is Bayes with respect to some prior. Together, these results characterize the class of admissible procedures—they are precisely the Bayes rules.

**Theorem 4.9** (Complete Class). *Let  $\Theta$  be a compact metric space<sup>1</sup> (equipped with the Borel  $\sigma$ -algebra) and  $\mathcal{C}$  a set of decision rules that is closed under randomization. Assume the risk functions  $\mathcal{R}(\cdot, \delta)$  are continuous on  $\Theta$  for each  $\delta \in \mathcal{C}$ . If  $\delta_0 \in \mathcal{C}$  is admissible (for  $\mathcal{C}$ ), then  $\delta_0$  is Bayes with respect to some prior  $\pi$  on  $\Theta$ .*

*Proof.* If  $\mathcal{C}$  is convex, then the set  $S = \{\mathcal{R}(\cdot, \delta) : \delta \in \mathcal{C}\}$  is also convex. To see this, note that for any  $\delta_1, \delta_2 \in \mathcal{C}$  and  $\lambda \in [0, 1]$ , we can define the decision rule

$$\delta_\lambda(x, U) = \begin{cases} \delta_1(x) & \text{with probability } \lambda, \\ \delta_2(x) & \text{with probability } 1 - \lambda, \end{cases}$$

Then, using independence of  $U$  and the data, we have

$$\mathcal{R}(\theta, \delta_\lambda) = \lambda\mathcal{R}(\theta, \delta_1) + (1 - \lambda)\mathcal{R}(\theta, \delta_2).$$

<sup>1</sup>More generally,  $\Theta$  can be a compact Hausdorff space.

Furthermore, admissibility means  $\mathcal{R}(\cdot, \delta_0)$  is not strictly dominated: there is no  $\delta \in \mathcal{C}$  with  $\mathcal{R}(\theta, \delta) < \mathcal{R}(\theta, \delta_0)$  for all  $\theta$ .

By Lemma 4.11, there exists a probability measure  $\pi$  on  $\Theta$  with

$$\int_{\Theta} \mathcal{R}(\theta, \delta_0) d\pi(\theta) \leq \int_{\Theta} \mathcal{R}(\theta, \delta) d\pi(\theta) \quad \text{for all } \delta \in \mathcal{C}.$$

Thus,  $\delta_0$  minimizes Bayes risk with respect to  $\pi$ .  $\square$

*Remark 4.10.* The attentive reader may object to the mixing of decision rules in (4.2): what do we do if  $\delta_1$  and  $\delta_2$  are themselves randomized decision rules? The answer is that in this case, we could instead use

$$\delta_{\lambda}(x, U) = \begin{cases} \delta_1(x, U/\lambda) & \text{if } U \leq \lambda, \\ \delta_2(x, (U - \lambda)/(1 - \lambda)) & \text{if } U > \lambda, \end{cases}$$

combined with the fact that  $U/\lambda | [U \leq \lambda] \sim \text{Uniform}(0, 1)$  (check).

Many extensions to the complete class theorem exist, the formulation above is one that does not require too heavy machinery to prove. Continuity of the risk functions follows typically from mild continuity assumptions on the model and the loss function. Convexity of the set  $\mathcal{C}$  is satisfied when it includes randomized decision rules: if given two decision rules  $\delta_1$  and  $\delta_2$  in  $\mathcal{C}$ , mixing them with probability  $\lambda$  and  $1 - \lambda$  yields a decision rule in  $\mathcal{C}$ . Hence, if we take  $\mathcal{C}$  to be class of all randomized decision rules, the complete class theorem applies. Remarkably, it remains true for many other restricted classes of decision rules as well, such as the class of all (possibly randomized) unbiased estimators or invariant decision rules (check).

The key ingredient is proving the existence of a prior for which  $\delta_0$  minimizes the Bayes risk – this is the following lemma, which uses the Hahn-Banach separation theorem to produce a supporting prior.

**Lemma 4.11.** *Let  $\Theta$  be a compact metric space (equipped with the Borel  $\sigma$ -algebra) and consider  $S$  a convex subset of the space of continuous functions on  $\Theta$ .*

*If  $r : \Theta \rightarrow \mathbb{R}$  is a continuous function and there does not exist  $s \in S$  with  $s(\theta) \leq r(\theta)$  for all  $\theta \in \Theta$ , then there exists a probability measure  $\pi$  on  $\Theta$  such that*

$$\int_{\Theta} r(\theta) d\pi(\theta) \leq \int_{\Theta} s(\theta) d\pi(\theta) \quad \text{for all } s \in S.$$

*Proof* ( $\spadesuit$ ). Define

$$N = \{f \in C(\Theta) : f(\theta) < 0 \text{ for all } \theta \in \Theta\},$$

where  $C(\Theta)$  is the space of continuous (real-valued) functions on  $\Theta$ . The set  $N$  is an open convex subset of  $C(\Theta)$ .

The hypothesis says  $(r + N) \cap S = \emptyset$ . Since  $r + N$  is open and convex, and  $S$  is convex, the geometric form of Hahn-Banach (Theorem C.17) provides a nonzero continuous linear functional  $\varphi : C(\Theta) \rightarrow \mathbb{R}$  and a constant  $\alpha$  such that

$$\varphi(r + n) \leq \alpha \leq \varphi(s) \quad \text{for all } n \in N, s \in S.$$

Taking  $n \rightarrow 0$  gives  $\varphi(r) \leq \varphi(s)$  for all  $s \in S$ .

By the Riesz-Markov theorem (Theorem C.35), the continuous linear functional  $\varphi$  corresponds to a signed Radon measure  $\mu$  on  $\Theta$ :  $\varphi(f) = \int_{\Theta} f d\mu$  for all  $f \in C(\Theta)$ . The proof is finished by showing the **claim** that  $\mu \geq 0$ . Indeed, if the claim holds, then  $\theta \mapsto 1$  is a continuous function on  $\Theta$  and hence  $\varphi(1) = \int_{\Theta} 1 d\mu = \mu(\Theta) < \infty$ . Since  $\varphi \neq 0$ , we have  $\mu(\Theta) > 0$ . Therefore, setting  $\pi = \mu/\mu(\Theta)$  gives the required probability measure.

We proceed to prove the claim: for any  $n \in N$  and  $t > 0$ , we have  $tn \in N$  ( $N$  is a cone), so  $\varphi(r + tn) \leq \alpha$  for all  $t > 0$ . If  $\varphi(n) > 0$  for some  $n \in N$ , the linearity of  $\varphi$  violates this bound for some large  $t$ . Hence,  $\varphi(n) \leq 0$  for all  $n \in N$ , which implies  $\mu \geq 0$ .  $\square$

*Remark 4.12.* The compactness of  $\Theta$  ensures the Riesz-Markov theorem applies. For non-compact  $\Theta$ , additional conditions are needed to guarantee the separating functional corresponds to a countably additive probability measure. However, one can rest assured that for any space that is locally compact (e.g.  $\mathbb{R}^d$ ), we can take some (sequence of) arbitrary large compacts  $K \subset \Theta$  to apply the theorem to.

Together with Theorem 4.4, the complete class theorem provides a full characterization of admissibility: a decision rule is admissible if and only if it is Bayes. This has two practical consequences. First, finding admissible decision rules is natural and easy if we are Bayesian. Second, if we use an admissible decision rule, we are being Bayesian —perhaps without knowing what our prior is.

## 4.3 Minimaxity and Bayes

Recall from our earlier discussions on estimation (Chapter 2) and hypothesis testing (Chapter 3) that a decision rule is minimax if it minimizes the worst-case risk. The minimax theorem connects this to Bayes optimality: the minimax risk equals the maximum Bayes risk, achieved by a least favorable prior.

Recall that the *minimax risk* of a given class of decision rules  $\mathcal{C}$  and a parameter

space  $\Theta$  is

$$\bar{\mathcal{R}}_{\mathcal{C},\Theta} \equiv \bar{\mathcal{R}} = \inf_{\delta \in \mathcal{C}} \sup_{\theta \in \Theta} \mathcal{R}(\theta, \delta).$$

A decision rule  $\delta^*$  is *minimax* for the class  $\mathcal{C}$  and parameter space  $\Theta$  if  $\sup_{\theta} \mathcal{R}(\theta, \delta^*) = \bar{\mathcal{R}}_{\mathcal{C},\Theta}$ .

A straightforward connection between minimax risk and Bayes risk is provided by the observation that for any prior  $\pi$  on  $\Theta$ ,

$$\sup_{\theta} \mathcal{R}(\theta, \delta) \geq \int \mathcal{R}(\theta, \delta) d\pi(\theta) \geq \mathcal{R}_{\pi}(\delta_{\pi}). \quad (4.1)$$

That is, Bayes risk always lower bounds the worst-case risk. This observation forms the starting point of many arguments to establish minimaxity: in order to establish a lower bound on the minimax risk, it suffices to find a prior for which the Bayes risk is provably large.

In other cases,

**Definition 4.13** (Least Favorable Prior). A prior  $\pi^*$  is *least favorable* if it maximizes the best-case Bayes risk:

$$\check{\mathcal{R}}(\pi^*) = \sup_{\pi \in \mathcal{P}(\Theta)} \check{\mathcal{R}}(\pi), \quad \text{where } \check{\mathcal{R}}(\pi) = \inf_{\delta \in \mathcal{C}} \int_{\Theta} \mathcal{R}(\theta, \delta) d\pi(\theta),$$

and  $\mathcal{P}(\Theta)$  is the space of all probability measures on  $\Theta$ .

Why would we consider a least favorable prior? The original motivation for Bayesian statistics is often to incorporate expert knowledge to improve performance. However, in many scientific contexts—such as drug approval or policy making—subjectivity is undesirable. We want a procedure that is robust and convincing even to a skeptic. A least favorable prior represents the “worst-case” belief; if a procedure performs well under this prior, it performs well under any prior. In this sense, choosing a least favorable prior is a principled way to select a prior that provides best-worst case “frequentist” guarantees.

A key tool for identifying least favorable priors is the following property.

**Proposition 4.14.** *If  $\delta^*$  is a Bayes rule with respect to some prior  $\pi$ , and  $\mathcal{R}(\theta, \delta^*)$  is constant in  $\theta$ , then  $\delta^*$  is minimax.*

*Proof.* For any competing estimator  $\delta'$ ,

$$\sup_{\theta} \mathcal{R}(\theta, \delta') \geq \int \mathcal{R}(\theta, \delta') d\pi(\theta) \geq \int \mathcal{R}(\theta, \delta^*) d\pi(\theta) = \mathcal{R}(\theta, \delta^*) = \sup_{\theta} \mathcal{R}(\theta, \delta^*),$$

where the first inequality holds because the supremum is at least the average, the second

because  $\delta^*$  minimizes the Bayes risk  $\int \mathcal{R}(\theta, \delta) d\pi(\theta)$ , and the final equality because  $\mathcal{R}(\theta, \delta^*)$  is constant in  $\theta$ .  $\square$

We also have the converse: if  $\delta^*$  is minimax, and if a least favorable prior exists, then  $\delta^*$  is Bayes with respect to this least favorable prior.

**Proposition 4.15.** *If  $\delta^*$  is minimax and  $\pi^*$  is least favorable, then  $\delta^*$  is Bayes with respect to  $\pi^*$ .*

*Proof.* Since  $\delta^*$  is minimax,  $\sup_{\theta} \mathcal{R}(\theta, \delta^*) = \bar{\mathcal{R}}$ . For any prior  $\pi$ ,

$$\int \mathcal{R}(\theta, \delta^*) d\pi(\theta) \leq \sup_{\theta} \mathcal{R}(\theta, \delta^*) = \bar{\mathcal{R}}.$$

In particular,  $\int \mathcal{R}(\theta, \delta^*) d\pi^*(\theta) \leq \bar{\mathcal{R}} = r(\pi^*)$ . But  $r(\pi^*) = \inf_{\delta} \int \mathcal{R}(\theta, \delta) d\pi^*$  by definition, so

$$\int \mathcal{R}(\theta, \delta^*) d\pi^*(\theta) = r(\pi^*).$$

Hence  $\delta^*$  is Bayes for  $\pi^*$ .  $\square$

However, it remains for us to answer when these least favorable priors and minimax rules exist.

**Theorem 4.16** (Minimax Theorem). *Under the assumptions of Theorem 4.9, the minimax risk equals the maximum Bayes risk:*

$$\inf_{\delta \in \mathcal{C}} \sup_{\theta \in \Theta} \mathcal{R}(\theta, \delta) = \sup_{\pi \in \mathcal{P}(\Theta)} \inf_{\delta \in \mathcal{C}} \int_{\Theta} \mathcal{R}(\theta, \delta) d\pi(\theta).$$

*Moreover, a least favorable prior  $\pi^*$  exists. If a minimax rule exists, then it is Bayes with respect to  $\pi^*$ .*

*Proof.* Let  $\bar{\mathcal{R}} = \inf_{\delta} \sup_{\theta} \mathcal{R}(\theta, \delta)$ .

*The inequality  $\geq$ :* Established in (4.1).

*The inequality  $\leq$ :* The constant function  $r(\theta) \equiv \bar{\mathcal{R}}$  is not strictly dominated by the risk set  $S = \{\mathcal{R}(\cdot, \delta) : \delta \in \mathcal{C}\}$ . Indeed, if  $\mathcal{R}(\theta, \delta) < \bar{\mathcal{R}}$  for all  $\theta$  for some  $\delta$ , then  $\sup_{\theta} \mathcal{R}(\theta, \delta) < \bar{\mathcal{R}}$ , contradicting the definition of  $\bar{\mathcal{R}}$ .

By Lemma 4.11, there exists  $\pi^*$  with

$$\bar{\mathcal{R}} = \int_{\Theta} \bar{\mathcal{R}} d\pi^* \leq \int_{\Theta} \mathcal{R}(\theta, \delta) d\pi^*(\theta) \quad \text{for all } \delta \in \mathcal{C}.$$

Hence,  $r(\pi^*) \geq \bar{\mathcal{R}}$ , giving equality. The prior  $\pi^*$  is least favorable. The second part of the theorem follows from Proposition 4.15.  $\square$

*Remark 4.17.* Various conditions on the loss function guarantee the existence of minimax rule, for example if the loss is convex or appropriately continuous in the decision.

## 4.4 Bayesian testing

There are many ways to approach hypothesis testing from a Bayesian perspective, and the literature reflects genuine disagreement about which is most appropriate. One places a prior probability on each hypothesis being true and computes posterior odds, turning the question into one of belief updating. A second, more model-oriented approach uses posterior predictive checks to assess whether the observed data is consistent with a posited model. Each of these carries its own philosophical commitments about what testing is meant to accomplish.

In this section, we take the decision-theoretic perspective developed throughout this chapter. Rather than interpreting priors necessarily as beliefs, we simply consider the consequence of placing priors  $\pi_0$  on  $\Theta_0$  and  $\pi_1$  on  $\Theta_1$ . That is, given a possibly composite testing problem  $H_0 : \theta \in \Theta_0$  versus  $H_1 : \theta \in \Theta_1$ , choose prior distributions  $\pi_0$  on  $\Theta_0$  and  $\pi_1$  on  $\Theta_1$ , and consider the *collapsed hypotheses*

$$H_0 : X \sim P_{\pi_0} \quad \text{versus} \quad H_1 : X \sim P_{\pi_1},$$

where  $P_{\pi_i}(\cdot) = \int P_{\theta}(\cdot) d\pi_i(\theta)$  is the prior predictive under  $\pi_i$ . This is now a simple-versus-simple testing problem, and the Neyman-Pearson lemma (Theorem 3.14) tells us that the optimal test rejects when the (possibly infinite) likelihood ratio  $dP_{\pi_1}/dP_{\pi_0}(x)$  exceeds a threshold. This likelihood ratio is called the *Bayes factor*.

Calibrating the threshold requires care. For a simple null  $H_0 : \theta = \theta_0$ , the prior  $\pi_0$  is a point mass, and the likelihood ratio test rejects when  $\int p_{\theta}(x) d\pi_1(\theta) > c \cdot p_{\theta_0}(x)$ . A conservative choice is  $c = \alpha^{-1}$ : by Markov's inequality (check),

$$P_{\theta_0} \left( \int p_{\theta}(X) d\pi_1(\theta) > \alpha^{-1} \cdot p_{\theta_0}(X) \right) \leq \alpha,$$

since  $\mathbb{E}_{\theta_0}[\int p_{\theta}(X) d\pi_1(\theta)/p_{\theta_0}(X)] = 1$ . For composite nulls, the threshold must ensure level  $\alpha$  uniformly over  $\Theta_0$ , which generally depends on the structure of the problem.

Properties of the priors are inherited by the resulting test. If the testing problem is invariant under a group  $G$  (Definition 3.32) and the priors  $\pi_0, \pi_1$  are invariant under the induced action on  $\Theta$ , then the prior predictives  $P_{\pi_0}$  and  $P_{\pi_1}$  are invariant under  $G$ , and the likelihood ratio  $dP_{\pi_1}/dP_{\pi_0}$  is a function of the maximal invariant. The resulting Neyman-Pearson test is therefore invariant—invariance of the Bayesian test comes for free from invariance of the priors.

Which priors should we choose? If we have genuine prior knowledge about the likely location of  $\theta$  under each hypothesis, we can encode it directly. But if our goal is to produce a test with strong worst-case guarantees—one that is convincing regardless of the true parameter—we could choose priors that are least favorable in the sense of Definition 4.13. Theorem 4.18 guarantees that such priors exist under mild conditions, and that the resulting tests trace out the efficient frontier as we vary the relative cost of worst case Type I vs worst case Type II error probabilities.

**Theorem 4.18** (Optimal tests for composite hypotheses). *Let  $\Theta_0$  and  $\Theta_1$  be disjoint compact subsets of  $\Theta$ , and suppose a  $\mu$ -dominated model such that its likelihood function  $\theta \mapsto p_\theta(x)$  is continuous for  $\mu$ -a.e.  $x$ , and there exists  $g \in L^1(\mu)$  such that  $p_\theta(x) \leq g(x)$  for  $\mu$ -a.e.  $x$  and all  $\theta \in \Theta$ .*

*For testing  $H_0 : \theta \in \Theta_0$  versus  $H_1 : \theta \in \Theta_1$ , consider the weighted error criterion*

$$\mathcal{R}_{a,b}(\delta) = \sup_{\theta \in \Theta} \mathcal{R}(\theta, \delta) = \max\{a \cdot \sup_{\theta \in \Theta_0} \mathbb{E}_\theta[\delta], b \cdot \sup_{\theta \in \Theta_1} \mathbb{E}_\theta[1 - \delta]\}$$

where the weights  $a, b > 0$ .

*If the testing problem is non-trivial (i.e.  $\inf_\delta \mathcal{R}_{a,b}(\delta) > 0$ ), then:*

- (a) *There exists a test  $\delta^* \equiv \delta_{a,b}^*$  minimizing  $\mathcal{R}_{a,b}(\delta)$  over all tests.*
- (b) *There exist prior distributions  $\pi_0^*$  on  $\Theta_0$  and  $\pi_1^*$  on  $\Theta_1$  respectively, such that  $\delta^*$  is a likelihood ratio test:*

$$\delta^*(x, u) = \begin{cases} 1 & \text{if } \int p_\theta(x) d\pi_1^*(\theta) > c \int p_\theta(x) d\pi_0^*(\theta), \\ \mathbb{1}_{\{u \leq \gamma\}} & \text{if } \int p_\theta(x) d\pi_1^*(\theta) = c \int p_\theta(x) d\pi_0^*(\theta), \\ 0 & \text{if } \int p_\theta(x) d\pi_1^*(\theta) < c \int p_\theta(x) d\pi_0^*(\theta), \end{cases}$$

for some  $c \geq 0$  and  $\gamma \in [0, 1]$ .

- (c) *As  $a/b$  varies over  $(0, \infty)$ , the optimal tests trace out the efficient frontier of achievable (size, worst-case Type II error) pairs.*

*Proof.* Consider the loss function

$$L(\theta, d) = a \mathbb{1}_{\theta \in \Theta_0} d + b \mathbb{1}_{\theta \in \Theta_1} (1 - d),$$

and note that the corresponding risk function  $\mathcal{R}_{a,b}(\theta, \delta)$  satisfies

$$\sup_{\theta} \mathcal{R}_{a,b}(\theta, \delta) = \max\{a \cdot \sup_{\theta \in \Theta_0} \mathbb{E}_\theta[\delta], b \cdot \sup_{\theta \in \Theta_1} \mathbb{E}_\theta[1 - \delta]\}.$$

We first establish the existence of a least favorable prior, which turns out to be a

consequence of the minimax theorem. The risk function  $\theta \mapsto \mathcal{R}_{a,b}(\theta, \delta)$  is continuous for each  $\delta$ . Indeed, by the dominated convergence theorem (using the fact that  $\delta$  is bounded and that  $p_\theta$  is ‘enveloped’ by  $g$ ), we have

$$\lim_{n \rightarrow \infty} \int \delta(x, u) p_{\theta_n}(x) d\mu(x) du = \int \delta(x, u) p_\theta(x) d\mu(x) du,$$

for any sequence of parameter values  $\theta_n \rightarrow \theta$ . The set of randomized tests is convex, so Theorem 4.16 applies and yields us the existence of a least favorable prior  $\pi^*$  on  $\Theta$ :

$$\inf_{\delta} \sup_{\theta} \mathcal{R}_{a,b}(\theta, \delta) = \inf_{\delta} \int \mathcal{R}_{a,b}(\theta, \delta) d\pi^*(\theta). \quad (4.2)$$

We can conclude from the fact that the testing problem is non-trivial that  $\pi^*$  has positive mass on both  $\Theta_0$  and  $\Theta_1$ : if  $\pi^*(\Theta_1) = 0$ , then for every  $\delta$ ,

$$\int_{\Theta} \mathcal{R}_{a,b}(\theta, \delta) d\pi^*(\theta) = a \int_{\Theta_0} \mathbb{E}_{\theta}[\delta] d\pi^*(\theta),$$

which is minimized by  $\delta \equiv 0$ , giving  $\inf_{\delta} \int \mathcal{R}_{a,b} d\pi^* = 0$ . By the same argument,  $\pi^*(\Theta_0) > 0$ . Consider the respective renormalized restrictions of the priors,  $\pi_i^* = \pi_{|\Theta_i}^*/\pi^*(\Theta_i)$ . We have

$$\begin{aligned} \int \mathcal{R}_{a,b}(\theta, \delta) d\pi^*(\theta) &= a\pi^*(\Theta_0) \int \mathcal{R}_{a,b}(\theta, \delta) d\pi_0^*(\theta) + b\pi^*(\Theta_1) \int \mathcal{R}_{a,b}(\theta, \delta) d\pi_1^*(\theta) \\ &= c_0 \int \int \delta(x, u) dP_{\pi_0^*}(x) du + c_1 \int \int (1 - \delta(x, u)) dP_{\pi_1^*}(x) du. \end{aligned}$$

The Neyman-Pearson theorem yields that the optimal test  $\delta^*$  is a likelihood ratio test, of the form provided in the theorem. Part (a) and part (b) can now be concluded from (4.2).

Part (c) can be proven in a similar fashion to Exercise 3.5.  $\square$

Theorem 4.18 guarantees the existence of least favorable priors under mild conditions. The result highlights that tests using Bayes factors need not be subjective at all: they can provide perfectly valid frequentist guarantees in terms of power and type I error, and above all, they are even minimax optimal.

Existence is one thing—finding the least favorable priors is another. In general, it is difficult to find a closed-form expression for  $\pi_0^*$  and  $\pi_1^*$ , and computing them requires solving an infinite-dimensional optimization problem. There are practical limits to the reach of this Bayesian approach to composite testing: while the theoretical picture is clean, it is most useful in settings where the structure of the problem constrains the least favorable priors to a tractable form. Notable examples include testing in location

families, where invariance pins down the priors (as in the Hunt-Stein theorem), and problems with finite or low-dimensional parameter spaces, where the optimization over priors can be carried out explicitly. Outside of such structured settings, the minimax testing framework of Section 3.2.3 is often invoked at a more abstract level—establishing that optimal tests exist and characterizing their form—without explicitly constructing the least favorable priors. For example, in a high-dimensional setting, we may be happy to know that a test distinguishes two hypotheses when they are sufficiently separated, without knowing the exact optimal constants  $c_0$  and  $c_1$ . We can at the very least rest assured that our corresponding test is admissible.

## 4.5 Reflections on Bayesian statistics and decision theory

Which prior should we choose? The decision-theoretic perspective developed in this chapter suggests a perhaps uncomfortable answer: it depends on what we want our decision rule to achieve.

If we care only about admissibility, the choice is easy—any prior will do. Theorem 4.4 guarantees that unique Bayes rules are admissible, so every prior yields a decision rule that is not strictly dominated. But admissibility is a weak requirement, and we typically want more. If we would like our decision rule to be unbiased, we are largely out of luck: Bayes estimators are typically biased (Exercise 4.5), and this bias is precisely what buys them lower risk elsewhere. If we would like invariance under group transformations, we should choose a prior that is itself invariant—this is the content of the Hunt-Stein theorem (Theorem 2.47), which identifies the Haar measure on compact groups as the natural prior for invariant decision problems. If we want good worst-case performance, we should choose a prior that is least favorable (see Section 4.3), so that the resulting Bayes rule is minimax.

In modern high-dimensional statistics, a common aspiration is to find decision rules that are both admissible and minimax rate-optimal. In settings that force a bias-variance trade-off—and high-dimensional problems almost always do—a Bayesian approach guarantees admissibility by construction, and with a well-chosen prior, the resulting estimator can attain the minimax rate. This combination of adaptivity and optimality has made Bayesian methods a central tool in nonparametric and high-dimensional inference. The cost is typically computational: posterior distributions in complex models are often intractable, requiring computational methods such as Markov chain Monte Carlo or variational methods.

For testing, the Bayesian approach is similarly appealing in principle. Once priors

$\pi_0$  and  $\pi_1$  are specified on the null and alternative, the optimal test on the collapsed hypotheses is immediate: the Neyman-Pearson lemma applied to the collapsed hypotheses  $P_{\pi_0}$  versus  $P_{\pi_1}$ . But how should these priors be specified? Should they reflect genuine beliefs about the location of  $\theta$ , or should they be chosen to produce the most convincing test—that is, to be least favorable? Least favorable priors yield tests with the strongest worst-case guarantees, but finding them is difficult, outside of structured settings. There does not appear to be a singular principled answer to this question.

These lines of thinking may seem somewhat removed from the view in which a single prior on  $\Theta$  encodes the analyst's beliefs and is used uniformly across all inferential tasks. The decision-theoretic perspective suggests something different: the prior should be chosen as part of the decision problem at hand. If we face multiple decision problems concerning the same model—say, estimating different functionals of the same parameter—we may need different priors for each. This is not merely a theoretical possibility: Recent work (Ritov et al. 2014, Arbel, Gayraud, and Rousseau 2013, Zhao 2000, Rivoirard and Rousseau 2012, Castillo and Nickl 2013) has shown that for certain high-dimensional models, no single prior yields Bayes estimators that are simultaneously minimax rate-optimal for two different estimation targets (with corresponding different loss functions) within the same model; a different prior seems needed for each.

## Exercises

*Exercise 4.1.* Let  $\pi(\cdot | x)$  denote the posterior distribution of  $\theta \in \Theta \subseteq \mathbb{R}$  given  $X = x$ . Determine the Bayes rule under each of the following loss functions.

- (a) *Squared error loss:*  $L(\theta, d) = (\theta - d)^2$ .
- (b) *Absolute error loss:*  $L(\theta, d) = |\theta - d|$ .
- (c) *Weighted squared error loss:*  $L(\theta, d) = w(\theta)(\theta - d)^2$ , where  $w : \Theta \rightarrow (0, \infty)$  is a known weight function.

You may assume all relevant expectations exist and that minimizers are unique.

*Exercise 4.2* (Revisiting the James–Stein estimator via Empirical Bayes). Let  $X \sim N_d(\theta, I_d)$  with  $d \geq 3$  and total squared error loss  $L(\theta, \delta) = \|\delta - \theta\|^2$ . Consider the conjugate prior  $\theta \sim N_d(0, \tau^2 I_d)$  with  $\tau > 0$ .

- (a) Derive the Bayes estimator  $\delta_\tau(X)$  and express it in the form  $(1 - B)X$ . Identify the shrinkage factor  $B$  as a function of  $\tau$ .
- (b) Compute the prior predictive distribution (the marginal distribution of  $X$ , integrating out  $\theta$ ).
- (c) Suppose the hyperparameter  $\tau$  is unknown. We wish to estimate the shrinkage factor  $B$  from the data using the marginal distribution derived in (b). Show that  $B = \frac{1}{\tau^2 + 1}$  can be unbiasedly estimated by  $\hat{B} = \frac{d-2}{\|X\|^2}$ .  
*Hint:* If  $Y \sim \chi_d^2$ , what is  $\mathbb{E}[1/Y]$ ?
- (d) Substitute  $\hat{B}$  for  $B$  in the Bayes estimator form from (a). What estimator do you obtain? Would you prefer this estimator over the one from (a)?

*Exercise 4.3* (Spike-and-slab priors and pre-testing). Consider the normal mean problem  $X \sim N(\theta, 1)$  with squared error loss.

Recall the “test-first” estimator from Example 2.42:

$$\delta_{PT}(X) = X \mathbb{1}\{|X| > c\}.$$

This estimator implicitly assumes  $\theta$  is either exactly 0 or “large”. Formalize this by considering a *spike-and-slab prior*:

$$\theta \sim (1 - w)\delta_0 + wN(0, \tau^2),$$

where  $\delta_0$  is a point mass at 0 (the “spike”),  $N(0, \tau^2)$  is the “slab” representing non-zero effects, and  $w \in (0, 1)$  is the prior probability of a signal.

1. Derive the posterior probability of the slab component,  $p(x) = P(\theta \neq 0 \mid X = x)$ . Show that it is a sigmoid-like function of  $x^2$ .
2. Show that the Bayes estimator (the posterior mean) takes the form

$$\delta^*(X) = p(X) \cdot \frac{\tau^2}{\tau^2 + 1} X.$$

Interpret this as adaptive shrinkage: how does the shrinkage factor depend on  $|X|$ ?

3. Compare  $\delta^*$  with  $\delta_{PT}$ . In what sense is  $\delta^*$  a “smoothed” version of  $\delta_{PT}$ ?
4. (*Admissibility*) Is the pre-test estimator  $\delta_{PT}$  admissible? Explain why or why not. *Hint: Consider the continuity of the risk function or the estimator itself.*

*Exercise 4.4* (Minimax estimation for the Bernoulli model). Let  $X_1, \dots, X_n \stackrel{iid}{\sim} \text{Bernoulli}(p)$  with  $p \in (0, 1)$ . Consider the symmetric Beta prior  $p \sim \text{Beta}(\alpha, \alpha)$  for  $\alpha > 0$ , and squared error loss  $L(p, \delta) = (\delta - p)^2$ . Let  $T = \sum_{i=1}^n X_i$ .

- (a) Derive the Bayes estimator  $\delta_\alpha(T)$  under squared error loss.
- (b) Show that  $\delta_\alpha$  is admissible.
- (c) Compute the risk function  $R(p, \delta_\alpha) = \mathbb{E}_p[(\delta_\alpha(T) - p)^2]$  explicitly as a function of  $p$ .
- (d) Find  $\alpha^*$  such that  $R(p, \delta_{\alpha^*})$  is constant in  $p$ , and give the resulting estimator and its risk.
- (e) Conclude that  $\delta_{\alpha^*}$  is simultaneously Bayes, admissible, and minimax, and provide a least favorable prior for the decision problem.

*Exercise 4.5* (Bias of Bayes estimators). Let  $X \sim N(\theta, 1)$  (single observation) with squared error loss.

- (a) Consider the prior  $\theta \sim N(0, \tau^2)$ . Find the Bayes estimator  $\delta_\tau(X)$  and compute its bias  $b(\theta) = \mathbb{E}_\theta[\delta_\tau(X)] - \theta$  as a function of  $\theta$ .
- (b) Compute the mean squared error  $R(\theta, \delta_\tau)$  and show that  $R(\theta, \delta_\tau) < R(\theta, X) = 1$  for all  $\theta$ .
- (c) Show more generally that for any proper prior  $\pi$  with finite mean  $\mu = \mathbb{E}_\pi[\theta]$ , the Bayes estimator  $\delta_\pi(X) = \mathbb{E}[\theta \mid X]$  satisfies  $\mathbb{E}_\theta[\delta_\pi(X)] \neq \theta$  for at least some  $\theta$ .

*Hint:* Suppose  $\delta_\pi$  is unbiased, i.e.,  $\mathbb{E}_\theta[\delta_\pi(X)] = \theta$  for all  $\theta$ . Consider the Bayes risk.

*Exercise 4.6* (Least favorable sequences and minimax estimators). Let  $\{\pi_k\}$  be a sequence of prior distributions with corresponding Bayes estimators  $\delta_k$ , and let  $\delta$  be an estimator such that

$$R(\pi_k, \delta_k) \rightarrow \sup_{\theta} R(\theta, \delta).$$

- (a) Show that  $\delta$  is minimax.  
 (b) A sequence  $\{\pi_k\}$  of priors is called *least favorable* if for every prior  $\pi$ ,

$$R(\pi, \delta_\pi) \leq \lim_{k \rightarrow \infty} R(\pi_k, \delta_k).$$

Show that  $\{\pi_k\}$  is least favorable.

*Exercise 4.7* (♠ The posterior as a Bayes rule). Let  $(\Theta, \mathcal{T}, \mu)$  be a  $\sigma$ -finite measure space and suppose the prior  $\pi$  is absolutely continuous with respect to  $\mu$ , with density  $p = d\pi/d\mu$ . Assume the posterior distribution satisfies  $\pi(\cdot | x) \ll \mu$  for  $P$ -almost every  $x$ , and write  $\pi(\theta | x) = d\pi(\cdot | x)/d\mu(\theta)$  for the posterior density. Let the action space be

$$\mathcal{D} = \left\{ Q \ll \mu : q = \frac{dQ}{d\mu}, \int_{\Theta} q d\mu = 1 \right\},$$

and consider the logarithmic loss  $L(\theta, Q) = -\log q(\theta)$ .

1. Show that the Bayes rule under logarithmic loss is to report the posterior distribution:  $\delta^*(x) = \pi(\cdot | x)$ .

*Hint:* Write the posterior expected loss of an arbitrary  $Q \in \mathcal{D}$  in terms of the Kullback–Leibler divergence from  $\pi(\cdot | x)$  to  $Q$ .

2. Conclude that the Bayes risk equals the conditional entropy:

$$\mathcal{R}_\pi(\delta^*) = H(\theta | X) := -E[\log \pi(\theta | X)],$$

where the expectation is taken under the joint distribution of  $(\theta, X)$ .

3. Show that if no data were observed, the optimal action under logarithmic loss would be to report the prior, with expected loss equal to the entropy  $H(\theta) = -\int_{\Theta} \log p(\theta) d\pi(\theta)$ . Conclude that the reduction in Bayes risk from observing  $X$  is the mutual information:

$$H(\theta) - H(\theta | X) = I(\theta; X).$$

You may assume all entropies are finite.

*Exercise 4.8* (Mixing randomized decision rules). Let  $\delta_1(x, \cdot)$  and  $\delta_2(x, \cdot)$  be two randomized decision rules, where the randomization is implemented via a uniform random variable  $U \sim \text{Uniform}(0, 1)$ . For any  $\lambda \in (0, 1)$ , consider the mixed decision rule  $\delta_\lambda$  defined by

$$\delta_\lambda(x, U) = \begin{cases} \delta_1(x, U/\lambda) & \text{if } U \leq \lambda, \\ \delta_2(x, (U - \lambda)/(1 - \lambda)) & \text{if } U > \lambda. \end{cases}$$

- (a) Show that conditional on the event  $\{U \leq \lambda\}$ , the random variable  $U' = U/\lambda$  follows a  $\text{Uniform}(0, 1)$  distribution.
- (b) Show that conditional on the event  $\{U > \lambda\}$ , the random variable  $U'' = (U - \lambda)/(1 - \lambda)$  follows a  $\text{Uniform}(0, 1)$  distribution.
- (c) Conclude that for any  $\theta$ , the risk of  $\delta_\lambda$  satisfies

$$\mathcal{R}(\theta, \delta_\lambda) = \lambda \mathcal{R}(\theta, \delta_1) + (1 - \lambda) \mathcal{R}(\theta, \delta_2).$$

**Part II**

**Asymptotic Statistics**

**Part III**

**Appendix**

# A Metric Spaces

## A.1 Metrics

**Definition A.1** (Metric). Let  $X$  be a set. A *metric* on  $X$  is a function  $d : X \times X \rightarrow \mathbb{R}$  such that for all  $x, y, z \in X$ :

- (i)  $d(x, y) \geq 0$  (non-negativity);
- (ii)  $d(x, y) = 0$  if and only if  $x = y$  (identity of indiscernibles);
- (iii)  $d(x, y) = d(y, x)$  (symmetry);
- (iv)  $d(x, z) \leq d(x, y) + d(y, z)$  (triangle inequality).

**Definition A.2** (Metric Space). A *metric space* is a pair  $(X, d)$ , where  $X$  is a set and  $d$  is a metric on  $X$ .

**Example A.3** (Euclidean Space). Let  $X = \mathbb{R}^n$ . The Euclidean metric is defined by

$$d(x, y) = \|x - y\|_2 = \sqrt{\sum_{i=1}^n (x_i - y_i)^2}.$$

Then  $(\mathbb{R}^n, d)$  is a metric space. ◇

**Example A.4** (Function Space). Let  $X = C[0, 1]$ , the set of continuous real-valued functions on the interval  $[0, 1]$ . The supremum metric (or uniform metric) is defined by

$$d(f, g) = \sup_{t \in [0, 1]} |f(t) - g(t)|.$$

Then  $(C[0, 1], d)$  is a metric space. ◇

## A.2 Topology

**Definition A.5** (Open Ball). Let  $(X, d)$  be a metric space. The *open ball* of radius  $r > 0$  centered at  $x \in X$  is the set

$$B_r(x) = \{y \in X : d(x, y) < r\}.$$

**Definition A.6** (Open Set in Metric Spaces). A subset  $U \subseteq X$  is called *open* if for every  $x \in U$ , there exists an  $\epsilon > 0$  such that  $B_\epsilon(x) \subseteq U$ .

**Definition A.7** (Closed Set). A subset  $F \subseteq X$  is *closed* if its complement  $X \setminus F$  is open.

**Definition A.8** (Closure). The *closure* of a subset  $A \subseteq X$ , denoted  $\bar{A}$ , is the intersection of all closed sets containing  $A$ . It is the smallest closed set containing  $A$ .

**Definition A.9** (Neighborhood). A subset  $N \subseteq X$  is called a *neighborhood* of a point  $x \in X$  if there exists an open set  $U$  such that  $x \in U \subseteq N$ . Equivalently,  $N$  is a neighborhood of  $x$  if there exists an  $\epsilon > 0$  such that  $B_\epsilon(x) \subseteq N$ .

**Proposition A.10.** Let  $(X, d)$  be a metric space. The collection  $\mathcal{T}$  of open sets in  $X$  (as defined in Definition A.6) satisfies the following properties:

- (i)  $\emptyset \in \mathcal{T}$  and  $X \in \mathcal{T}$ ;
- (ii) The union of any collection of open sets is open;
- (iii) The intersection of any finite collection of open sets is open.

**Definition A.11** (Continuous Function). Let  $(X, d_X)$  and  $(Y, d_Y)$  be metric spaces. A function  $f : X \rightarrow Y$  is *continuous* at a point  $x \in X$  if for every  $\epsilon > 0$ , there exists a  $\delta > 0$  such that  $d_X(x, y) < \delta$  implies  $d_Y(f(x), f(y)) < \epsilon$ . The function  $f$  is *continuous* if it is continuous at every point in  $X$ .

**Proposition A.12.** Let  $(X, d_X)$  and  $(Y, d_Y)$  be metric spaces. A function  $f : X \rightarrow Y$  is continuous if and only if for every open set  $V \subseteq Y$ , the preimage  $f^{-1}(V)$  is open in  $X$ .

Proposition A.12 reveals that continuity can be characterized entirely in terms of open sets, without explicit reference to the underlying metric.

**Definition A.13** (Topology Generated by a Metric). The collection of all open sets in a metric space  $(X, d)$  forms a topology on  $X$ , called the *topology induced by the metric*  $d$ .

This motivates the generalization of continuity in metric spaces to spaces where only the notion of “openness” is defined, which leads to the definition of a topological space. It turns out that the properties of Proposition A.10 are precisely the properties needed to have things function the way they do for metrics.

**Definition A.14** (Topology). A *topology* on a set  $X$  is a collection  $\mathcal{T}$  of subsets of  $X$  satisfying:

- (i)  $\emptyset \in \mathcal{T}$  and  $X \in \mathcal{T}$ ;
- (ii) The union of any collection of sets in  $\mathcal{T}$  is in  $\mathcal{T}$ ;

(iii) The intersection of any finite collection of sets in  $\mathcal{T}$  is in  $\mathcal{T}$ .

The pair  $(X, \mathcal{T})$  is called a *topological space*. The elements of  $\mathcal{T}$  are called *open sets*.

*Remark A.15.* Every metric induces a topology, but not every topology arises from a metric. A topological space whose topology is induced by a metric is called *metrizable*.

**Definition A.16** (Separable Space). A topological space  $X$  is called *separable* if it contains a countable dense subset. That is, there exists a countable set  $D \subseteq X$  such that  $\overline{D} = X$ .

**Definition A.17** (Polish Space). A topological space  $X$  is called a *Polish space* if it is separable and completely metrizable. That is, there exists a metric  $d$  on  $X$  which induces the topology of  $X$  such that  $(X, d)$  is a complete metric space.

## A.3 Compactness

**Definition A.18** (Bounded Set). A subset  $A$  of a metric space  $(X, d)$  is *bounded* if there exists  $x \in X$  and  $R > 0$  such that  $A \subseteq B_R(x)$ .

**Definition A.19** (Compactness). A subset  $K$  of a topological space  $X$  is *compact* if every open cover of  $K$  has a finite subcover. That is, if  $K \subseteq \bigcup_{i \in I} U_i$  where each  $U_i$  is open, then there exists a finite subset  $J \subseteq I$  such that  $K \subseteq \bigcup_{j \in J} U_j$ .

**Definition A.20** (Sequential Compactness). A subset  $K$  of a metric space is *sequentially compact* if every sequence in  $K$  has a convergent subsequence whose limit belongs to  $K$ .

In metric spaces, compactness and sequential compactness are equivalent.

**Definition A.21** (Locally Compact Space). A topological space  $X$  is *locally compact* if every point  $x \in X$  has a compact neighborhood. That is, for every  $x \in X$ , there exists an open set  $U$  containing  $x$  such that  $\overline{U}$  is compact.

**Example A.22** (Euclidean space is locally compact). The space  $\mathbb{R}^d$  with the Euclidean topology is locally compact. For any  $x \in \mathbb{R}^d$ , the open ball  $B_1(x)$  has closure  $\overline{B_1(x)}$  equal to the closed ball  $\{y : \|y - x\| \leq 1\}$ , which is compact by the Heine–Borel theorem.

More generally, any open or closed subset of  $\mathbb{R}^d$  is locally compact. Compact spaces are trivially locally compact.  $\diamond$

**Definition A.23** (Limit Point). A point  $x \in X$  is a *limit point* (or accumulation point) of a set  $A$  if every open neighborhood of  $x$  contains a point of  $A$  distinct from  $x$ .

**Definition A.24** (Generated Topology). Let  $X$  be a set and  $\mathcal{S}$  be a collection of subsets of  $X$ . The *topology generated by  $\mathcal{S}$*  is the smallest topology on  $X$  containing  $\mathcal{S}$ . It consists of all arbitrary unions of finite intersections of elements of  $\mathcal{S}$ . The elements of  $\mathcal{S}$  are called a *subbasis* for the topology.

**Example A.25** (Standard Topology on  $\mathbb{R}$ ). Let  $X = \mathbb{R}$ . The standard topology on  $\mathbb{R}$  is the topology generated by the collection of all open intervals  $(a, b)$ . In fact, this is the same as the topology induced by the Euclidean metric  $d(x, y) = |x - y|$ .  $\diamond$

**Example A.26** (Topology of Pointwise Convergence). Let  $X$  be the set of all functions  $f : [0, 1] \rightarrow \mathbb{R}$ . The topology of pointwise convergence is the topology generated by sets of the form

$$S_{t,(a,b)} = \{f \in X : a < f(t) < b\}$$

where  $t \in [0, 1]$  and  $a < b$  are real numbers. Convergence in this topology corresponds exactly to pointwise convergence: a sequence  $f_n \rightarrow f$  if and only if  $f_n(t) \rightarrow f(t)$  for all  $t \in [0, 1]$ .  $\diamond$

# B Measure Theory

## B.1 Measure and Probability

The foundational concept in measure theory is the sigma-algebra, which defines the collection of subsets to which we can assign a measure.

**Definition B.1.** A  $\sigma$ -algebra  $\mathcal{F}$  on a set  $\Omega$  is a collection of subsets of  $\Omega$  that satisfies the following properties:

- (i)  $\emptyset \in \mathcal{F}$
- (ii) If  $A \in \mathcal{F}$ , then  $A^c \in \mathcal{F}$
- (iii) If  $A_1, A_2, \dots \in \mathcal{F}$ , then  $\bigcup_{i=1}^{\infty} A_i \in \mathcal{F}$

Once we have a  $\sigma$ -algebra, we can define a measure, which generalizes the concepts of length, area, and probability.

**Definition B.2.** Consider a measurable space  $(\Omega, \mathcal{F})$ . A *measure*  $\mu$  on a  $\sigma$ -algebra  $\mathcal{F}$  is a function that assigns a non-negative real number to each set in  $\mathcal{F}$  and satisfies the following properties:

1.  $\mu(\emptyset) = 0$
2. If  $A_1, A_2, \dots \in \mathcal{F}$  are disjoint, then  $\mu(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} \mu(A_i)$

If  $\mu(\Omega) < \infty$ , then  $\mu$  is called a *finite measure*. If in addition  $\mu(\Omega) = 1$ , then  $\mu$  is a *probability measure*.

These components form the standard objects of study in measure theory.

**Definition B.3.** A pair  $(\Omega, \mathcal{F})$  consisting of a set  $\Omega$  and a  $\sigma$ -algebra  $\mathcal{F}$  is called a *measurable space*. A triple  $(\Omega, \mathcal{F}, \mu)$  consisting of a measurable space and a measure  $\mu$  is called a *measure space*. If  $\mu$  is a probability measure, the triple is called a *probability space*.

Many important measures are not finite, but satisfy a weaker condition called  $\sigma$ -finiteness.

**Definition B.4.** A measure  $\mu$  on  $(\Omega, \mathcal{F})$  is called  *$\sigma$ -finite* if there exists a sequence of sets  $A_1, A_2, \dots \in \mathcal{F}$  such that  $\bigcup_{i=1}^{\infty} A_i = \Omega$  and  $\mu(A_i) < \infty$  for all  $i$ .

A simple example of a measure that can be finite or  $\sigma$ -finite is the counting measure.

**Example B.5** (Counting Measure). Let  $\Omega$  be a countable set and  $\mathcal{F} = 2^\Omega$ . The counting measure  $\mu$  is defined by  $\mu(A) = |A|$  (the number of elements in  $A$ ) for any  $A \subseteq \Omega$ . This measure is  $\sigma$ -finite since  $\Omega$  is countable (take  $A_i = \{\omega_i\}$ ).  $\diamond$

Measures are often defined on a smaller class of sets (like intervals in  $\mathbb{R}$ ) and then extended to the full  $\sigma$ -algebra. Carathéodory's Extension Theorem guarantees that this extension is unique for  $\sigma$ -finite measures.

**Theorem B.6** (Uniqueness of Measure Extension). *Let  $\mathcal{A}$  be a collection of subsets of  $\Omega$  that is closed under finite intersections (a  $\pi$ -system) and generates the  $\sigma$ -algebra  $\mathcal{F} = \sigma(\mathcal{A})$ . If two measures  $\mu$  and  $\nu$  on  $(\Omega, \mathcal{F})$  agree on  $\mathcal{A}$  (i.e.,  $\mu(A) = \nu(A)$  for all  $A \in \mathcal{A}$ ), and they are  $\sigma$ -finite on  $\mathcal{A}$ , then  $\mu = \nu$  on  $\mathcal{F}$ .*

Measures also behave continuously with respect to increasing or decreasing sequences of sets.

**Proposition B.7.** *Let  $\mu$  be a measure on  $(\Omega, \mathcal{F})$ .*

1. (**Continuity from below**) *If  $A_1 \subseteq A_2 \subseteq \dots$  is an increasing sequence of sets in  $\mathcal{F}$  and  $A = \bigcup_{n=1}^{\infty} A_n$ , then*

$$\mu(A) = \lim_{n \rightarrow \infty} \mu(A_n).$$

2. (**Continuity from above**) *If  $A_1 \supseteq A_2 \supseteq \dots$  is a decreasing sequence of sets in  $\mathcal{F}$  with  $\mu(A_1) < \infty$  and  $A = \bigcap_{n=1}^{\infty} A_n$ , then*

$$\mu(A) = \lim_{n \rightarrow \infty} \mu(A_n).$$

We now turn to the functions between measurable spaces, which must preserve the measurable structure.

**Definition B.8.** Let  $(\Omega, \mathcal{F})$  and  $(S, \mathcal{G})$  be measurable spaces. A function  $f : \Omega \rightarrow S$  is *measurable* (or  $\mathcal{F}/\mathcal{G}$ -measurable) if for every  $B \in \mathcal{G}$ , the preimage  $f^{-1}(B) \in \mathcal{F}$ .

That is,  $f$  is measurable if

$$f^{-1}(B) = \{\omega \in \Omega : f(\omega) \in B\} \in \mathcal{F} \quad \text{for all } B \in \mathcal{G}.$$

Conversely, any function induces a  $\sigma$ -algebra on its domain.

**Definition B.9.** Let  $(\Omega, \mathcal{F})$  and  $(S, \mathcal{G})$  be measurable spaces, and let  $f : \Omega \rightarrow S$  be a measurable function. The  $\sigma$ -algebra generated by  $f$ , denoted by  $\sigma(f)$ , is the collection of all preimages of sets in  $\mathcal{G}$ :

$$\sigma(f) = \{f^{-1}(B) : B \in \mathcal{G}\}.$$

This is the smallest  $\sigma$ -algebra on  $\Omega$  with respect to which  $f$  is measurable. Note that  $\sigma(f) \subseteq \mathcal{F}$  since  $f$  is measurable.

**Definition B.10.** The *Borel  $\sigma$ -algebra* on a topological space  $(X, \mathcal{T})$ , denoted by  $\mathcal{B}(X)$ , is the  $\sigma$ -algebra generated by the open sets  $\mathcal{T}$ . In particular, if  $(X, d)$  is a metric space,  $\mathcal{B}(X)$  is generated by the open balls.

If  $(X, \mathcal{B}(X))$  and  $(Y, \mathcal{B}(Y))$  are two measurable spaces equipped with their Borel  $\sigma$ -algebras, then any continuous function  $f : X \rightarrow Y$  is measurable.

For  $X = \mathbb{R}$ ,  $\mathcal{B}(\mathbb{R})$  is the  $\sigma$ -algebra generated by the collection of all open intervals in  $\mathbb{R}$ . Sets in  $\mathcal{B}(\mathbb{R})$  are called *Borel sets*. This is the standard  $\sigma$ -algebra used when the sample space is  $\mathbb{R}$  (or  $\mathbb{R}^d$ ).

On the real line, the most important measure is the one that assigns lengths to intervals.

**Definition B.11** (Lebesgue Measure). The Lebesgue measure  $\lambda$  on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$  is the unique measure satisfying  $\lambda((a, b]) = b - a$  for all intervals  $(a, b]$ .

The Lebesgue measure is  $\sigma$ -finite since  $\mathbb{R} = \bigcup_{n=1}^{\infty} (-n, n]$ .

Measurable functions are closed under various operations.

**Proposition B.12.** Let  $(\Omega, \mathcal{F})$ ,  $(S, \mathcal{G})$ , and  $(T, \mathcal{H})$  be measurable spaces.

1. (**Composition**) If  $f : \Omega \rightarrow S$  is  $\mathcal{F}/\mathcal{G}$ -measurable and  $g : S \rightarrow T$  is  $\mathcal{G}/\mathcal{H}$ -measurable, then the composition  $g \circ f : \Omega \rightarrow T$  is  $\mathcal{F}/\mathcal{H}$ -measurable.

A measurable function can be used to transport a measure from its domain to its codomain.

**Definition B.13** (Push-forward Measure). Let  $(\Omega, \mathcal{F}, \mu)$  be a measure space,  $(S, \mathcal{G})$  a measurable space, and  $T : \Omega \rightarrow S$  a measurable function. The *push-forward measure* of  $\mu$  by  $T$ , denoted  $\mu^T$  (or sometimes  $T_{\#}\mu$  or  $\mu \circ T^{-1}$ ), is the measure on  $(S, \mathcal{G})$  defined by

$$\mu^T(B) = \mu(T^{-1}(B)) \quad \text{for all } B \in \mathcal{G}.$$

Intuitively,  $\mu^T$  describes the distribution of the random element  $T(\omega)$  when  $\omega$  is distributed according to  $\mu$ .

The relationship between integrals under the original and push-forward measures is given by the change of variables formula.

**Theorem B.14** (Change of Variables Formula). Let  $T : (\Omega, \mathcal{F}, \mu) \rightarrow (S, \mathcal{G})$  be measurable. For any measurable function  $g : S \rightarrow \mathbb{R}$ ,  $g$  is integrable with respect to  $\mu^T$  if and only if  $g \circ T$  is integrable with respect to  $\mu$ , and

$$\int_S g(y) d\mu^T(y) = \int_{\Omega} g(T(\omega)) d\mu(\omega).$$

**Definition B.15** (Equivalence Relation). An *equivalence relation*  $\sim$  on a set  $X$  is a binary relation that satisfies three properties for all  $a, b, c \in X$ :

1. **Reflexivity:**  $a \sim a$ .
2. **Symmetry:** If  $a \sim b$ , then  $b \sim a$ .
3. **Transitivity:** If  $a \sim b$  and  $b \sim c$ , then  $a \sim c$ .

Given an equivalence relation  $\sim$  on a set  $X$ , the *equivalence class* of an element  $x \in X$ , denoted  $[x]$ , is the set of all elements in  $X$  equivalent to  $x$ :

$$[x] = \{y \in X : y \sim x\}.$$

The set of all equivalence classes is called the *quotient set* and denoted by  $X/\sim$ .

Equivalence relations allow us to define measurable structures on quotient spaces.

**Definition B.16** (Quotient  $\sigma$ -algebra). Let  $(X, \Sigma)$  be a measurable space and  $\sim$  an equivalence relation on  $X$ . The *quotient  $\sigma$ -algebra* on the quotient space  $X/\sim$ , denoted by  $\Sigma/\sim$ , is defined as

$$\Sigma/\sim = \{B \subseteq X/\sim \mid \pi^{-1}(B) \in \Sigma\},$$

where  $\pi : X \rightarrow X/\sim$  is the canonical projection map  $\pi(x) = [x]$ .

This is the largest  $\sigma$ -algebra on  $X/\sim$  making the projection  $\pi$  measurable.

## B.2 Integration

### B.2.1 The Standard Machinery

A common strategy in measure theory to prove a property  $\mathbf{p}$  for all measurable functions is the so-called “standard machine” or “approximation by simple functions”. The steps are typically:

1. **Indicator Functions:** Prove that  $\mathbf{p}$  holds for indicator functions  $\mathbb{1}_A$  for all measurable sets  $A$ .
2. **Simple Functions:** Extend the result to non-negative simple functions  $s = \sum_{i=1}^n c_i \mathbb{1}_{A_i}$  by linearity.
3. **Non-negative Measurable Functions:** Use the fact that any non-negative measurable function  $f$  is the limit of an increasing sequence of non-negative simple functions  $s_n \uparrow f$ . Prove that  $\mathbf{p}$  is preserved under this limit (often using the Monotone Convergence Theorem).

4. **General Measurable Functions:** For a general measurable function  $f$ , write  $f = f^+ - f^-$  where  $f^+ = \max(f, 0)$  and  $f^- = \max(-f, 0)$ . Extend the result by linearity, provided integrability conditions are met.

Key theorems supporting this machinery include:

**Theorem B.17** (Monotone Class Theorem). *Let  $\mathcal{A}$  be an algebra of sets generating a  $\sigma$ -algebra  $\mathcal{F}$ . Let  $\mathcal{M}$  be a collection of subsets of  $\Omega$  that is a monotone class (i.e., closed under countable increasing unions and countable decreasing intersections). If  $\mathcal{A} \subseteq \mathcal{M}$ , then  $\mathcal{F} \subseteq \mathcal{M}$ .*

**Theorem B.18** (Monotone Convergence Theorem). *If  $\{f_n\}$  is a sequence of non-negative measurable functions such that  $f_n \uparrow f$  pointwise, then*

$$\lim_{n \rightarrow \infty} \int f_n d\mu = \int f d\mu.$$

**Lemma B.19** (Fatou's Lemma). *If  $\{f_n\}$  is a sequence of non-negative measurable functions, then*

$$\int \liminf_{n \rightarrow \infty} f_n d\mu \leq \liminf_{n \rightarrow \infty} \int f_n d\mu.$$

**Theorem B.20** (Dominated Convergence Theorem). *Let  $\{f_n\}$  be a sequence of measurable functions converging pointwise to  $f$ . If there exists an integrable function  $g$  such that  $|f_n| \leq g$  for all  $n$ , then  $f$  is integrable and*

$$\lim_{n \rightarrow \infty} \int f_n d\mu = \int f d\mu.$$

The condition of a single dominating function in the DCT can be relaxed to uniform integrability, which controls the integrals of the sequence uniformly over sets of small measure.

**Definition B.21** (Uniform Integrability). Let  $(\Omega, \mathcal{F}, \mu)$  be a measure space. A collection of measurable functions  $\{f_i\}_{i \in I}$  is called *uniformly integrable* if for every  $\varepsilon > 0$ , there exists  $M > 0$  such that

$$\sup_{i \in I} \int_{\{|f_i| > M\}} |f_i| d\mu < \varepsilon.$$

When  $\mu$  is a finite measure, uniform integrability admits an equivalent characterization in terms of sets of small measure.

**Proposition B.22.** *Let  $(\Omega, \mathcal{F}, \mu)$  be a finite measure space. A collection  $\{f_i\}_{i \in I}$  of integrable functions is uniformly integrable if and only if:*

1.  $\sup_{i \in I} \int |f_i| d\mu < \infty$ , and

2. for every  $\varepsilon > 0$ , there exists  $\delta > 0$  such that for all  $A \in \mathcal{F}$  with  $\mu(A) < \delta$ ,

$$\sup_{i \in I} \int_A |f_i| d\mu < \varepsilon.$$

Uniform integrability provides a necessary and sufficient condition for  $L^1$  convergence.

**Theorem B.23** (Vitali Convergence Theorem). *Let  $(\Omega, \mathcal{F}, \mu)$  be a finite measure space and let  $\{f_n\}$  be a sequence of integrable functions converging in measure to  $f$ . Then  $f_n \rightarrow f$  in  $L^1(\mu)$  if and only if  $\{f_n\}$  is uniformly integrable.*

## B.2.2 Differentiation of integrals

A function  $F : [a, b] \rightarrow \mathbb{R}$  is called *absolutely continuous* if for every  $\varepsilon > 0$  there exists  $\delta > 0$  such that for any finite collection of disjoint intervals  $(a_k, b_k) \subseteq [a, b]$ ,

$$\sum_k (b_k - a_k) < \delta \implies \sum_k |F(b_k) - F(a_k)| < \varepsilon.$$

Absolute continuity is strictly stronger than continuity and uniform continuity, but weaker than Lipschitz continuity.

**Theorem B.24** (Lebesgue Fundamental Theorem of Calculus). *Let  $[a, b] \subseteq \mathbb{R}$ .*

1. (**First form.**) *If  $f \in L^1([a, b])$  and  $F(x) = \int_a^x f(t) dt$ , then  $F$  is absolutely continuous on  $[a, b]$  and  $F'(x) = f(x)$  for Lebesgue-almost every  $x \in [a, b]$ .*
2. (**Second form.**) *If  $F : [a, b] \rightarrow \mathbb{R}$  is absolutely continuous, then  $F$  is differentiable almost everywhere,  $F' \in L^1([a, b])$ , and*

$$F(x) - F(a) = \int_a^x F'(t) dt \quad \text{for all } x \in [a, b].$$

The two forms are converses of each other: the first says that integrating and then differentiating recovers the original function (a.e.), while the second says that differentiating and then integrating recovers the original function (exactly, for absolutely continuous  $F$ ). Together, they establish that the absolutely continuous functions are precisely those that arise as indefinite integrals of  $L^1$  functions.

### B.2.3 Function spaces

**Definition B.25** ( $\mathcal{L}^p$  spaces). Let  $(\Omega, \mathcal{F}, \mu)$  be a measure space. For  $1 \leq p < \infty$ , let  $\mathcal{L}^p(\Omega, \mathcal{F}, \mu)$  denote the set of all measurable functions  $f : \Omega \rightarrow \mathbb{R}$  such that

$$\|f\|_p := \left( \int_{\Omega} |f|^p d\mu \right)^{1/p} < \infty.$$

Similarly,  $\mathcal{L}^\infty(\Omega, \mathcal{F}, \mu)$  consists of all essentially bounded measurable functions, i.e., those for which there exists a constant  $C$  such that  $|f(\omega)| \leq C$  for almost all  $\omega$ . The essential supremum is defined as:

$$\|f\|_\infty := \inf\{C \geq 0 : |f(\omega)| \leq C \text{ for } \mu\text{-almost all } \omega\}.$$

The quantity  $\|\cdot\|_p$  satisfies most properties of a norm (non-negativity, homogeneity, triangle inequality), but it is only a *semi-norm* on  $\mathcal{L}^p$ , because  $\|f\|_p = 0$  implies  $f = 0$  only almost everywhere (not everywhere). To obtain a Banach space, we must identify functions that are equal almost everywhere.

**Definition B.26** ( $L^p$  spaces). We define an equivalence relation  $\sim$  on  $\mathcal{L}^p$  by  $f \sim g$  if and only if  $f = g$   $\mu$ -almost everywhere. The  $L^p$  space is the quotient space of equivalence classes:

$$L^p(\Omega, \mathcal{F}, \mu) := \mathcal{L}^p(\Omega, \mathcal{F}, \mu) / \sim.$$

Elements of  $L^p$  are equivalence classes  $[f]$ , but it is standard practice to abuse notation and refer to them as functions  $f$ .

Equipped with the norm  $\|[f]\|_p := \|f\|_p$ , the space  $L^p$  becomes a Banach space (a complete normed vector space).

Important special cases include:

- $L^p(\mathbb{R}^d)$ : When  $\Omega = \mathbb{R}^d$  equipped with the Lebesgue measure.
- $L^p([0, 1])$ : The space of functions on the unit interval square-integrable with respect to Lebesgue measure. This is a standard setting for functional analysis.
- $\ell^p$ : When  $\mu$  is the counting measure on  $\mathbb{N}$ , the space is the set of sequences  $(x_n)$  with  $\sum |x_n|^p < \infty$ .
- $L^2(\mu)$ : For  $p = 2$ , the space is a Hilbert space with inner product  $\langle f, g \rangle = \int fg d\mu$ .

### B.2.4 Change of measure

Let  $\mu$  be a measure on  $(\Omega, \mathcal{F})$  and let  $f : \Omega \rightarrow [0, \infty]$  be a non-negative measurable function. We can define a new measure  $\nu$  on  $(\Omega, \mathcal{F})$  by setting

$$\nu(A) = \int_A f d\mu \quad \text{for all } A \in \mathcal{F}.$$

It is a standard exercise in measure theory to verify that  $\nu$  indeed satisfies the properties of a measure.

**Definition B.27** (Probability Density). If the function  $f$  is non-negative and the induced measure  $\nu$  satisfies  $\nu(\Omega) = 1$  (i.e.,  $\nu$  is a probability measure), then  $f$  is called a *probability density* of  $\nu$  with respect to the reference measure  $\mu$ .

The relationship between  $\nu$  and  $\mu$  constructed above implies a specific property called absolute continuity.

**Definition B.28** (Absolute Continuity). Let  $\nu$  and  $\mu$  be two measures on a measurable space  $(\Omega, \mathcal{F})$ . We say  $\nu$  is *absolutely continuous* with respect to  $\mu$  (denoted  $\nu \ll \mu$ ) if for all  $A \in \mathcal{F}$ ,

$$\mu(A) = 0 \implies \nu(A) = 0.$$

The fundamental result connecting these concepts is the Radon-Nikodym theorem, which states that under mild conditions, absolute continuity is sufficient to guarantee the existence of a density.

**Theorem B.29** (Radon-Nikodym Theorem). *Let  $\nu$  and  $\mu$  be two measures on a measurable space  $(\Omega, \mathcal{F})$ , and assume that  $\mu$  is  $\sigma$ -finite. If  $\nu \ll \mu$ , then there exists a non-negative measurable function  $f : \Omega \rightarrow [0, \infty)$  such that for all  $A \in \mathcal{F}$ ,*

$$\nu(A) = \int_A f d\mu.$$

*The function  $f$  is unique up to a set of  $\mu$ -measure zero. We call  $f$  the Radon-Nikodym derivative or density of  $\nu$  with respect to  $\mu$ , and denote it by  $f = \frac{d\nu}{d\mu}$ .*

The next theorem provides a characterization of sufficient statistics (Definition 1.9). The theorem provides the measure-theoretic foundation for the Factorization Theorem (Theorem 1.12) encountered in the main text. Its proof is quite involved and is omitted here, but one can find it in Halmos and Savage 1949.

**Theorem B.30** (Halmos–Savage). *Let  $\mathcal{P}$  be a family of probability measures dominated by a  $\sigma$ -finite measure. A statistic  $T$  is sufficient for  $\mathcal{P}$  if and only if for all  $P, Q \in \mathcal{P}$ , the likelihood ratio  $dP/dQ$  admits a  $\sigma(T)$ -measurable version.*

## B.3 Joint distributions

### B.3.1 Product measures and independence

Given two measurable spaces  $(\Omega_1, \mathcal{F}_1)$  and  $(\Omega_2, \mathcal{F}_2)$ , the *product  $\sigma$ -algebra*, denoted  $\mathcal{F}_1 \otimes \mathcal{F}_2$ , is the  $\sigma$ -algebra on  $\Omega_1 \times \Omega_2$  generated by the collection of measurable rectangles  $\{A \times B : A \in \mathcal{F}_1, B \in \mathcal{F}_2\}$ .

If  $\mu_1$  and  $\mu_2$  are  $\sigma$ -finite measures on  $(\Omega_1, \mathcal{F}_1)$  and  $(\Omega_2, \mathcal{F}_2)$  respectively, there exists a unique measure  $\mu = \mu_1 \otimes \mu_2$  on the product space such that

$$\mu(A \times B) = \mu_1(A)\mu_2(B) \quad \text{for all } A \in \mathcal{F}_1, B \in \mathcal{F}_2.$$

**Definition B.31** (Independence). Let  $(\Omega, \mathcal{F}, P)$  be a probability space. Two events  $A, B \in \mathcal{F}$  are *independent* if  $P(A \cap B) = P(A)P(B)$ . Two random variables  $X : \Omega \rightarrow \mathcal{X}$  and  $Y : \Omega \rightarrow \mathcal{Y}$  are *independent* if for all  $A \in \mathcal{X}$  and  $B \in \mathcal{Y}$ , the events  $\{X \in A\}$  and  $\{Y \in B\}$  are independent.

In terms of joint distributions, independence means the joint distribution is the product measure of the marginals. That is, the joint law of  $(X, Y)$  is  $P_{(X,Y)} = P_X \otimes P_Y$ .

**Definition B.32** (i.i.d.). A sequence of random variables  $X_1, X_2, \dots, X_n$  is *independent and identically distributed (i.i.d.)* if they are mutually independent and all have the same marginal distribution.

If  $X_1, \dots, X_n \stackrel{\text{iid}}{\sim} P$ , their joint distribution on the product space  $(\mathcal{X}^n, \mathcal{X}^{\otimes n})$  is the product measure  $P^{\otimes n}$ , defined inductively by  $P^{\otimes 1} = P$  and  $P^{\otimes(n+1)} = P^{\otimes n} \otimes P$ .

### B.3.2 Conditional probability and expectation

The definition of conditional probability is based on the concept of conditional expectation.

**Definition B.33** (Conditional Expectation). Let  $(\Omega, \mathcal{F}, P)$  be a probability space,  $\mathcal{G} \subseteq \mathcal{F}$  a sub- $\sigma$ -algebra, and  $X$  an integrable random variable (i.e.,  $E|X| < \infty$ ). The *conditional expectation* of  $X$  given  $\mathcal{G}$ , denoted  $E[X \mid \mathcal{G}]$ , is the equivalence class of  $\mathcal{G}$ -measurable random variables  $Z$  such that

$$\int_G Z dP = \int_G X dP \quad \text{for all } G \in \mathcal{G}.$$

The existence and uniqueness (up to almost sure equivalence) of  $Z$  are guaranteed by the Radon-Nikodym theorem.

**Theorem B.34** (Existence and Uniqueness of Conditional Expectation). *Let  $(\Omega, \mathcal{F}, P)$  be a probability space,  $\mathcal{G} \subseteq \mathcal{F}$  a sub- $\sigma$ -algebra, and  $X$  an integrable random variable. Then there exists a unique (up to almost sure equivalence)  $\mathcal{G}$ -measurable random variable  $Z$  such that*

$$\int_G Z dP = \int_G X dP \quad \text{for all } G \in \mathcal{G}.$$

With this tool, we can rigorously define the probability of an event given partial information.

**Definition B.35** (Conditional Probability). The *conditional probability* of an event  $A \in \mathcal{F}$  given a sub- $\sigma$ -algebra  $\mathcal{G}$ , denoted  $P(A \mid \mathcal{G})$ , is defined as the conditional expectation of the indicator function of  $A$ :

$$P(A \mid \mathcal{G}) := E[\mathbb{1}_A \mid \mathcal{G}].$$

When conditioning on a random variable  $Y$ , we mean conditioning on the  $\sigma$ -algebra generated by  $Y$ , i.e.,  $E[X \mid Y] := E[X \mid \sigma(Y)]$ .

Conditional expectations satisfy a generalized version of Bayes' theorem.

**Theorem B.36** (Abstract Bayes Formula). *Let  $P$  and  $Q$  be probability measures on  $(\Omega, \mathcal{F})$  such that  $P \ll Q$ , and let  $L = dP/dQ$  be the Radon-Nikodym derivative. For any sub- $\sigma$ -algebra  $\mathcal{G} \subseteq \mathcal{F}$  and any  $P$ -integrable random variable  $f$ ,*

$$E_P[f \mid \mathcal{G}] = \frac{E_Q[fL \mid \mathcal{G}]}{E_Q[L \mid \mathcal{G}]} \quad P\text{-a.s.}$$

Often, we want to view the conditional probability  $P(\cdot \mid \mathcal{G})(\omega)$  as a probability measure on  $(\Omega, \mathcal{F})$  for each fixed  $\omega$ . This is not guaranteed by the general definition (due to null sets for each  $A$ ). However, it is possible in sufficiently “nice” spaces.

A crucial property relating measurability with respect to a random variable and functions of that random variable is given by the Doob-Dynkin Lemma.

**Lemma B.37** (Doob–Dynkin Lemma). *Let  $(S, \mathcal{S})$  be a standard Borel space and let  $X : (\Omega, \mathcal{F}) \rightarrow (S, \mathcal{S})$  be measurable. Then a random variable  $Y : (\Omega, \mathcal{F}) \rightarrow (\mathbb{R}, \mathcal{B}(\mathbb{R}))$  is  $\sigma(X)$ -measurable if and only if there exists a measurable function  $g : S \rightarrow \mathbb{R}$  such that  $Y = g(X)$ .*

This lemma implies that  $E[Z \mid X] = g(X)$  for some measurable function  $g$ . Specifically, if  $Y$  is  $\sigma(X)$ -measurable, it is a function of  $X$ .

Under certain conditions, conditional probabilities can be realized as a kernel that is a measure for each fixed  $\omega$ .

**Definition B.38** (Regular Conditional Probability). Let  $(\Omega, \mathcal{F}, P)$  be a probability space and  $\mathcal{G} \subseteq \mathcal{F}$  a sub- $\sigma$ -algebra. A *regular conditional probability* is a function  $\kappa : \Omega \times \mathcal{F} \rightarrow [0, 1]$  such that:

1. For each  $\omega \in \Omega$ ,  $\kappa(\omega, \cdot)$  is a probability measure on  $(\Omega, \mathcal{F})$ .
2. For each  $A \in \mathcal{F}$ ,  $\omega \mapsto \kappa(\omega, A)$  is a version of  $P(A \mid \mathcal{G})$ .

Regular conditional probabilities are guaranteed to exist when  $\Omega$  is a standard Borel space (e.g. a Polish space (see Definition A.17 in Appendix A) equipped with its Borel  $\sigma$ -algebra).

**Theorem B.39** (Existence of Regular Conditional Probabilities). *Let  $(\Omega, \mathcal{F}, P)$  be a probability space where  $\Omega$  is a Polish space and  $\mathcal{F} = \mathcal{B}(\Omega)$  is its Borel  $\sigma$ -algebra. For any sub- $\sigma$ -algebra  $\mathcal{G} \subseteq \mathcal{F}$ , there exists a regular conditional probability given  $\mathcal{G}$ .*

A related concept is the Markov kernel, which generalizes the idea of a transition matrix.

**Definition B.40** (Markov Kernel). Let  $(X, \mathcal{X})$  and  $(Y, \mathcal{Y})$  be measurable spaces. A *Markov kernel* (or probability kernel) from  $(X, \mathcal{X})$  to  $(Y, \mathcal{Y})$  is a function  $K : X \times \mathcal{Y} \rightarrow [0, 1]$  such that:

1. For each  $x \in X$ , the map  $B \mapsto K(x, B)$  is a probability measure on  $(Y, \mathcal{Y})$ .
2. For each  $B \in \mathcal{Y}$ , the map  $x \mapsto K(x, B)$  is  $\mathcal{X}$ -measurable.

Markov kernels are used to model random mappings where the output distribution depends on the input, such as in conditional distributions  $P(Y \in B \mid X = x)$ .

Finally, we state the version of Bayes' rule for densities, which is the most common form used in statistical inference.

**Theorem B.41** (Bayes' Rule for Densities). *Let  $\Theta$  and  $\mathcal{X}$  be random variables taking values in measurable spaces  $(\Omega_\Theta, \mathcal{F}_\Theta)$  and  $(\Omega_{\mathcal{X}}, \mathcal{F}_{\mathcal{X}})$ , respectively. Suppose the joint distribution of  $(\Theta, \mathcal{X})$  is dominated by a product measure  $\nu \otimes \mu$ , with joint density  $p(\theta, x)$ . Then the conditional distribution of  $\Theta$  given  $\mathcal{X} = x$  has density (with respect to  $\nu$ ):*

$$p(\theta \mid x) = \frac{p(\theta, x)}{\int_{\Omega_\Theta} p(\vartheta, x) d\nu(\vartheta)},$$

*provided the denominator is positive and finite. In the common case where  $p(\theta, x) = p(x \mid \theta)\pi(\theta)$  (likelihood  $\times$  prior), this becomes the familiar form:*

$$p(\theta \mid x) = \frac{p(x \mid \theta)\pi(\theta)}{\int p(x \mid \vartheta)\pi(\vartheta) d\nu(\vartheta)}.$$

## B.4 Concentration of measure

**Lemma B.42** (Jensen’s Inequality). *Let  $(\Omega, \mathcal{F}, P)$  be a probability space, let  $X \in L^1(P)$  be real-valued, and let  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$  be convex such that  $\mathbb{E}|\varphi(X)| < \infty$ . Then*

$$\varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi(X)].$$

*If  $\varphi$  is strictly convex, then equality holds if and only if  $X$  is constant  $P$ -a.s. Moreover, for any sub- $\sigma$ -algebra  $\mathcal{G} \subseteq \mathcal{F}$ ,*

$$\varphi(\mathbb{E}[X \mid \mathcal{G}]) \leq \mathbb{E}[\varphi(X) \mid \mathcal{G}] \quad P\text{-a.s.}$$

**Lemma B.43** (Markov’s inequality). *If  $X \geq 0$ , then for any  $a > 0$ ,*

$$\mathbb{P}(X \geq a) \leq \frac{\mathbb{E}[X]}{a}.$$

*Proof.* Note that  $a \cdot \mathbb{1}_{X \geq a} \leq X$ . Taking expectations gives  $a \cdot \mathbb{P}(X \geq a) \leq \mathbb{E}[X]$ .  $\square$

The following concentration inequalities are immediate consequences.

**Lemma B.44** (Chebyshev’s inequality). *If  $\text{Var}(X) < \infty$ , then for any  $k > 0$ ,*

$$\mathbb{P}(|X - \mathbb{E}[X]| \geq k) \leq \frac{\text{Var}(X)}{k^2}.$$

*Proof.* Apply Markov’s inequality to  $(X - \mathbb{E}[X])^2$  with threshold  $k^2$ .  $\square$

**Lemma B.45** (Chernoff’s bound). *For any random variable  $X$  and any  $a \in \mathbb{R}$ ,*

$$\mathbb{P}(X \geq a) \leq \inf_{t>0} e^{-ta} \mathbb{E}[e^{tX}].$$

*Proof.* For any  $t > 0$ , the event  $\{X \geq a\}$  implies  $\{e^{tX} \geq e^{ta}\}$ . Apply Markov’s inequality to  $e^{tX}$  and take the infimum over  $t > 0$ .  $\square$

## B.5 Transforms

**Definition B.46** (Laplace Transform). Let  $\mu$  be a finite measure on  $(\mathbb{R}^k, \mathcal{B}(\mathbb{R}^k))$ . The *Laplace transform* of  $\mu$  is the function  $\psi : \mathbb{R}^k \rightarrow \mathbb{R}$  defined by

$$\psi(t) = \int_{\mathbb{R}^k} e^{\langle t, x \rangle} d\mu(x),$$

provided the integral exists.

The Laplace transform is a powerful tool for characterizing measures. A key property is its uniqueness:

**Theorem B.47** (Uniqueness of Laplace Transform). *Let  $\mu$  and  $\nu$  be two finite measures on  $\mathbb{R}^k$ . If their Laplace transforms agree on an open set containing the origin, then  $\mu = \nu$ .*

*Proof Sketch.* We sketch the argument for  $k = 1$  and compact support. Suppose  $\mu$  and  $\nu$  are supported on a compact interval  $[a, b]$ . The Laplace transform condition implies

$$\int_a^b e^{tx} d\mu(x) = \int_a^b e^{tx} d\nu(x)$$

for all  $t$  in a neighborhood of 0. By analyticity, this equality extends to all  $t \in \mathbb{R}$ . By linearity,

$$\int_a^b P(e^x) d\mu(x) = \int_a^b P(e^x) d\nu(x)$$

for any polynomial  $P$ . The algebra of functions of the form  $x \mapsto P(e^x)$  separates points on  $[a, b]$  and vanishes at no point. By the Stone-Weierstrass theorem, such functions are dense in the space of continuous functions  $C([a, b])$  with respect to the uniform norm.

Thus, for any continuous function  $f$ ,  $\int f d\mu = \int f d\nu$ . Since measures on Borel  $\sigma$ -algebras are determined by their integrals against continuous functions (Riesz Representation Theorem), we conclude  $\mu = \nu$ . The extension to non-compact support requires more careful analysis involving truncation or compactification, but the core idea remains the density of exponential families in function spaces.  $\square$

This uniqueness property extends to signed measures. If  $\mu$  is a signed measure with  $\int e^{\langle t, x \rangle} d\mu(x) = 0$  for all  $t$  in an open set, then  $\mu$  is the zero measure. This fact is crucial for proving completeness of exponential families.

Another important transform is the characteristic function, which similarly provides a powerful tool for characterizing measures.

**Definition B.48** (Characteristic Function). Let  $\mu$  be a finite measure on  $(\mathbb{R}^k, \mathcal{B}(\mathbb{R}^k))$ . The *characteristic function* of  $\mu$  is the function  $\phi : \mathbb{R}^k \rightarrow \mathbb{C}$  defined by

$$\phi(t) = \int_{\mathbb{R}^k} e^{i\langle t, x \rangle} d\mu(x),$$

where  $i = \sqrt{-1}$ .

Unlike the Laplace transform, the characteristic function is always defined for any finite measure (since  $|e^{i\langle t, x \rangle}| = 1$  is bounded). It also uniquely determines the measure.

**Theorem B.49** (Uniqueness of Characteristic Functions). *Let  $\mu$  and  $\nu$  be two finite measures on  $\mathbb{R}^k$ . If their characteristic functions agree, i.e.,  $\phi_\mu(t) = \phi_\nu(t)$  for all  $t \in \mathbb{R}^k$ , then  $\mu = \nu$ .*

This theorem is a direct consequence of the Fourier Inversion Theorem. Since the characteristic function is essentially the Fourier transform of the measure, and the Fourier transform is injective, the measure is uniquely determined.

# C Linear Algebra and (♠) Functional Analysis

The part of this appendix that concerns functional analysis is not prerequisite material for the course, nor will it be covered in lectures. However, many results in statistical decision theory—particularly existence theorems for optimal procedures—rely on functional analysis in essential ways. For students already familiar with functional analysis, this appendix clarifies those connections. For motivated students encountering these ideas for the first time, it provides a self-contained introduction to the key results.

The start of the appendix is devoted to linear algebra, which is a prerequisite for the course, but for which it may be helpful to review some concepts.

We note that our treatment of both topics will be rather brief and incomplete. For a more thorough treatment, we refer the reader to the books by Conway 1990 and Rudin 1991, on which this appendix is based. The interested student may find it motivating to follow a course on functional analysis.

The central object is the *vector space*, and the central theme is understanding *linear maps* between vector spaces. Finite-dimensional linear algebra—the study of matrices—is the special case where everything can be computed explicitly. Functional analysis extends these ideas to infinite-dimensional spaces, where new phenomena emerge but the core intuitions remain.

**Definition C.1** (Vector Space). A *vector space* is a set  $V$  equipped with two operations: vector addition and scalar multiplication, satisfying the following axioms:

1. Vector addition is associative and commutative.
2. There exists an element  $0 \in V$  such that  $v + 0 = v$  for all  $v \in V$ .
3. For each  $v \in V$ , there exists an element  $-v \in V$  such that  $v + (-v) = 0$ .

**Definition C.2** (Convexity). A set  $C$  in a vector space  $V$  is *convex* if for any  $x, y \in C$  and any  $\lambda \in [0, 1]$ , the point  $\lambda x + (1 - \lambda)y$  is also in  $C$ .

**Definition C.3** (Span). The *span* of a subset  $S$  of a vector space  $V$ , denoted  $\text{span}(S)$ , is the set of all finite linear combinations of elements in  $S$ .

**Definition C.4** (Basis and Dimension). A *Hamel basis* for a vector space  $V$  is a minimal spanning set: a set  $B \subseteq V$  with  $\text{span}(B) = V$  such that no proper subset of

$B$  spans  $V$ . Equivalently,  $B$  is a basis if every  $v \in V$  can be written uniquely as a finite linear combination of elements of  $B$ .

If  $V$  has a basis with  $d$  elements, we say  $\dim(V) = d$ . If no finite basis exists,  $V$  is *infinite-dimensional*.

Equip with topogloy for which addition and scalar multiplication are continuous, we get a *topological vector space*.

**Definition C.5** (Topological Vector Space). A *topological vector space* is a vector space  $V$  equipped with a topology  $\mathcal{T}$  for which addition and scalar multiplication are continuous. That is, for all  $v, w \in V$  and  $c \in \mathbb{R}$ ,

1.  $v + w \in V$  and  $cv \in V$ .
2. The maps  $+: V \times V \rightarrow V$  and  $\cdot: \mathbb{R} \times V \rightarrow V$  are continuous.

We can have multiple sources of topology on a vector space. For example, we can have equipped with metric distance. A particular type of distance is defined by a norm.

**Definition C.6** (Norm). A *norm* on a vector space  $V$  is a function  $\|\cdot\|: V \rightarrow \mathbb{R}$  satisfying the following axioms:

1. Non-negativity:  $\|v\| \geq 0$  for all  $v \in V$ .
2. Positive definiteness:  $\|v\| = 0$  if and only if  $v = 0$ .
3. Homogeneity:  $\|\lambda v\| = |\lambda| \|v\|$  for all  $\lambda \in \mathbb{R}$  and  $v \in V$ .
4. Triangle inequality:  $\|v + w\| \leq \|v\| + \|w\|$  for all  $v, w \in V$ .

A norm *respects* the vector space structure in all kinds of ways. The topology induced by a norm plays nice with the norm operations.

A normed vector space is a vector space equipped with a norm.

**Definition C.7** (Normed Vector Space). A *normed vector space* is a vector space  $V$  equipped with a norm  $\|\cdot\|$  and its topology induced by the norm.

Most structure encountered is inner product spaces.

**Definition C.8** (Inner Product). An *inner product* on a vector space  $V$  is a function  $\langle \cdot, \cdot \rangle: V \times V \rightarrow \mathbb{R}$  satisfying the following axioms:

1. Symmetry:  $\langle v, w \rangle = \langle w, v \rangle$  for all  $v, w \in V$ .
2. Linearity in the first argument:  $\langle \lambda v, w \rangle = \lambda \langle v, w \rangle$  for all  $\lambda \in \mathbb{R}$  and  $v, w \in V$ .
3. Positive definiteness:  $\langle v, v \rangle \geq 0$  for all  $v \in V$ .

An inner product space is a vector space equipped with an inner product. Any inner product space is a normed vector space with norm  $\|v\| = \sqrt{\langle v, v \rangle}$ .

In from introductory linear algebra courses, we are very familiar with a particular type of inner product space: the Euclidean space  $\mathbb{R}^d$ .

**Example C.9** (Euclidean Space). The *Euclidean space*  $\mathbb{R}^d$  is the vector space of  $d$ -dimensional vectors with the inner product  $\langle x, y \rangle = x^\top y$ . The Euclidean space has all kinds of nice properties. Linear algebra is that geometric intuition—angles, lengths, projections—can guide algebraic computation. It is where our intuition of dimension easily matches rigorous definitions.

Convexity.

One is that is a complete metric space (see Appendix A).

Its compact subsets are precisely the closed and bounded subsets (see Appendix A). Every linear operator between Euclidean spaces can be represented by a matrix. Matrices we can study very well: decompositions, inverse, eigenvalues, etc.

What is more, any finite dimensional vector space is ‘isomorphic’ to  $\mathbb{R}^d$  for some  $d$ . If the finite dimensional vector space is normed, its norm is equivalent to the Euclidean norm.

We will make all the properties precise Section C.1. ◇

Many spaces of interest in statistics are (subsets of) topological vector spaces, and many of these are infinite-dimensional. Some examples include:

- The space of square-integrable functions  $L^2(\mu)$  (see Chapter 2). This is a Hilbert space, essential for understanding the geometry of statistical models and concepts like differentiability in quadratic mean.
- The space of continuous functions  $C(K)$  on a compact set  $K$ . This space plays a central role in Chapter 4 via the Riesz–Markov theorem, allowing us to view priors as linear functionals.
- The space of finite signed measures  $\mathcal{M}(K)$ , which is the dual of  $C(K)$ . In decision theory, we often view the set of priors as a convex subset of this space.
- The space of integrable functions  $L^1(\mu)$ , which contains a set of probability densities.

Many of these spaces lose much of the nice structure that we are used to from finite-dimensional linear algebra.

## C.1 Finite dimensional vector spaces

**Definition C.10** (Loewner Order). Let  $A$  and  $B$  be symmetric matrices in  $\mathbb{R}^{d \times d}$ . We say that  $A$  is greater than or equal to  $B$  in the *Loewner order*, denoted by  $A \geq B$ , if the matrix  $A - B$  is positive semi-definite. That is, for all vectors  $v \in \mathbb{R}^d$ ,

$$v^\top (A - B)v \geq 0.$$

If  $A - B$  is positive definite, we write  $A > B$ .

**Theorem C.11** (Heine-Borel). *A subset of Euclidean space  $\mathbb{R}^n$  is compact if and only if it is closed and bounded.*

**Example C.12.** The Heine-Borel theorem does not hold in general metric spaces. For instance, consider the space  $C[0, 1]$  with the supremum metric. The closed unit ball  $B = \{f \in C[0, 1] : \|f\|_\infty \leq 1\}$  is closed and bounded, but it is not compact. The sequence of functions  $f_n(x) = x^n$  is in  $B$ , but it does not have a subsequence that converges uniformly to a continuous function (it converges pointwise to a discontinuous function).  $\diamond$

In  $\mathbb{R}^d$ , the following result is fundamental to convex analysis and optimization.

**Theorem C.13** (Separating Hyperplane Theorem in  $\mathbb{R}^d$ ). *Let  $A, B \subseteq \mathbb{R}^d$  be nonempty disjoint convex sets. Then there exists a nonzero vector  $a \in \mathbb{R}^d$  and a scalar  $c \in \mathbb{R}$  such that*

$$a^\top x \leq c \leq a^\top y \quad \text{for all } x \in A, y \in B.$$

*If  $A$  is closed,  $B$  is compact, and  $A \cap B = \emptyset$ , then strict separation holds: there exists  $\varepsilon > 0$  such that  $a^\top x \leq c - \varepsilon < c + \varepsilon \leq a^\top y$  for all  $x \in A, y \in B$ .*

The set  $\{z \in \mathbb{R}^d : a^\top z = c\}$  is a hyperplane separating  $A$  from  $B$ . This result has a clean proof in finite dimensions using the projection theorem: if  $A$  and  $B$  are closed with  $B$  compact, the continuous function  $(x, y) \mapsto \|x - y\|$  attains its minimum on  $A \times B$ , giving closest points  $x^* \in A$  and  $y^* \in B$ . The vector  $a = y^* - x^*$  defines the separating hyperplane.

## C.2 Functional analysis

Functional analysis extends linear algebra to infinite-dimensional spaces. We develop three fundamental results—the Hahn-Banach theorem, the Banach-Alaoglu theorem, and the Riesz representation theorem—each with direct applications the results in the course.

A *linear functional* on a vector space  $V$  is a linear map  $\varphi : V \rightarrow \mathbb{R}$ . In finite dimensions, every linear functional on  $\mathbb{R}^d$  has the form  $\varphi(x) = a^\top x$  for some  $a \in \mathbb{R}^d$ . In infinite dimensions, the situation is more subtle.

**Definition C.14** (Dual Space). The *algebraic dual* of a vector space  $V$  is the vector space  $V^*$  of all linear functionals on  $V$ . If  $V$  is a normed space, the *topological dual* (or simply *dual*) is the space  $V'$  of all *bounded* (equivalently, continuous) linear functionals, equipped with the operator norm

$$\|\varphi\| = \sup_{\|x\| \leq 1} |\varphi(x)|.$$

Boundedness and continuity coincide for linear functionals:  $\varphi$  is continuous if and only if  $\|\varphi\| < \infty$ . In infinite dimensions, unbounded linear functionals exist but require the axiom of choice to construct; we focus on bounded functionals.

### C.2.1 The Hahn-Banach theorem

The Hahn-Banach theorem guarantees that linear functionals can be extended from subspaces to the whole space without increasing the norm. It is the foundation for duality arguments throughout functional analysis.

**Theorem C.15** (Hahn-Banach, Analytic Form). *Let  $V$  be a real vector space and  $p : V \rightarrow \mathbb{R}$  a sublinear functional, i.e.,*

1.  $p(\alpha x) = \alpha p(x)$  for all  $\alpha \geq 0$  and  $x \in V$ ,
2.  $p(x + y) \leq p(x) + p(y)$  for all  $x, y \in V$ .

*Let  $M \subseteq V$  be a subspace and  $\varphi : M \rightarrow \mathbb{R}$  a linear functional satisfying  $\varphi(x) \leq p(x)$  for all  $x \in M$ . Then there exists a linear extension  $\tilde{\varphi} : V \rightarrow \mathbb{R}$  with  $\tilde{\varphi}|_M = \varphi$  and  $\tilde{\varphi}(x) \leq p(x)$  for all  $x \in V$ .*

*Proof sketch.* The proof proceeds in two steps. First, one shows that  $\varphi$  can be extended by one dimension: if  $x_0 \notin M$ , there exists  $c \in \mathbb{R}$  such that extending  $\varphi$  to  $M + \mathbb{R}x_0$  by  $\tilde{\varphi}(m + tx_0) = \varphi(m) + tc$  preserves the bound  $\tilde{\varphi} \leq p$ . The constraint on  $c$  is

$$\sup_{m \in M} (\varphi(m) - p(m + x_0)) \leq c \leq \inf_{m' \in M} (p(m' + x_0) - \varphi(m')),$$

and sublinearity of  $p$  ensures this interval is nonempty. Second, Zorn's lemma (a version of the axiom of choice) extends this one-dimensional argument to the whole space: the collection of all extensions of  $\varphi$  dominated by  $p$  is partially ordered by extension, and every chain has an upper bound, so a maximal element exists. Maximality forces the domain to be all of  $V$ .  $\square$

**Corollary C.16** (Extension of Bounded Functionals). *Let  $V$  be a normed space,  $M \subseteq V$  a subspace, and  $\varphi : M \rightarrow \mathbb{R}$  a bounded linear functional. Then there exists a bounded linear extension  $\tilde{\varphi} : V \rightarrow \mathbb{R}$  with  $\|\tilde{\varphi}\| = \|\varphi\|$ .*

*Proof.* Apply Theorem C.15 with  $p(x) = \|\varphi\|_M \cdot \|x\|$ , where  $\|\varphi\|_M = \sup_{\|m\| \leq 1, m \in M} |\varphi(m)|$ . The extension  $\tilde{\varphi}$  satisfies  $|\tilde{\varphi}(x)| \leq \|\varphi\|_M \|x\|$  for all  $x \in V$ , so  $\|\tilde{\varphi}\| \leq \|\varphi\|_M$ . The reverse inequality is immediate since  $\tilde{\varphi}$  extends  $\varphi$ .  $\square$

**Theorem C.17** (Hahn-Banach, Geometric Form). *Let  $V$  be a real topological vector space,  $A, B \subseteq V$  nonempty disjoint convex sets with  $A$  open. Then there exists a continuous linear functional  $\varphi : V \rightarrow \mathbb{R}$  and  $c \in \mathbb{R}$  such that*

$$\varphi(a) < c \leq \varphi(b) \quad \text{for all } a \in A, b \in B.$$

**Corollary C.18** (Strict Separation). *Let  $V$  be a locally convex topological vector space,  $A \subseteq V$  compact and convex, and  $B \subseteq V$  closed and convex, with  $A \cap B = \emptyset$ . Then there exists a continuous linear functional  $\varphi : V \rightarrow \mathbb{R}$  and  $c_1 < c_2$  such that*

$$\varphi(a) < c_1 < c_2 < \varphi(b) \quad \text{for all } a \in A, b \in B.$$

## C.2.2 The Banach-Alaoglu theorem

In  $\mathbb{R}^d$ , the Heine-Borel theorem characterizes compact sets: a subset of  $\mathbb{R}^d$  is compact if and only if it is closed and bounded. In particular, the closed unit ball  $\{x \in \mathbb{R}^d : \|x\| \leq 1\}$  is compact. This fails dramatically in infinite dimensions.

**Proposition C.19.** *The closed unit ball in an infinite-dimensional normed space is not compact in the norm topology.*

*Proof sketch.* Let  $V$  be infinite-dimensional. One can construct a sequence  $(x_n)$  in the unit ball with  $\|x_n - x_m\| \geq 1$  for all  $n \neq m$  (e.g., using Riesz's lemma). Such a sequence has no convergent subsequence, so the unit ball is not sequentially compact, hence not compact.  $\square$

The failure of compactness is a serious obstacle: many existence arguments rely on extracting convergent subsequences from bounded sets. The Banach-Alaoglu theorem recovers compactness by using a weaker topology.

### Weak and Weak\* Topologies

The norm topology on an infinite-dimensional space has “too many” open sets for the unit ball to be compact. Coarser topologies—those with fewer open sets—can restore compactness while preserving enough structure for analysis.

**Definition C.20** (Weak Topology). The *weak topology* on a normed space  $V$  is the coarsest topology making every bounded linear functional  $\varphi \in V'$  continuous. A sequence  $(x_n)$  converges weakly to  $x$ , written  $x_n \rightharpoonup x$ , if and only if

$$\varphi(x_n) \rightarrow \varphi(x) \quad \text{for all } \varphi \in V'.$$

**Definition C.21** (Weak\* Topology). The *weak\* topology* on the dual space  $V'$  is the coarsest topology making every evaluation functional  $\text{ev}_x : \varphi \mapsto \varphi(x)$  continuous for  $x \in V$ . A sequence  $(\varphi_n)$  converges weak\* to  $\varphi$ , written  $\varphi_n \xrightarrow{w^*} \varphi$ , if and only if

$$\varphi_n(x) \rightarrow \varphi(x) \quad \text{for all } x \in V.$$

The weak\* topology on  $V'$  is generally coarser than the weak topology on  $V'$ , which is coarser than the norm topology. In finite dimensions all three coincide, but in infinite dimensions the distinctions are crucial.

**Proposition C.22.** *Let  $V$  be a normed space.*

1. *Norm convergence implies weak convergence:  $\|x_n - x\| \rightarrow 0$  implies  $x_n \rightharpoonup x$ .*
2. *The converse fails in infinite dimensions.*
3. *Weakly convergent sequences are norm-bounded (uniform boundedness principle).*
4. *The norm is weakly lower semicontinuous: if  $x_n \rightharpoonup x$ , then  $\|x\| \leq \liminf_n \|x_n\|$ .*

*Remark C.23* (Terminological Warning). In probability theory, “weak convergence” of measures  $\mu_n \rightarrow \mu$  means  $\int f d\mu_n \rightarrow \int f d\mu$  for all bounded continuous  $f$ . This is weak\* convergence in the functional-analytic sense: measures are elements of  $C_b(\mathcal{X})'$ , and the convergence tests against elements of  $C_b(\mathcal{X})$ . The terminology is unfortunate.

**Theorem C.24** (Banach-Alaoglu). *Let  $V$  be a normed space. The closed unit ball*

$$B_{V'} = \{\varphi \in V' : \|\varphi\| \leq 1\}$$

*is compact in the weak\* topology.*

*Proof sketch.* For each  $x \in V$ , the set of possible values  $\{\varphi(x) : \varphi \in B_{V'}\}$  is contained in the interval  $[-\|x\|, \|x\|]$ . Define the product space

$$P = \prod_{x \in V} [-\|x\|, \|x\|].$$

By Tychonoff’s theorem,  $P$  is compact in the product topology. There is a natural embedding  $\iota : B_{V'} \rightarrow P$  given by  $\iota(\varphi) = (\varphi(x))_{x \in V}$ . One verifies:

1. The map  $\iota$  is injective (functionals are determined by their values).
2. The weak\* topology on  $B_{V'}$  coincides with the subspace topology inherited from  $P$ .
3. The image  $\iota(B_{V'})$  is closed in  $P$  (limits of linear functionals are linear).

Since  $\iota(B_{V'})$  is a closed subset of a compact space, it is compact. □

The use of Tychonoff's theorem (which is equivalent to the axiom of choice) is essential.

*Remark C.25 (Why Weak\*, Not Weak?).* The theorem concerns the weak\* topology, not the weak topology on  $V'$ . The weak topology on  $V'$  uses functionals from the bidual  $V''$ , which may be strictly larger than  $V$ . For non-reflexive spaces, the unit ball of  $V'$  is *not* weakly compact in general.

**Corollary C.26.** *For any  $r > 0$ , the ball  $\{\varphi \in V' : \|\varphi\| \leq r\}$  is weak\* compact.*

## C.3 The Riesz representation theorem

In  $\mathbb{R}^d$  with the standard inner product, every linear functional has a simple form.

**Proposition C.27.** *Every linear functional  $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}$  can be written as  $\varphi(x) = \langle x, y \rangle$  for a unique  $y \in \mathbb{R}^d$ . Moreover, if we equip  $\mathbb{R}^d$  with the Euclidean norm, then  $\|\varphi\| = \|y\|$ .*

*Proof.* Define  $y = (\varphi(e_1), \dots, \varphi(e_d))^T$  where  $e_i$  are the standard basis vectors. By linearity,  $\varphi(x) = \sum_{i=1}^d x_i \varphi(e_i) = \langle x, y \rangle$ . For the norm equality, Cauchy-Schwarz gives  $|\varphi(x)| = |\langle x, y \rangle| \leq \|x\| \|y\|$ , so  $\|\varphi\| \leq \|y\|$ . Equality is attained at  $x = y/\|y\|$ . □

This says  $(\mathbb{R}^d)' \cong \mathbb{R}^d$ : the dual space is isometrically isomorphic to the original space. The Riesz representation theorem extends this to infinite-dimensional Hilbert spaces.

### Hilbert Spaces

**Definition C.28 (Hilbert Space).** A *Hilbert space* is a complete inner product space: a vector space  $H$  with inner product  $\langle \cdot, \cdot \rangle$  such that the induced norm  $\|x\| = \sqrt{\langle x, x \rangle}$  makes  $H$  a complete metric space (every Cauchy sequence converges).

Completeness is automatic in finite dimensions but must be verified in infinite dimensions. The verification is often nontrivial.

**Example C.29.** The following are Hilbert spaces:

1.  $\mathbb{R}^d$  with  $\langle x, y \rangle = x^T y$ .

2.  $\ell^2 = \{(x_n)_{n=1}^\infty : \sum_{n=1}^\infty x_n^2 < \infty\}$  with  $\langle x, y \rangle = \sum_{n=1}^\infty x_n y_n$ .

3.  $L^2(\mu)$  for any measure  $\mu$ , with  $\langle f, g \rangle = \int fg d\mu$ .

The space  $C[0, 1]$  with the  $L^2$  inner product is *not* complete: Cauchy sequences of continuous functions can converge to discontinuous limits in  $L^2$ .  $\diamond$

Hilbert spaces admit orthogonal projections onto closed subspaces, just as in finite dimensions.

**Theorem C.30** (Projection Theorem). *Let  $H$  be a Hilbert space and  $M \subseteq H$  a closed subspace. For every  $x \in H$ , there exists a unique  $\hat{x} \in M$  such that*

$$\|x - \hat{x}\| = \inf_{m \in M} \|x - m\|.$$

The minimizer  $\hat{x}$  is characterized by the orthogonality condition:  $(x - \hat{x}) \perp M$ , i.e.,  $\langle x - \hat{x}, m \rangle = 0$  for all  $m \in M$ .

*Proof.* Let  $d = \inf_{m \in M} \|x - m\|$  and choose a minimizing sequence  $(m_n)$  in  $M$  with  $\|x - m_n\| \rightarrow d$ . The parallelogram law states

$$\|u + v\|^2 + \|u - v\|^2 = 2\|u\|^2 + 2\|v\|^2$$

for all  $u, v$  in an inner product space. Applying this to  $u = x - m_n$  and  $v = x - m_k$ :

$$\|m_n - m_k\|^2 = 2\|x - m_n\|^2 + 2\|x - m_k\|^2 - 4\left\|x - \frac{m_n + m_k}{2}\right\|^2.$$

Since  $(m_n + m_k)/2 \in M$ , we have  $\|x - (m_n + m_k)/2\| \geq d$ , so

$$\|m_n - m_k\|^2 \leq 2\|x - m_n\|^2 + 2\|x - m_k\|^2 - 4d^2 \rightarrow 0$$

as  $n, k \rightarrow \infty$ . Thus  $(m_n)$  is Cauchy. By completeness of  $H$ , it converges to some  $\hat{x}$ ; since  $M$  is closed,  $\hat{x} \in M$ .

For the orthogonality condition: if  $\langle x - \hat{x}, m \rangle \neq 0$  for some  $m \in M$  with  $\|m\| = 1$ , then for  $t = \langle x - \hat{x}, m \rangle$ ,

$$\|x - (\hat{x} + tm)\|^2 = \|x - \hat{x}\|^2 - 2t\langle x - \hat{x}, m \rangle + t^2 = \|x - \hat{x}\|^2 - t^2 < \|x - \hat{x}\|^2,$$

contradicting minimality. Uniqueness follows from strict convexity of the norm.  $\square$

The map  $P_M : H \rightarrow M$  sending  $x$  to  $\hat{x}$  is the *orthogonal projection* onto  $M$ . It is linear, satisfies  $P_M^2 = P_M$  (idempotent), and  $\langle P_M x, y \rangle = \langle x, P_M y \rangle$  (self-adjoint).

*Remark C.31.* The hypothesis that  $M$  is closed is essential. If  $M$  is not closed, the infimum need not be attained. For instance, in  $L^2[0, 1]$ , the subspace of polynomials is dense but not closed; for generic  $f \in L^2[0, 1]$ , no polynomial achieves the infimal distance.

### The Theorem

**Theorem C.32** (Riesz Representation). *Let  $H$  be a Hilbert space. For every bounded linear functional  $\varphi : H \rightarrow \mathbb{R}$ , there exists a unique  $y \in H$  such that*

$$\varphi(x) = \langle x, y \rangle \quad \text{for all } x \in H.$$

Moreover,  $\|\varphi\| = \|y\|$ .

*Proof.* If  $\varphi = 0$ , take  $y = 0$ . Otherwise, the kernel  $M = \ker(\varphi) = \{x \in H : \varphi(x) = 0\}$  is a closed subspace (closed because  $\varphi$  is continuous, a subspace by linearity). Since  $\varphi \neq 0$ , the kernel  $M$  is proper.

The orthogonal complement  $M^\perp = \{z \in H : \langle z, m \rangle = 0 \text{ for all } m \in M\}$  is nonzero. We claim  $\dim(M^\perp) = 1$ . Indeed,  $\varphi$  maps  $M^\perp$  into  $\mathbb{R}$  with kernel  $M^\perp \cap M = \{0\}$ , so  $\varphi|_{M^\perp}$  is injective; since  $\varphi$  is surjective onto  $\mathbb{R}$  and  $M^\perp$  injects into  $\mathbb{R}$ , we have  $\dim(M^\perp) = 1$ .

Choose  $z \in M^\perp$  with  $\varphi(z) = 1$  (possible by rescaling any nonzero element of  $M^\perp$ ). Every  $x \in H$  decomposes as  $x = (x - \varphi(x)z) + \varphi(x)z$ . Since  $\varphi(x - \varphi(x)z) = \varphi(x) - \varphi(x) = 0$ , we have  $x - \varphi(x)z \in M$ , hence

$$\langle x, z \rangle = \langle x - \varphi(x)z, z \rangle + \varphi(x)\langle z, z \rangle = 0 + \varphi(x)\|z\|^2.$$

Thus  $\varphi(x) = \langle x, z/\|z\|^2 \rangle$ . Taking  $y = z/\|z\|^2$  gives the representation.

For the norm equality:  $|\varphi(x)| = |\langle x, y \rangle| \leq \|x\|\|y\|$  by Cauchy-Schwarz, so  $\|\varphi\| \leq \|y\|$ . Equality is attained at  $x = y/\|y\|$ :  $\varphi(y/\|y\|) = \langle y, y \rangle/\|y\| = \|y\|$ .

Uniqueness: if  $\langle x, y \rangle = \langle x, y' \rangle$  for all  $x$ , then  $\langle x, y - y' \rangle = 0$  for all  $x$ ; taking  $x = y - y'$  gives  $\|y - y'\|^2 = 0$ .  $\square$

The Riesz representation theorem establishes that  $H' \cong H$  isometrically: every Hilbert space is isomorphic to its own dual. This self-duality is a defining feature of Hilbert spaces and fails for other Banach spaces. For instance,  $(L^1)' \cong L^\infty$  but  $L^1 \not\cong L^\infty$ .

**Corollary C.33** (Reflexivity of Hilbert Spaces). *Every Hilbert space is reflexive: the natural embedding  $J : H \rightarrow H''$  is surjective.*

*Proof.* By Riesz representation,  $H' \cong H$  and  $H'' \cong H' \cong H$ . The natural embedding  $J$  composed with these isomorphisms is the identity.  $\square$

For general Banach spaces, the dual need not be isomorphic to the original space. Nevertheless, concrete dualities exist. For instance, given a  $\sigma$ -finite measure space  $(\Omega, \mathcal{A}, \mu)$ , the dual of  $L^1(\Omega, \mathcal{A}, \mu)$  is  $L^\infty(\Omega, \mathcal{A}, \mu)$ : every bounded linear functional on  $L^1$  is integration against some  $L^\infty$  function.

**Proposition C.34.** *Let  $(\Omega, \mathcal{A}, \mu)$  be a  $\sigma$ -finite measure space. For every bounded linear functional  $\varphi : L^1(\Omega, \mathcal{A}, \mu) \rightarrow \mathbb{R}$ , there exists a unique  $g \in L^\infty(\Omega, \mathcal{A}, \mu)$  such that*

$$\varphi(f) = \int_{\Omega} fg \, d\mu \quad \text{for all } f \in L^1(\Omega, \mathcal{A}, \mu).$$

Moreover,  $\|\varphi\| = \|g\|_\infty$ .

A similar duality identifies the dual of  $C(K)$ —the space of continuous functions on a compact metric space—with the space of signed Radon measures  $\mathcal{M}(K)$ . Unlike Hilbert spaces,  $C(K)$  is not reflexive:  $\mathcal{M}(K)$  is a much larger space than  $C(K)$ . Nevertheless, the duality  $C(K)' \cong \mathcal{M}(K)$  is equally concrete: every continuous linear functional on  $C(K)$  is integration against some measure.

**Theorem C.35** (Riesz–Markov). *Let  $K$  be a compact metric space. For every bounded linear functional  $\varphi : C(K) \rightarrow \mathbb{R}$ , there exists a unique signed Radon measure  $\mu$  on  $(K, \mathcal{B}(K))$  such that*

$$\varphi(f) = \int_K f \, d\mu \quad \text{for all } f \in C(K).$$

Moreover,  $\|\varphi\| = |\mu|(K)$ , where  $|\mu|$  denotes the total variation of  $\mu$ .

*Proof.* See Rudin 1991, Chapter 2.  $\square$

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