MATH 598

Bayesian Inference, Computational Methods and Monte Carlo

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Introduction

The objective of a statistical analysis is to use data to make *optimal* and *coherent* decisions, including

- *inference*: making statements about the unknown data generating mechanism;
- *prediction*: making statements about as yet unobserved ('future') data,

whilst appropriately representing the uncertainty associated with these decisions.

Typically, the analysis is based on a probabilistic (or statistical) model.

Notation and Basic Concepts

Let Y denote a single random variable taking values on $\mathcal{Y} \subseteq \mathbb{R}$.

- Y records the result of some measurement procedure;
- $\mathcal{Y}$ could be countable (so that Y is 'discrete').

Let y denote an observed value associated with Y.

Notation and Basic Concepts

A *probability model* for Y is encapsulated in a *probability function*, $P_Y(.)$, where (informally) for set $A \subseteq \mathbb{R}$,

$$P_Y(A) \equiv \Pr[Y \in A]$$

and more specifically

$$P_Y\left(\ (-\infty, c]\ \right) \equiv \Pr[Y \leqslant c].$$

We define the *distribution function*, $F_Y(.)$, via the specification

$$F_Y(c) \equiv P_Y\left(\ (-\infty, c]\ \right) = \Pr[Y \leqslant c] \qquad c \in \mathbb{R}.$$

Notation and Basic Concepts

If Y is *discrete*, then

$$\mathcal{Y} = \{y_1^*, y_2^*, \ldots, \}$$

and for any $y \in \mathbb{R}$, we have

$$F_Y(y) = \sum_{j:y_j^* \leqslant y} \Pr[Y = y_j^*] = \sum_{j:y_j^* \leqslant y} p_Y(y_j^*)$$

say, where

$$p_Y(y_j^*) = \Pr[Y = y_j^*]$$

is the *probability mass function* (pmf) for Y.

Notation and Basic Concepts

If we can write

$$F_Y(y) = \int_{-\infty}^{y} f_Y(t)\, dt \qquad y \in \mathbb{R}$$

then we term F_Y an *absolutely continuous distribution*, with

$$f_Y(y)$$

termed the *probability density function* (pdf) for Y. In this case

$$f_Y(y) = \left. \frac{dF_Y(t)}{dt} \right|_{t=y}$$

Note: more generally a distribution can have both discrete and continuous components.

Notation and Basic Concepts

For simplicity we can unify notation for the discrete and continuous cases by writing

$$\Pr(Y \in A) = \int_A F_Y(dy) \equiv \begin{cases} \sum_{y \in A} p_Y(y) & Y \text{ discrete} \\ \int_A f_Y(y)\, dy & Y \text{ continuous} \end{cases}$$

The notation

$$\Pr(Y \in A) = \int_A dF_Y(y)$$

is also used.

Notation and Basic Concepts

In practice, we observe data ('*observables*')

$$y_1, \ldots, y_n$$

and use them to learn about the unknown ('*unobservable*') model P_Y or F_Y, or features of it such as its expectation

$$\theta = \int y \; F_Y(dy)$$

That is, it is the distribution F_Y that is unknown.

Notation and Basic Concepts

The data are realizations of random variables $Y_1, \ldots, Y_n$, and we have observed the event

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \in \{y_i\})\right].$$

This is a *joint* probability, so we need to consider the *joint probability model*

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \in A_i)\right]$$

for arbitrary subsets $A_1, \ldots, A_n$ of $\mathbb{R}$.

Notation and Basic Concepts

Specifically, we consider the *joint cdf*

$$F_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n) = \Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\right] \qquad (y_1,\ldots,y_n) \in \mathbb{R}^n$$

or quantities derived from it (*joint pdf* etc).

Notation and Basic Concepts

A typical assumption is that $Y_1, \ldots, Y_n$ are *independent*, that is that for all $(y_1, \ldots, y_n) \in \mathbb{R}^n$

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\right] = \prod_{i=1}^{n} \Pr\left[Y_i \leqslant y_i\right]$$

so that

$$F_{Y_1,\ldots,Y_n}(y_1, \ldots, y_n) = \prod_{i=1}^{n} F_{Y_i}(y_i).$$

Notation and Basic Concepts

Further, it is often assumed that the $Y_1, \ldots, Y_n$ are *identically distributed*

$$F_{Y_1,\ldots,Y_n}(y_1, \ldots, y_n) = \prod_{i=1}^{n} F_Y(y_i).$$

However, these are quite strong assumptions.

Notation and Basic Concepts

A weaker assumption is that of *infinite exchangeability*: we consider an infinite sequence

$$Y_1, Y_2, Y_3, \ldots$$

for which, for all $n \geqslant 1$ and sets $A_1, \ldots, A_n$ we have that

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \in A_i)\right] = \Pr\left[\bigcap_{i=1}^{n}(Y_i \in A_{\sigma(i)})\right]$$

for all permutations $(\sigma_{(1)}, \ldots, \sigma_{(n)})$ of indices $(1, \ldots, n)$.

Notation and Basic Concepts

$n = 2$:

$$\Pr\left[(Y_1 \leqslant y_1) \cap (Y_2 \leqslant y_2)\right] = \Pr\left[(Y_1 \leqslant y_2) \cap (Y_2 \leqslant y_1)\right]$$

$n = 3$:

$$\begin{aligned}
&\Pr\left[(Y_1 \leqslant y_1) \cap (Y_2 \leqslant y_2) \cap (Y_3 \leqslant y_3)\right] \\
&\qquad = \Pr\left[(Y_1 \leqslant y_2) \cap (Y_2 \leqslant y_1) \cap (Y_3 \leqslant y_3)\right] \\
&\qquad = \Pr\left[(Y_1 \leqslant y_3) \cap (Y_2 \leqslant y_2) \cap (Y_3 \leqslant y_1)\right] \\
&\qquad = \Pr\left[(Y_1 \leqslant y_3) \cap (Y_2 \leqslant y_1) \cap (Y_3 \leqslant y_2)\right] \\
&\qquad = \cdots
\end{aligned}$$

Notation and Basic Concepts

For infinite exchangeability: need this kind of relationship

(a) to hold for any finite n drawn from the infinite sequence

(b) to respect marginalization conditions; that is

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\right]$$

must be compatible with

$$\Pr\left[\bigcap_{i=1}^{n+1}(Y_i \leqslant y_i)\right]$$

in the sense that

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\right] = \lim_{y_{n+1}\longrightarrow\infty} \Pr\left[\bigcap_{i=1}^{n+1}(Y_i \leqslant y_i)\right]$$

Example: Binary case

Suppose we have an infinitely exchangeable sequence $\{Y_n\}$, where for each i, $Y_i \in \{0, 1\}$. Consider for $n \geqslant 1$

$$\Pr[(Y_1 = y_1) \cap \cdots \cap (Y_n = y_n)]$$

which we may write in short

$$\Pr[Y_1 = y_1, \ldots, Y_n = y_n],$$

where we consider vector arguments

$$(y_1, \ldots, y_n) \in \{0, 1\}^n$$

Example: Binary case

Then under infinite exchangeability, we must have that

$$\Pr[Y_1 = y_1, \ldots, Y_n = y_n]$$

depends only on the value of

$$s_n = \sum_{i=1}^{n} y_i.$$

For each n, there are 2^n possible binary vectors of length n, but

$$s_n \in \{0, 1, \ldots, n\}$$

so there are a maximum of $(n + 1)$ different probabilities, although these probabilities must sum to 1.

Notation and Basic Concepts

Example: Binary case

- $n = 1$: $s_n \in \{0, 1\}$, so denote the probabilities $p_{1,0}$ and $p_{1,1}$, where we must have

$$p_{1,0} = 1 - p_{1,1}$$

Example: Binary case

- $n = 2$: $s_n \in \{0, 1, 2\}$, so denote the probabilities $p_{2,0}, p_{2,1}$ and $p_{2,2}$, where we must have that

$$p_{2,0} = 1 - p_{2,1} - p_{2,2}$$

but also due to marginalization that

$$\begin{aligned} p_{1,y_1} &= \Pr[Y_1 = y_1] \\ &= \Pr[Y_1 = y_1, Y_2 = 0] + \Pr[Y_1 = y_1, Y_2 = 1] \\ &= p_{2,y_1} + p_{2,y_1+1} \end{aligned}$$

for $y_1 \in \{0, 1\}$.

Example: Binary case

This construction be extended to define the required relations for any n.

However, to specify the distribution in this way, we need to specify and compute the relations for all n.

Example: Binary case

Assuming *independence*, we have

$$\Pr[Y_1 = y_1, \ldots, Y_n = y_n] = \prod_{i=1}^{n} \Pr[Y_i = y_i] = p^{s_n}(1-p)^{n-s_n}$$

where

$$p = \Pr[Y_i = y_i] \qquad i = 1, \ldots, n.$$

Conditional probability

For two events, E_1, E_2 with $P(E_2) > 0$, we have that

$$P(E_1|E_2) = \frac{P(E_1 \cap E_2)}{P(E_2)}$$

is the *conditional probability* for E_1 given E_2.

- $P(E_1)$ is the probability that E_1 occurs;
- $P(E_1|E_2)$ is the probability that E_1 occurs *if we have information* that E_2 occurs.
- *relative* to the probability of E_2, what is the probability that *both* E_1 and E_2 occur ?
- E_1 and E_2 are *independent* if and only if $P(E_1|E_2) = P(E_1)$

Conditional probability

For two events, E_1, E_2 with both $P(E_1) > 0$ and $P(E_2) > 0$, we have by the definition that

$$P(E_1|E_2) = \frac{P(E_2|E_1)P(E_1)}{P(E_2)}.$$

We know this result as *Bayes Theorem*.

Conditional probability

Exchangeability assumptions allow for *dependence*: that is, for example

$$\Pr[Y_{n+1} \in A_{n+1} | Y_1 = y_1, \ldots, Y_n = y_n]$$

does not reduce to

$$\Pr[Y_{n+1} \in A_{n+1}]$$

as in the independence case. That is, for all i and j, Y_i and Y_j are identically distributed, but not independent.

Conditional probability

Example: Infinitely exchangeable binary case

$$\begin{aligned}
&\Pr[Y_{n+1} = 1 | Y_1 = y_1, \ldots, Y_n = y_n] \\
&\qquad = \frac{\Pr[Y_1 = y_1, \ldots, Y_n = y_n, Y_{n+1} = 1]}{\Pr[Y_1 = y_1, \ldots, Y_n = y_n]} \\
&\qquad = \frac{p_{n+1, s_n + 1}}{p_{n, s_n}}
\end{aligned}$$

where

$$s_n = \sum_{i=1}^{n} y_i .$$

Conditional probability

Example: Independent binary case

$$
\begin{aligned}
&\Pr\left[Y_{n+1} = 1 \middle| Y_1 = y_1, \ldots, Y_n = y_n\right] \\
&\qquad = \frac{\Pr\left[Y_1 = y_1, \ldots, Y_n = y_n, Y_{n+1} = 1\right]}{\Pr\left[Y_1 = y_1, \ldots, Y_n = y_n\right]} \\
&\qquad = \frac{p^{s_n+1}(1-p)^{n-s_n}}{p^{s_n}(1-p)^{n-s_n}} \\
&\qquad = p \\
&\qquad = \Pr\left[Y_{n+1} = 1\right]
\end{aligned}
$$

Conditional probability

Note

It is possible to consider *finite exchangeability*, where the exchangeability holds for a *finite* collection of random variables, that is, for a *specific* $n \geqslant 1$

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\right] = \Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_{\sigma(i)})\right]$$

for all permutations $(\sigma_{(1)}, \ldots, \sigma_{(n)})$ of indices $(1, \ldots, n)$.

Inference and prediction

In *statistical* calculations

- we observe data $y_1, \ldots, y_n$ and wish to make statements about unknown quantities in light of the data;
- given the data, *what do we think about the model* ?

If F_Y is *known*, there is no *inference* problem, and prediction can be carried out via F_Y.

Inference and prediction

If F_Y is *unknown*, then it is the focus of our inference.

- we treat F_Y as an unknown, and make statements about it in light of the data;
- given the data, *what do we think about* F_Y ?

We treat F_Y as a *random variable*.

Inference and prediction

If F_Y is *unknown*, then an independent and identically distributed (IID) statement of the sort above is really a *conditional* statement given F_Y.

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\middle| F_Y\right] = \prod_{i=1}^{n} F_Y(y_i)$$

Inference and prediction

If F_Y is a random variable, we must be able to specify a probability distribution for it:

- in general, F_Y is an *infinite-dimensional* object;
- F_Y has certain specific properties.

Need the capability to build a probability distribution on the space of functions. $\mathcal{F}$ say, that satisfy the properties of distribution functions.

Parametric modelling

The most common approach involves using a *finite* dimensional '*parameter*', $\theta \in \mathbb{R}^d$ say, and specifying that

$$F_Y(y) \equiv F_Y(y;\theta) \qquad y \in \mathbb{R}$$

so that the unknown quantity is now θ, and $F_Y(.;\theta)$ is a *known functional form*. Then

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\middle|\theta\right] = \prod_{i=1}^{n} F_Y(y_i;\theta)$$

Non-parametric modelling

The *non-parametric* approach involves using an *infinite* dimensional parameter, the function $F_Y(.)$ itself. We write

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\middle| F_Y\right] = \prod_{i=1}^{n} F_Y(y_i)$$

Semi-parametric modelling

The *semi-parametric* approach involves using a model that is specified in terms of both

- a *finite* dimensional parameter, $\theta \in \mathbb{R}^d$
- an *infinite* dimensional parameter.

Example: Semi-parametric location model

The model

$$F_Y(y;\theta) \equiv F(y-\theta)$$

where $\theta \in \mathbb{R}$ and F is an arbitrary cdf is a semi-parametric location model for a univariate random variable Y.

Interest and nuisance parameters

We often partition parameters into two components

- *parameters of interest*: the focus of inference;
- *nuisance parameters*: parameters necessary for the specification of the probability model, but which are not the focus of interest.

In the parametric case, we might partition $\theta = (\psi, \lambda)$ where ψ is the parameter of interest.

In the semi-parametric case, the non-parametric component is usually regarded as nuisance parameter.

Interest and nuisance parameters

In the non-parametric case, inference focusses on F_Y itself, or possibly some functional of F_Y, for example the *expectation* of F_Y:

$$\mu(F_Y) = \mathbb{E}_Y[Y; F_Y] = \int y \; dF_Y(y) \equiv \int y \; F_Y(dy)$$

Part 1
Bayesian Theory

1.1 De Finetti's Representation

The first key result of Bayesian theory is a representation result for the probability distribution of infinitely exchangeable random variables.

- the theorem characterizes all possible forms for the distribution;
- it gives a straightforward mechanism for the construction of arbitrary distributions for infinitely exchangeable sequences;
- this result underpins the logic of Bayesian inference and prediction.

1.1 De Finetti's Representation

Theorem: 0-1 representation theorem

Suppose that $Y_1, Y_2, \ldots$ is an infinitely exchangeable sequence of 0-1 variables. Then there exists a distribution function $\pi_0(.)$ such that for all $n \geqslant 1$, the joint mass function of $(Y_1, Y_2, \ldots, Y_n)$ can be represented

$$p_{Y_1,Y_2,\ldots,Y_n}(y_1, y_2, \ldots, y_n) = \int_0^1 \left\{ \prod_{i=1}^{n} \theta^{y_i} (1-\theta)^{1-y_i} \right\} \pi_0(d\theta)$$

for some probability distribution $\pi_0(.)$.

de Finetti, Hewitt-Savage

1.1 De Finetti's Representation

Theorem: 0-1 representation theorem

Furthermore, $\pi_0(.)$ is defined for $0 \leqslant \theta \leqslant 1$ by

$$\int_0^{\theta} \pi_0 (dt) = \lim_{n \to \infty} \Pr [R_n \leqslant \theta] \qquad (\blacklozenge)$$

and where

$$S_n = \sum_{i=1}^{n} Y_i \qquad R_n = \frac{S_n}{n}.$$

1.1 De Finetti's Representation

Theorem: 0-1 representation theorem

We define

$$\theta_0 = \lim_{n \to \infty} R_n$$

that is, $R_n \xrightarrow{a.s.} \theta_0$; the quantity θ_0 is the limiting relative frequency of 1s in the infinitely exchangeable binary sequence.

Proof: See Handout 01.

Note

(i) The converse of the theorem is also true: it is straightforward to see that the distributions formed by computing the integral for a given $\pi_0(.)$ are finite dimensional distributions derived for an infinitely exchangeable sequence.

(ii) The quantity θ parameterizes the conditional distribution of the Y_i; we can interpret

$$\prod_{i=1}^{n} \theta^{y_i} (1-\theta)^{1-y_i} = \prod_{i=1}^{n} p_{Y_i}(y_i;\theta)$$

and deduce that for each n, $Y_1, \ldots, Y_n$ are *conditionally independent* given θ.

Note

(iii) The quantity θ parameterizes the conditional distribution of the Y_i; we can interpret

$$\prod_{i=1}^{n} \theta^{y_i} (1-\theta)^{1-y_i} = \prod_{i=1}^{n} p_{Y_i}(y_i;\theta)$$

and deduce that for each n, $Y_1, \ldots, Y_n$ are *conditionally independent* given θ.

Note

(iv) $\pi_0(.)$ is a probability distribution for θ, but the generality of the construction *does not specify* what form $\pi_0(d\theta)$ should take; different choices for $\pi_0(.)$ will lead to different exchangeable forms.

(v) We often relax notation and allow $\pi_0(.)$ to denote either the cdf or the pdf whenever convenient to do so.

1.1 De Finetti's Representation

The theorem extends to arbitrary infinitely exchangeable sequences.

Theorem: General representation theorem

Suppose that

- $Y_1, Y_2, \ldots$ is an infinitely exchangeable sequence of variables taking values on $\mathbb{R}$;
- P_Y is a probability measure on $\mathbb{R}^\infty$ that defines all finite dimensional distributions for $\{Y_n\}_{n=1}^\infty$;
- $\mathcal{F}$ denotes the set of all distribution functions on $\mathbb{R}$.

Theorem: General representation theorem

Then there exists a distribution function $\pi_0(.)$ on $\mathcal{F}$, such that the joint distribution of $(Y_1, Y_2, \ldots, Y_n)$ has the form

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\right] = \int_{\mathcal{F}} \left\{\prod_{i=1}^{n} F(y_i)\right\} \pi_0(dF)$$

where F parameterizes the model: F is an unobservable distribution function.

1.1 De Finetti's Representation

Theorem: General representation theorem

We interpret F via its limiting form; let F_0 be a distribution function defined for $y \in \mathbb{R}$ by

$$F_0(y) = \lim_{n\to\infty} F_n(y) = \lim_{n\to\infty} \left\{ \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{(-\infty,y]}(Y_i) \right\}$$

is a distribution on the space of functions $\mathcal{F}$, defined as a limit as $n \longrightarrow \infty$ of the *empirical distribution function*, F_n, defined for $Y_1, \ldots, Y_n$.

Note

(i) The unknown distribution F parameterizes the conditional distribution of the Y_i;

$$\prod_{i=1}^{n} F(y_i)$$

indicates that for each n, $Y_1, \ldots, Y_n$ are *conditionally independent* given F.

(ii) $\pi_0(.)$ is a probability distribution for F; that is, it is a probability distribution on the space $\mathcal{F}$ of distribution functions. Calculations require (Lebesgue) integrals over $\mathcal{F}$ taken with respect to π_0.

Note

(iii) F_0 is the *limiting empirical distribution function*:

- classical results tell us that this limiting distribution can be interpreted as the *true* marginal distribution function for the Y_i;
- the limiting form does not tell us about the joint structure of the Y_i.

(iv) $\pi_0(.)$ is a probability distribution for F; therefore it is a probability distribution on the space $\mathcal{F}$ of distribution functions.

Note

(v) F_n is the *empirical distribution function*:

- this is the classical estimator of the distribution function based on $Y_1, \ldots, Y_n$;
- pointwise behaviour (at each individual y) easy to study;
- function-wise behaviour (at all y simultaneously) requires *empirical process theory*.

1.1 De Finetti's Representation

The general representation theorem can be made specific by

- imposing *symmetry* or *invariance constraints* on the observables;
- requiring the existence of *sufficient statistics*;
  - the *exponential family*.
- allowing for *partial exchangeability* to construct conditional forms of exchangeable sequences
  - *regression*, *hierarchical models* etc.

These considerations lead to the use of specific *parametric* models.

Example: Partial exchangeability

Let $\{O_n\}_{n=1}^{\infty}$ be an infinitely exchangeable sequence of random vectors in $\mathbb{R}^2$

$$O_i = (X_i, Y_i) \qquad i = 1, 2, \ldots.$$

Then

- $\{X_n\}_{n=1}^{\infty}$ is also an infinitely exchangeable sequence;
- for each $n \geqslant 1$, and *given* $X_1 = x_1, \ldots, X_n = x_n$, the variables

  $$Y_1, \ldots, Y_n$$

  are *partially exchangeable*.

1.1 De Finetti's Representation

A typical form of the de Finetti representation is in terms of parametric densities: for $n \geqslant 1$

$$f_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n) = \int \prod_{i=1}^{n} f(y_i;\theta)\, \pi_0\,(d\theta)$$

where

$$f_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n)$$

is the *joint pdf* for $Y_1,\ldots,Y_n$.

Note

The de Finetti calculation is a standard type of '*marginalization*' calculation; for example, for two continuous random variables

$$f_Y(y) = \int f_{Y|X}(y|x) f_X(x)\, dx.$$

We can think of $f_X(x)$ as a '*mixing*' distribution.

In the de Finetti representation, the two random variables are

- the observables $Y_1, \ldots, Y_n$;
- the 'parameter' θ or F.

Note

The terms

$$\prod_{i=1}^{n} p_{Y_i}(y_i;\theta) \qquad \text{or} \qquad \prod_{i=1}^{n} f_{Y_i}(y_i;\theta)$$

in parametric case, or in the non-parametric case

$$\prod_{i=1}^{n} F(y_i)$$

are equivalent to the familiar *likelihood function* that forms the basis of much statistical theory.

Prediction

The assumption of infinite exchangeability and the de Finetti representation give an automatic rule for constructing predictions. For $n, m \geqslant 1$ consider the prediction of

$$Y_{n+1}, \ldots, Y_{n+m}$$

conditional on observed values of

$$Y_1, \ldots, Y_n.$$

We focus first on the binary case for simplicity.

Prediction

By de Finetti, recall that for each $n \geqslant 1$

$$p_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n) = \int_0^1 \left\{ \prod_{i=1}^{n} \theta^{y_i} (1-\theta)^{1-y_i} \right\} \pi_0(d\theta) \qquad (\S)$$

Prediction

Similarly

$$p_{Y_1,\ldots,Y_{n+m}}\left(y_1,\ldots,y_{n+m}\right)=\int_0^1\left\{\prod_{i=1}^{n+m}\theta^{y_i}\left(1-\theta\right)^{1-y_i}\right\}\pi_0\left(d\theta\right)$$

Prediction

Then for the *predictive* distribution, by the conditional probability definition, we have

$$p_{Y_{n+1},\ldots,Y_{n+m}|Y_1,\ldots,Y_n}\left(y_{n+1},\ \ldots,y_{n+m}|y_1,\ldots,y_n\right)$$

$$= \frac{p_{Y_1,\ldots,Y_{n+m}}\left(y_1,\ldots,y_{n+m}\right)}{p_{Y_1,\ldots,Y_n}\left(y_1,\ldots,y_n\right)}$$

$$= \frac{\int_0^1 \left\{\prod_{i=1}^{n+m} \theta^{y_i}\left(1-\theta\right)^{1-y_i}\right\}\pi_0\left(d\theta\right)}{\int_0^1 \left\{\prod_{i=1}^{n} t^{y_i}\left(1-t\right)^{1-y_i}\right\}\pi_0\left(dt\right)}$$

where t is a dummy integrating variable.

Prediction

We may rewrite this expression by noting that the denominator can be treated as a constant in the integral in the numerator, and that the product in the numerator can be split

$$\prod_{i=1}^{n+m} \theta^{y_i} (1-\theta)^{1-y_i}$$

$$= \left\{ \prod_{i=1}^{n} \theta^{y_i} (1-\theta)^{1-y_i} \right\} \times \left\{ \prod_{i=n+1}^{n+m} \theta^{y_i} (1-\theta)^{1-y_i} \right\}.$$

Prediction

That is

$$p_{Y_{n+1},\ldots,Y_{n+m}|Y_1,\ldots,Y_n}\left(y_{n+1},\ \ldots,y_{n+m}\middle|y_1,\ldots,y_n\right)$$

$$= \int_0^1 \left\{ \prod_{i=n+1}^{n+m} \theta^{y_i} \left(1-\theta\right)^{1-y_i} \right\} \pi_n\left(d\theta\right) \qquad (\dagger)$$

where

$$\pi_n(d\theta) = \frac{\prod_{i=1}^{n} \theta^{y_i} \left(1-\theta\right)^{1-y_i} \pi_0\left(d\theta\right)}{\int_0^1 \left\{ \prod_{i=1}^{n} t^{y_i} \left(1-t\right)^{1-y_i} \right\} \pi_0\left(dt\right)} \qquad (\ddagger)$$

Prediction

Comparing (§) to (†), we see that the forms of the two representations for

$$p_{Y_1,\ldots,Y_n}\left(y_1,\ldots,y_n\right)$$

and

$$p_{Y_{n+1},\ldots,Y_{n+m}|Y_1,\ldots,Y_n}\left(y_{n+1},\ldots,y_{n+m}\middle|y_1,\ldots,y_n\right)$$

are *identical* with $\pi_0(d\theta)$ in the former replaced by $\pi_n(d\theta)$ in the latter.

Prediction

We can therefore think of

$$\pi_n(d\theta)$$

as being an *updated* version of

$$\pi_0(d\theta)$$

in light of observing $y_1, \ldots, y_n$. Note that

$$\int \pi_n(d\theta) = 1$$

from (‡), so $\pi_n(d\theta)$ does define a *valid probability distribution*.

Terminology

- $\pi_0(d\theta)$ is the *prior distribution* for θ;
- $\pi_n(d\theta)$ is the *posterior distribution* for θ;
- $p_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n)$ is the *prior predictive distribution*
  - also termed the *marginal likelihood*;
- $p_{Y_{n+1},\ldots,Y_{n+m}|Y_1,\ldots,Y_n}(y_{n+1},\ldots,y_{n+m}|y_1,\ldots,y_n)$ is the *posterior predictive distribution*.

Limiting predictions

Let

$$S_{1,n} = \sum_{i=1}^{n} Y_i \qquad\qquad S_{n+1,n+m} = \sum_{i=n+1}^{n+m} Y_i$$

By direct calculation from (§), by the theorem of total probability, we have

$$\Pr[S_{1,n} = s_{1,n}] = \binom{n}{s_{1,n}} \int_0^1 t^{s_{1,n}} (1-t)^{n-s_{1,n}} \, \pi_0(dt)$$

using t as the integrating variable; this holds for

$$s_{1,n} \in \{0, 1, \ldots, n\}.$$

Limiting predictions

Note from (‡) that $\pi_n(d\theta)$ depends on the data $y_1, \ldots, y_n$ only via

$$s_{1,n} = \sum_{i=1}^{n} y_i$$

as

$$\pi_n(d\theta) = \frac{\theta^{s_{1,n}} (1-\theta)^{n-s_{1,n}} \pi_0(d\theta)}{\int_0^1 t^{s_{1,n}} (1-t)^{n-s_{1,n}} \pi_0(dt)}$$

Thus we can interpret $S_{1,n}$ as a (Bayesian) *sufficient statistic*.

Limiting predictions

Therefore for $s \in \{0, 1, \ldots, m\}$,

$$\Pr[S_{n+1,n+m} = s | S_{1,n} = s_{1,n}]$$

$$= \binom{m}{s} \int_0^1 t^s (1-t)^{m-s} \, \pi_n(dt).$$

Limiting predictions

Now let

$$R_{n+1,n+m} = \frac{S_{n+1,n+m}}{m}.$$

Then, by the form of (†), and the result from the theorem (♦), we may conclude directly that

$$\lim_{m\to\infty} \Pr\left[R_{n+1,n+m} \leqslant \theta \middle| S_{1,n} = s_{1,n}\right] = \int_0^\theta \pi_n\left(dt\right)$$

that is, the *posterior distribution* is a *limiting form of the predictive distribution* for a particular summary statistic.

Limiting predictions

Note

In the above formulation, if we consider $n \longrightarrow \infty$, we observe that for $\theta \in [0, 1]$,

$$\lim_{n \longrightarrow \infty} \pi_n(\theta) = \delta_{\{\theta_0\}}(\theta) = \begin{cases} 1 & \theta = \theta_0 \\ 0 & \theta \neq \theta_0 \end{cases}$$

that is, the posterior distribution is *degenerate* at θ_0.

True values

In our specifications, we have defined

- in the binary case

$$\theta_0 = \lim_{n \longrightarrow \infty} \frac{1}{n} \sum_{i=1}^{n} Y_i$$

- in the general case

$$F_0(y) = \lim_{n \longrightarrow \infty} \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{(-\infty, y]}(Y_i)$$

We can regard θ_0 and $F_0(.)$ as the '*true*' parameters that render the observables independent if conditioned upon.

Model mis-specification

In any real example, we observe $y_1, \ldots, y_n$, but whereas we can *propose* a model for the joint distribution of the variables under exchangeability, we do not know that our selected model is the correct (data generating) one.

The limit results hold under the assumption that the model is *correctly specified*, but in reality our model may be *mis-specified*.

Model mis-specification

Example: Binary case

In the exchangeable binary case, we must have

$$p_{Y_i}(y_i;\theta) = \theta^{y_i}(1-\theta)^{1-y_i}$$

for each $0 \leqslant \theta \leqslant 1$; however different choices of $\pi_0(d\theta)$ lead to different models for the joint distribution of $Y_1, \ldots, Y_n$.

θ_0 is the hypothetical value of θ that renders the Y_is independent if conditioned upon: however,

- this *cannot be assessed in the data*, as we do not observe data from a conditional-on-θ model.

Model mis-specification

Example: Binary case

Suppose that

$$\pi_0(\theta) \equiv Beta(\alpha_0, \beta_0).$$

for $\alpha_0, \beta_0 > 0$. Then from (‡), we have for the posterior density

$$\pi_n(\theta) \propto \left\{ \prod_{i=1}^{n} \theta^{y_i} (1-\theta)^{1-y_i} \right\} \theta^{\alpha_0 - 1} (1-\theta)^{\beta_0 - 1}$$

$$= \theta^{s_n + \alpha_0 - 1} (1-\theta)^{n - s_n + \beta_0 - 1}$$

where

$$s_n = \sum_{i=1}^{n} y_i.$$

Model mis-specification

Example: Binary case

That is,

$$\pi_n(\theta) \equiv \mathit{Beta}(s_n + \alpha_0, n - s_n + \beta_0) \equiv \mathit{Beta}(\alpha_n, \beta_n)$$

say, so that

$$\pi_n(\theta) = \frac{\Gamma(\alpha_n + \beta_n)}{\Gamma(\alpha_n)\Gamma(\beta_n)} \theta^{\alpha_n - 1}(1-\theta)^{\beta_n - 1}.$$

Model mis-specification

Example: Binary case

From inspection of posterior $\pi_n(\theta)$, we may deduce that

$$\lim_{n \longrightarrow \infty} \pi_n(\theta) \longrightarrow \delta_{\theta_0}(\theta)$$

that is, the posterior is *degenerate* at θ_0 *irrespective* of the choice of prior parameters.

Model mis-specification

Example: Binary case

However, other choices of prior *may* lead to different behaviour: for example,

- if $\pi_0(\theta)$ is itself *degenerate* at a given value c say, then the posterior is also degenerate at c;
- if $\pi_0(\theta)$ is *uniform on a sub-interval* $(c_1, c_2) \subset [0, 1]$, then the posterior is also restricted to this interval.

Model mis-specification

Example: Binary case

From (§), we may conclude that the prior predictive

$$p_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n)$$

takes the form

$$p_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n) = \frac{\Gamma(\alpha_0+\beta_0)}{\Gamma(\alpha_0)\Gamma(\beta_0)}\frac{\Gamma(\alpha_n)\Gamma(\beta_n)}{\Gamma(\alpha_n+\beta_n)}$$

Model mis-specification

Example: Binary case

For $n = 1$:

$$p_{Y_1}(y_1) = \frac{\Gamma(\alpha_0 + \beta_0)}{\Gamma(\alpha_0)\Gamma(\beta_0)} \frac{\Gamma(\alpha_0 + y_1)\Gamma(\beta_0 + 1 - y_1)}{\Gamma(\alpha_0 + \beta_0 + 1)}$$

so that

$$\begin{aligned} \mathbb{E}_{Y_1}[Y_1] = \Pr[Y_1 = 1] &= \frac{\Gamma(\alpha_0 + \beta_0)}{\Gamma(\alpha_0)\Gamma(\beta_0)} \frac{\Gamma(\alpha_0 + 1)\Gamma(\beta_0)}{\Gamma(\alpha_0 + \beta_0 + 1)} \\ &= \frac{\alpha_0}{\alpha_0 + \beta_0} \end{aligned}$$

Model mis-specification

Example: Binary case

For $n = 2$:

$$p_{Y_1,Y_2}(y_1, y_2) = \frac{\Gamma(\alpha_0 + \beta_0)}{\Gamma(\alpha_0)\Gamma(\beta_0)} \frac{\Gamma(\alpha_0 + y_1 + y_2)\Gamma(\beta_0 + 2 - y_1 - y_2)}{\Gamma(\alpha_0 + \beta_0 + 2)}$$

$$\begin{aligned} \therefore \ \mathbb{E}_{Y_1,Y_2}[Y_1 Y_2] &= \Pr[Y_1 = 1, Y_2 = 1] \\ &= \frac{\Gamma(\alpha_0 + \beta_0)}{\Gamma(\alpha_0)\Gamma(\beta_0)} \frac{\Gamma(\alpha_0 + 2)\Gamma(\beta_0)}{\Gamma(\alpha_0 + \beta_0 + 2)} \\ &= \frac{\alpha_0(\alpha_0 + 1)}{(\alpha_0 + \beta_0)(\alpha_0 + \beta_0 + 1)} \end{aligned}$$

Model mis-specification

Example: Binary case

$$\text{Cov}_{Y_1,Y_2}[Y_1, Y_2] = \frac{\alpha_0(\alpha_0+1)}{(\alpha_0+\beta_0)(\alpha_0+\beta_0+1)} - \left(\frac{\alpha_0}{\alpha_0+\beta_0}\right)^2$$

Thus as the prior changes (that is, α_0 and β_0 change) the modelled covariance between pairs of Ys changes.

Model mis-specification

Example: Binary case

From (†), we may conclude that the posterior predictive

$$p_{Y_{n+1},\ldots,Y_{n+m}|Y_1,\ldots,Y_n}\left(y_{n+1},\ldots,y_{n+m}\middle|y_1,\ldots,y_n\right)$$

takes the form

$$\frac{\Gamma(\alpha_n+\beta_n)}{\Gamma(\alpha_n)\Gamma(\beta_n)}\frac{\Gamma(\alpha_n+s_{n+1,n+m})\Gamma(\beta_n+m-s_{n+1,n+m})}{\Gamma(\alpha_n+\beta_n+m)}$$

where

$$s_{n+1,n+m}=\sum_{i=n+1}^{n+m}y_i$$

Model mis-specification

Example: Binary case

If $n = m = 1$

$$p_{Y_2|Y_1}(y_2|y_1) = \frac{\Gamma(\alpha_0 + y_1 + y_2)\Gamma(\beta_0 + 2 - y_1 - y_2)}{\Gamma(\alpha_0 + y_1)\Gamma(\beta_0 + 1 - y_1)(\alpha_0 + \beta_0 + 1)}$$

so that for $y_2 \in \{0, 1\}$

$$p_{Y_2|Y_1}(y_2|0) = \frac{\Gamma(\alpha_0 + y_2)\Gamma(\beta_0 + 2 - y_2)}{\Gamma(\alpha_0)\Gamma(\beta_0 + 1)(\alpha_0 + \beta_0 + 1)}$$

$$p_{Y_2|Y_1}(y_2|1) = \frac{\Gamma(\alpha_0 + 1 + y_2)\Gamma(\beta_0 + 1 - y_2)}{\Gamma(\alpha_0 + 1)\Gamma(\beta_0)(\alpha_0 + \beta_0 + 1)}$$

Model mis-specification

In general, in the *parametric* case, we need to consider the possibility of mis-specification of a component of the model; the choice of

$$f_Y(y_i;\theta) \quad \text{or} \quad \pi_0(d\theta)$$

yields a prior predictive

$$f_{Y_1,\ldots,Y_n}(y_1,\ldots,y_n)$$

that may not match the *true* (data generating) model.

In the *non-parametric* case, the same considerations apply.

Model mis-specification

De Finetti's theorem tells us that under exchangeability, there must exist a representation of the data generating model such that

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\right] = \int \prod_{i=1}^{n} F^*(y_i;\theta)\ \pi_0^*\ (d\theta)$$

for at least one combination of

$$F_Y^*(y_i;\theta) \quad \text{and} \quad \pi_0^*(d\theta)$$

Model mis-specification

It may be that $\pi_0^*(d\theta)$ is a degenerate distribution at $\theta = \theta_0^*$ say, so that

$$\Pr\left[\bigcap_{i=1}^{n}(Y_i \leqslant y_i)\right] = \prod_{i=1}^{n} F^*(y_i;\theta_0^*)$$

and the Y_is are independent.

In most cases, we will assume correct specification.

Numerical Examples

Example: Normal model

See `knitr` handout 01.

Note the important identity: for scalar x, and constants A, a, B, b

$$A(x-a)^2 + B(x-b)^2 = (A+B)\left(x - \frac{Aa+Bb}{A+B}\right)^2 + \frac{AB}{A+B}(a-b)^2$$

Example: Bernoulli model

See `knitr` handout 02.

Extensions

- multivariate Ys: extension straightforward;
- regression problems: *partial exchangeability*;
- hierarchical models: *partial exchangeability*.

1.2 Bayesian calculations

- Bayesian updating
- Sufficiency concepts
- Prior specification

Bayesian updating

The Bayesian calculation acts *sequentially*; that is, for data $\mathbf{y}_1$

$$\pi_{n_1}(\theta) = \frac{f_{\mathbf{Y}_1}(\mathbf{y}_1;\theta)\pi_0(\theta)}{f_{\mathbf{Y}_1}(\mathbf{y}_1)} = \frac{f_{\mathbf{Y}_1}(\mathbf{y}_1;\theta)\pi_0(\theta)}{\int f_{\mathbf{Y}_1}(\mathbf{y}_1;t)\pi_0(t)\,dt}$$

contains the information about θ in light of the data $\mathbf{y}_1$ and prior assumptions.

Bayesian updating

If new (independent and identically distributed to $\mathbf{y}_1$) data $\mathbf{y}_2$ become available, then the posterior for θ in light of the combined data $(\mathbf{y}_1, \mathbf{y}_2)$ is

$$\pi_n(\theta) = \frac{f_{\mathbf{Y}_1,\mathbf{Y}_2}(\mathbf{y}_{1,}, \mathbf{y}_2; \theta)\pi_0(\theta)}{f_{\mathbf{Y}_1,\mathbf{Y}_2}(\mathbf{y}_1, \mathbf{y}_2)} = \frac{f_{\mathbf{Y}_1,\mathbf{Y}_2}(\mathbf{y}_1, \mathbf{y}_2; \theta)\pi_0(\theta)}{\int f_{\mathbf{Y}_1,\mathbf{Y}_2}(\mathbf{y}_1, \mathbf{y}_2; t)\pi_0(t)\, dt}$$

where $n = n_1 + n_2$ is the total sample size.

Bayesian updating

But note also that

$$\pi_n(\theta) = \frac{f_{\mathbf{Y}_2}(\mathbf{y}_2;\theta)\pi_{n_1}(\theta)}{f_{\mathbf{Y}_2|\mathbf{Y}_1}(\mathbf{y}_2|\mathbf{y}_1)}$$

where $\pi_{n_1}(\theta)$ is the posterior for θ based on $\mathbf{y}_1$, and

$$f_{\mathbf{Y}_2|\mathbf{Y}_1}(\mathbf{y}_2|\mathbf{y}_1) = \frac{f_{\mathbf{Y}_1,\mathbf{Y}_2}(\mathbf{y}_1,\mathbf{y}_2)}{f_{\mathbf{Y}_1}(\mathbf{y}_1)} = \frac{\int f_{\mathbf{Y}_1,\mathbf{Y}_2}(\mathbf{y}_1,\mathbf{y}_2;t)\pi_0(t)\,dt}{\int f_{\mathbf{Y}_1}(\mathbf{y}_1;s)\pi_0(s)\,ds}$$

Sufficiency

If $\mathbf{T}(\mathbf{Y})$ is a sufficient statistic for θ in the classical sense, then by the Neyman factorization result, we have for the joint distribution

$$f_{\mathbf{Y}}(\mathbf{y};\theta) = g(\mathbf{T}(\mathbf{y}),\theta)h(\mathbf{y})$$

It follows that

$$\pi_n(\theta) = \frac{f_{\mathbf{Y}}(\mathbf{y};\theta)\pi_0(\theta)}{f_{\mathbf{Y}}(\mathbf{y})} = \frac{g(\mathbf{T}(\mathbf{y}),\theta)h(\mathbf{y})\pi_0(\theta)}{f_{\mathbf{Y}}(\mathbf{y})}$$

$$= \left[\frac{h(\mathbf{y})}{f_{\mathbf{Y}}(\mathbf{y})}\right] g(\mathbf{T}(\mathbf{y}),\theta)\pi_0(\theta)$$

Thus the posterior distribution of θ only depends on the data through $\mathbf{T}(\mathbf{y})$.

Sufficiency

Lemma

If $\mathbf{T}(\mathbf{Y})$ *is a sufficient statistic for* θ *(in the classical sense) then* $\pi_n(\theta)$ *depends on* $\mathbf{y}$ *only through the value of*

$$\mathbf{T}(\mathbf{y})$$

for all prior specifications $\pi_0(\theta)$.

Sufficiency

Proof.

By definition

$$f_{\mathbf{Y}}(\mathbf{y};\theta) = f_{\mathbf{Y},\mathbf{T}}(\mathbf{y},\mathbf{t};\theta)$$

if $\mathbf{t} = \mathbf{T}(\mathbf{y})$, and zero otherwise. Thus, by sufficiency,

$$f_{\mathbf{Y}}(\mathbf{y};\theta) = f_{\mathbf{Y}|\mathbf{T}}(\mathbf{y}|\mathbf{t}) f_{\mathbf{T}}(\mathbf{t};\theta)$$

and hence

$$\pi_n(\theta) \propto f_{\mathbf{Y}}(\mathbf{y};\theta)\pi(\theta) \propto f_{\mathbf{T}}(\mathbf{t};\theta)\pi_0(\theta)$$

□

Sufficiency

Lemma

$\mathbf{T}(\mathbf{Y})$ *is sufficient in the Bayesian sense – the Bayesian posterior depends on* $\mathbf{y}$ *only through* $\mathbf{T}(\mathbf{y})$ *– if and only if it is sufficient in the classical sense.*

We need to establish the converse of the previous result.

Proof.

For the posterior based on $\mathbf{t}$,

$$\pi_n(\theta) = \frac{f_{\mathbf{T}}(\mathbf{t};\theta)\pi_0(\theta)}{f_{\mathbf{T}}(\mathbf{t})}.$$

This must be equal to the posterior based on $\mathbf{Y}$, that is,

$$\frac{f_{\mathbf{Y}}(\mathbf{y};\theta)}{f_{\mathbf{Y}}(\mathbf{y})} = \frac{\pi_n(\theta)}{\pi_0(\theta)} = \frac{f_{\mathbf{T}}(\mathbf{t};\theta)}{f_{\mathbf{T}}(\mathbf{t})}.$$

Hence we must have

$$f_{\mathbf{Y}}(\mathbf{y};\theta) = f_{\mathbf{T}}(\mathbf{t};\theta)\frac{f_{\mathbf{Y}}(\mathbf{y})}{f_{\mathbf{T}}(\mathbf{t})} = g(\mathbf{t},\theta)h(\mathbf{y})$$

say. Thus $\mathbf{T}(\mathbf{Y})$ is sufficient in the classical sense. □

Construction of Prior Distributions

In the Bayesian formulation, the prior density plays an important role. There are several methods via which the prior can be specified quantitatively;

- from *historical* or training data;
- by *subjective assessment*, similar to the subjective assessment of probabilities in elementary probability theory;
- by matching to a *desired functional form*;
- or in a *non-informative* or *vague* specification, where the prior probability is supposedly spread 'evenly' across the parameter space.

Construction of Prior Distributions

For some models, a *conjugate prior* can be chosen; this prior combines with the likelihood in such a way to give an analytically tractable posterior calculation.

Consider a class of distributions $\mathcal{F}$ indexed by parameter θ

$$\mathcal{F} = \{f_Y(y;\theta) : \theta \in \Theta\}$$

A class $\mathcal{P}$ of prior distributions for θ is a *conjugate family* for $\mathcal{F}$ if the posterior distribution for θ resulting from data $\mathbf{y}$ is an element of $\mathcal{P}$ for all $f_Y \in \mathcal{F}$, $\pi_0 \in \mathcal{P}$ and $\mathbf{y} \in \mathcal{Y}$.

Construction of Prior Distributions

Example: Exponential Family

Suppose that $f_Y(y;\theta)$ is an Exponential Family distribution

$$f_Y(y;\theta) = h(y)c(\theta)\exp\left\{\sum_{j=1}^{k} t_j(y)w_j(\theta)\right\}$$

so that for a random sample of size n

$$\mathcal{L}_n(\theta) = h(\mathbf{y})\{c(\theta)\}^n \exp\left\{\sum_{j=1}^{k} T_j(\mathbf{y})w_j(\theta)\right\} \quad (1)$$

for

$$T_j(\mathbf{y}) = \sum_{i=1}^{n} t_j(y_i).$$

Construction of Prior Distributions

Example: Exponential Family

Suppose that

$$\pi_0(\theta) = d(\alpha, \beta)\{c(\theta)\}^{\alpha} \exp\left\{\sum_{j=1}^{k} \beta_j w_j(\theta)\right\} \tag{2}$$

where α and $\beta = (\beta_1, \ldots, \beta_k)^\top$ are *hyperparameters*. Combining prior and likelihood yields the posterior as

$$\begin{aligned} \pi_n(\theta) &\propto \{c(\theta)\}^{\alpha+n} \exp\left\{\sum_{j=1}^{k} [\beta_j + T_j(\mathbf{y})] w_j(\theta)\right\} \\ &= \{c(\theta)\}^{\alpha^\star} \exp\left\{\sum_{j=1}^{k} \beta_j^\star w_j(\theta)\right\} \end{aligned}$$

Construction of Prior Distributions

Example: Exponential Family

The normalizing constant can be deduced to be

$$d(\alpha + n, \beta + \mathbf{T}(\mathbf{y})),$$

and hence the posterior distribution has the same functional form as the prior, but with parameters updated to

$$\alpha^\star = \alpha + n \qquad \beta^\star = (\beta_1^\star, \ldots, \beta_k^\star)^\top = (\beta_1 + T_1(\mathbf{y}), \ldots, \beta_1 + T_1(\mathbf{y}))^\top.$$

Construction of Prior Distributions

A non-informative prior expresses *prior ignorance* about the parameter of interest.

- If $\Theta = \{\theta_1, \ldots, \theta_k\}$ (that is, θ is known to take one of a finite number of possible values). Then a non-informative prior places equal probability on each value, that is,

$$\pi_0(\theta) = \frac{1}{k} \qquad \theta \in \Theta.$$

Construction of Prior Distributions

- If Θ is a *bounded region*, then a natural non-informative prior is *constant* on Θ.
- If the parameter space Θ is uncountable and unbounded, however, a non-informative prior specification is more difficult to construct.
  - A naive prior specification would be to set $\pi_0(\theta)$ to be a constant, although this prior does not give a valid probability measure as it does not integrate to 1 over Θ.
  - A prior distribution $\pi_0(\theta)$ for parameter θ is termed *improper* if it does not integrate to 1.

Construction of Prior Distributions

Even for improper priors can be used to compute the posterior density, which itself will often be *proper* (integrate to 1).

However, if $\phi = g(\theta)$ is a transformation of θ, then by elementary transformation results, including the Jacobian of the transform $J(\theta \to \phi)$, it follows that

$$\pi_{0,\theta}(\theta) = c \qquad \Longrightarrow \qquad \pi_{0,\phi}(\phi) = c \times J(\theta \to \phi)$$

which may *not* be constant, and hence a *non-uniform* prior on ϕ results. This is perhaps unsatisfactory, and so the following procedure may be preferable.

Construction of Prior Distributions

Consider the prior $\pi_0(\theta)$ for parameter θ in probability model $f_Y(y;\theta)$ determined by

$$\pi_0(\theta) \propto \{|\mathcal{I}_\theta(\theta)|\}^{1/2}$$

where $\mathcal{I}_\theta(\theta)$ is the *Fisher Information,*

$$\mathcal{I}_\theta(\theta) = \mathbb{E}_Y\left[S(Y;\theta)S(Y;\theta)^\top;\theta\right] = -\mathbb{E}_Y\left[\Psi(Y;\theta);\theta\right]$$

and $|\mathcal{I}_\theta(\theta)|$ indicates the absolute value of the determinant of $\mathcal{I}_\theta(\theta)$. The prior $\pi_0(\theta)$ defined in this way is termed the *Jeffreys* prior.

Construction of Prior Distributions

$S(y;\theta)$ is the $k \times 1$ vector *score function* with jth element

$$S_j(y;\theta) = \frac{\partial}{\partial \theta_j} \log f_Y(y;\theta) \qquad j = 1, \ldots, k$$

and $\Psi(Y;\theta)$ is the $k \times k$ matrix of second partial derivatives with (j,l)th element

$$\frac{\partial^2}{\partial \theta_j \partial \theta_l} \log f_Y(y;\theta)$$

Given these functional forms, $S(Y;\theta)$ and $\Psi(Y;\theta)$ are *random variables*.

Construction of Prior Distributions

Example: $Binomial(m, \theta)$

We have

$$\begin{aligned}
\log f_Y(y;\theta) &= \log \binom{m}{y} + y \log \theta + (m-y)\log(1-\theta) \\
S(y;\theta) &= \frac{y}{\theta} - \frac{(m-y)}{(1-\theta)} \\
\Psi(y;\theta) &= -\frac{y}{\theta^2} - \frac{(m-y)}{(1-\theta)^2}
\end{aligned}$$

Example: $Binomial(m, \theta)$

Therefore

$$\mathcal{I}_\theta(\theta) = -\mathbb{E}_Y\left[-\frac{Y}{\theta^2} - \frac{(m-Y)}{(1-\theta)^2}\right] = \frac{m\theta}{\theta^2} + \frac{m(1-\theta)}{(1-\theta)^2} = \frac{m}{\theta(1-\theta)}$$

and hence

$$\pi_0(\theta) \propto |\mathcal{I}_\theta(\theta)|^{1/2} = \{\theta(1-\theta)\}^{-1/2}$$

Construction of Prior Distributions

Lemma

Jeffreys's prior is invariant under 1-1 transformations, that is, if $\phi = \phi(\theta)$, then the prior for ϕ obtained by reparameterization from θ to ϕ in the prior for θ, is precisely Jeffreys's prior for ϕ.

Proof.

Let $\phi = \phi(\theta)$ be a 1-1 transformation. Denote by $\ell_\theta(y;\theta)$ and $\ell_\phi(y;\phi)$ the log pdfs in the two parameterizations. Then by the rules of partial differentiation

$$\frac{\partial \ell_\phi}{\partial \phi_j} = \sum_{l=1}^{k} \frac{\partial \ell_\theta}{\partial \theta_l} \frac{\partial \theta_l}{\partial \phi_j} \qquad j = 1, \ldots, k$$

so that

$$S(y;\phi) = \Lambda(\theta,\phi) S(y;\theta)$$

where $\Lambda(\theta,\phi)$ is the $k \times k$ matrix with (j,l)th element

$$\frac{\partial \theta_l}{\partial \phi_j}$$

□

Proof.

In fact, $\Lambda(\theta, \phi)$ is just the Jacobian of the transformation from θ to ϕ, $J(\theta \to \phi)$. Hence

$$\mathcal{I}_\phi(\phi) = \Lambda(\theta, \phi)\mathcal{I}_\theta(\theta)\Lambda(\theta, \phi)^\top$$

and so

$$|\mathcal{I}_\phi(\phi)| = |\Lambda(\theta, \phi)\mathcal{I}_\theta(\theta)\Lambda(\theta, \phi)^\top| = |\Lambda(\theta, \phi)|^2|\mathcal{I}_\theta(\theta)|$$

and

$$|\mathcal{I}_\phi(\phi)|^{1/2} = |\Lambda(\theta, \phi)||\mathcal{I}_\theta(\theta)|^{1/2}.$$

□

Proof.

Thus

$$\pi_0(\phi) \propto |\mathcal{I}_\phi(\phi)|^{1/2} = |\Lambda(\theta, \phi)||\mathcal{I}_\theta(\theta)|^{1/2} = |\Lambda(\theta, \phi)|\pi_0(\theta)$$

and Jeffreys's prior for ϕ is identical to the one that would be obtained by constructing Jeffreys's prior for θ and reparameterizing to ϕ. □

Construction of Prior Distributions

Example: $Binomial(m, \theta)$

Suppose that $\phi = \theta/(1-\theta)$ (so that $\theta = \phi/(1+\phi)$). Then

$$\begin{aligned}
\log f_Y(y;\phi) &= \log \binom{m}{y} + y \log \phi - m \log(1+\phi) \\
S(y;\phi) &= \frac{y}{\phi} - \frac{m}{(1+\phi)} \\
\Psi(y;\phi) &= -\frac{y}{\phi^2} + \frac{m}{(1+\phi)^2}
\end{aligned}$$

Example: $Binomial(m, \theta)$

Therefore

$$\begin{aligned}\mathcal{I}_\phi(\phi) &= -\mathbb{E}_Y\left[-\frac{Y}{\phi^2} + \frac{m}{(1+\phi)^2}; \phi\right] \\ &= \frac{m\phi}{(1+\phi)\phi^2} - \frac{m}{(1+\phi)^2} \\ &= \frac{m}{\phi(1+\phi)^2}\end{aligned}$$

and hence

$$\pi_0(\phi) \propto |\mathcal{I}_\phi(\phi)|^{1/2} = \{\phi(1+\phi)^2\}^{-1/2}.$$

Construction of Prior Distributions

Example: *Binomial*(m, θ)

Now, recall that Jeffreys's prior for θ takes the form

$$\pi_0(\theta) \propto \{\theta(1-\theta)\}^{-1/2}$$

The Jacobian of the transformation from θ to ϕ is $(1+\phi)^{-2}$, and thus using the univariate transformation theorem

$$\pi_0(\phi) \propto \{\phi/(1+\phi)^2\}^{-1/2}(1+\phi)^{-2} = \{\phi(1+\phi)^2\}^{-1/2}$$

matching the result found above.

Location and Scale Parameters

Parameter θ is a *location parameter* if

$$f_Y(y;\theta) = f(y-\theta)$$

and is a *scale parameter* if

$$f_Y(y;\theta) = \frac{1}{\theta} f\left(\frac{y}{\theta}\right)$$

for some pdf f.

A 'non-informative' prior can be constructed using invariance principles in the location and scale cases.

Location and Scale Parameters

- For a *location* parameter, for a non-informative prior, it is required to have, for set $A \subset \Theta$

$$\int_A \pi_0(\theta)\, d\theta = \int_{A_c} \pi_0(\theta)\, d\theta$$

where $A_c = \{\theta : \theta - c \in A\}$ for scalar c. Therefore, for all c, we must have

$$\int_{A_c} \pi_0(\theta)\, d\theta = \int_A \pi_0(\theta - c)\, d\theta$$

$$\therefore \quad \pi_0(\theta) = \pi_0(\theta - c) \Longrightarrow \pi_0(\theta) = \text{constant}.$$

Location and Scale Parameters

- For a *scale* parameter, it is required to have, for arbitrary set $A \subset \Theta$

$$\int_A \pi_0(\theta)\, d\theta = \int_{A_c} \pi_0(\theta)\, d\theta$$

where now $A_c = \{\theta : c\theta \in A\}$ for scalar c. Therefore, for all c, we must have

$$\int_{A_c} \pi_0(\theta)\, d\theta = \int_A c\pi_0(c\theta)\, d\theta$$

$$\therefore \quad \pi_0(\theta) = c\pi_0(c\theta) \Longrightarrow \pi_0(\theta) \propto \frac{1}{\theta}$$

Location and Scale Parameters

This follows by the usual 'scale invariance' definition: a function $g(y)$ is *scale invariant* if

$$g(cy) \propto g(y)$$

and all scale invariant functions are power laws; for some $\alpha > 0$,

$$g(y) \propto y^{-\alpha}.$$

Here, the condition $\pi_0(\theta) = c\pi_0(c\theta)$ means that we must have $\alpha = 1$.

1.3 Bayesian Optimal Decisions

Many statistical procedures involve *decision-making*, that is, taking actions in light of observed data.

- parameter estimation;
- hypothesis testing;
- prediction/classification;
- model selection.

1.3 Bayesian Optimal Decisions

Define

- $T(.)$ as a function of data $\mathbf{Y} = (Y_1, \ldots, Y_n)$;

$$T \ : \ \mathbb{R}^n \longrightarrow \mathcal{T}$$

For example

$$T(\mathbf{Y}) = \frac{1}{n} \sum_{i=1}^{n} Y_i \qquad \text{sample mean}$$

$$T(\mathbf{Y}) = \left(Y_{(1)}, \ldots, Y_{(n)}\right)^\top \qquad \text{order statistics}$$

$$T_y(\mathbf{Y}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{(-\infty, y]}(Y_i) \qquad \text{empirical cdf}$$

- Model space $\mathcal{F}$;

1.3 Bayesian Optimal Decisions

- Loss function, $L(.,.)$,

$$L \ : \ \mathcal{T} \times \mathcal{F} \longrightarrow \mathbb{R}^{+} \bigcup \{0\}.$$

  Defines the loss in reporting T when the truth is defined by $F \in \mathcal{F}$.

Example:

For cdf F_Y, let

$$\mu = \int y \; F_Y(dy).$$

Then could define

$$L(T, F_Y) = (T - \mu)^2$$

as the loss in reporting 'estimator' T when the true functional of interest is μ.

1.3 Bayesian Optimal Decisions

The *optimal decision* is one that minimizes the expected loss, where the expectation is taken with respect to the distribution of random quantities in the calculation.

For a parametric analysis parameterized by θ

- in a *frequentist* analysis, θ is a fixed constant and the data are treated as random;
- in a *Bayesian* analysis, the data $y_1, \ldots, y_n$ are fixed, and θ is a random variable.

Example: Frequentist calculation

For cdf F_Y, let

$$\mu = \int y \; F_Y(dy).$$

with

$$L(T, F_Y) = (T - \mu)^2$$

we have that

$$\begin{aligned}
&\arg\min_T \mathbb{E}_{F_Y}[(T-\mu)^2] \\
&\quad = \arg\min_T \left\{ \mathbb{E}_{F_Y}\left[(T - \mathbb{E}_{F_Y}[T])^2 \right] + (\mathbb{E}_{F_Y}[T] - \mu)^2 \right\} \\
&\quad = \arg\min_T \left\{ \mathrm{Var}_{F_Y}[T] + (\mathbb{E}_{F_Y}[T] - \mu)^2 \right\}
\end{aligned}$$

Example: Frequentist calculation

This does not define the optimal T, but it does tell us that we need to take into account

- the *variance* of T, $\mathrm{Var}_{F_Y}[T]$
- the squared *bias*, $b_{F_Y}(T)$

$$b_{F_Y}(T) = \mathbb{E}_{F_Y}[T] - \mu$$

Kullback-Leibler loss

The *Kullback-Leibler* (KL) loss is used when measuring the discrepancy between distributions. For two distributions with cdfs F_0, F_1

$$KL(F_0, F_1) = \int \log \left\{ \frac{F_0(dy)}{F_1(dy)} \right\} F_0(dy)$$

which is defined when F_1 is absolutely continuous with respect to F_0, that is for the corresponding probability measures

$$P_0(B) = 0 \quad \Longrightarrow P_1(B) = 0$$

for any set B.

Kullback-Leibler loss

- Discrete case:

$$KL(p_0, p_1) = \sum_y \log\left\{\frac{p_0(y)}{p_1(y)}\right\} p_0(y) = \mathbb{E}_{p_0}\left[\log\left\{\frac{p_0(Y)}{p_1(Y)}\right\}\right].$$

- Continuous case:

$$KL(f_0, f_1) = \int \log\left\{\frac{f_0(y)}{f_1(y)}\right\} f_0(y)\, dy = \mathbb{E}_{f_0}\left[\log\left\{\frac{f_0(Y)}{f_1(Y)}\right\}\right].$$

Kullback-Leibler loss

Note

1. $KL(F_0, F_1) \geqslant 0$;
2. $KL(F_0, F_1) \neq KL(F_1, F_0)$
3. $KL(F_0, F_1) = 0$ if and only if the two distributions are identical.

Kullback-Leibler loss

Example:

In a parametric problem, we might have pdf

$$f(y;\theta)$$

with $\theta = \theta_0$ presumed to be the data generating model. Then we may write

$$KL(\theta_0, \theta) = \int \log\left\{\frac{f(y;\theta_0)}{f(y;\theta)}\right\} f_0(y;\theta_0)\, dy$$

and we seek to use data to report an estimator $\widehat{\theta} = T(Y_{1:n})$ of the true value θ_0.

Decision theory concepts

The key components of a *decision problem* are as follows;

- a *decision* d is to be made, and the decision is selected from some set $\mathcal{D}$ of alternatives.
- a true *state of nature*, $v(\theta)$, lying in set Υ, defined by the data generating model, $F_Y(y;\theta)$.
- a *loss function*, $L(\mathsf{d}, v)$, for decision d and state v, which records the loss (or penalty) incurred when the true state of nature is v and the decision made is d.

We aim to select the decision to *minimize* the *expected loss*.

Decision theory concepts

In an *estimation* context, the decision is the *estimate* of the parameter, and the true state of nature is the true value of the parameter, $\upsilon(\theta) \equiv \theta$.

If data $\mathbf{y} = y_{1:n}$ are available, the optimal decision will intuitively become a function of the data. Suppose now that the decision in light of the data is now in the form of an estimate, denoted $\mathsf{d}(\mathbf{y}) = \widehat{\theta}_n$, say, with associated loss $L(\widehat{\theta}_n, \theta)$

Decision theory concepts

(i) The *frequentist risk* or *loss* associated with decision denoted $\mathsf{d}(\mathbf{Y})$ (given by estimator $\widehat{\theta}_n$) is the expected loss associated with $\mathsf{d}(\mathbf{Y})$, with the expectation taken over the distribution of $\mathbf{Y}$ given θ

$$R_n(\mathsf{d}, \theta) = \mathbb{E}_{F_{\mathbf{Y}}}[L(\widehat{\theta}_n, \theta)] = \int_{\mathcal{Y}} L(\widehat{\theta}_n, \theta) f_{\mathbf{Y}}(\mathbf{y}; \theta)\, d\mathbf{y}$$

Decision theory concepts

(ii) The *Bayes risk* for $\mathsf{d}(\mathbf{Y})$ is the expected risk over the *prior* distribution of θ

$$\begin{aligned} R_n(\mathsf{d}) &= \mathbb{E}_{\pi_0}[R_n(\mathsf{d},\theta)] \\ &= \mathbb{E}_{\pi_0}\left[\mathbb{E}_{F_{\mathbf{Y}}}\left[L(\widehat{\theta}_n,\theta)\right]\right] \\ &= \int_\Theta \left\{\int_{\mathcal{Y}} L(\widehat{\theta}_n,\theta) f_{\mathbf{Y}}(\mathbf{y};\theta)\, d\mathbf{y}\right\} \pi_0(\theta)\, d\theta \\ &= \int_\Theta \int_{\mathcal{Y}} L(\widehat{\theta}_n,\theta) f_{\mathbf{Y}}(\mathbf{y}) \pi_n(\theta)\, d\mathbf{y}\, d\theta \\ &= \int_{\mathcal{Y}} \left\{\int_\Theta L(\widehat{\theta}_n,\theta)\pi_n(\theta)\, d\theta\right\} f_{\mathbf{Y}}(\mathbf{y})\, d\mathbf{y} \end{aligned}$$

where by Bayes theorem $f_{\mathbf{Y}}(\mathbf{y};\theta)\pi_0(\theta) = f_{\mathbf{Y}}(\mathbf{y})\pi_n(\theta)$.

(iii) With prior $\pi_0(\theta)$ and fixed data $\mathbf{y}$ the optimal Bayesian decision, termed the *Bayes rule* is

$$\widehat{\mathsf{d}}_B = \arg\min_{\mathsf{d}\in\mathcal{D}} R(\mathsf{d})$$

so that, for the *Bayes estimate* $\widehat{\theta}_{nB}$

$$\widehat{\theta}_{nB} = \arg\min_{\mathsf{d}\in\mathcal{D}} \int_{\mathcal{Y}} \left\{ \int_{\Theta} L(\widehat{\theta}_n, \theta)\pi_n(\theta)\, d\theta \right\} f_{\mathbf{Y}}(\mathbf{y})\, d\mathbf{y}$$

$$= \arg\min_{\widehat{\theta}_n\in\Theta} \int_{\Theta} L(\widehat{\theta}_n, \theta)\pi_n(\theta)\, d\theta$$

as only the inner integral depends on the decision and the data.

Decision theory concepts

That is, the decision that minimizes the Bayes risk minimizes *posterior expected loss* in making decision d, with expectation taken with respect to the posterior distribution $\pi_n(\theta)$.

Results for Different Loss Functions

(I) Under *squared-error loss*

$$L(\widehat{\theta}_n, \theta) = (\widehat{\theta}_n - \theta)^2$$

the *Bayes rule* for estimating θ is

$$\widehat{\mathsf{d}}_B(\mathbf{y}) = \widehat{\theta}_{nB}(\mathbf{y}) = \mathbb{E}_{\pi_n}[\theta] = \int \theta \pi_n(\theta)\, d\theta$$

that is, the *posterior expectation*.

Results for Different Loss Functions

The *expected posterior loss* for any Bayes estimate $\widehat{\theta}_n$ is

$$\int L(\widehat{\theta}_n, \theta)\pi_n(\theta)\, d\theta = \int (\widehat{\theta}_n - \theta)^2 \pi_n(\theta)\, d\theta$$

which needs to be minimized with respect to $\widehat{\theta}_n$.

Results for Different Loss Functions

Write $t = \widehat{\theta}_n$. Then

$$\frac{d}{dt}\left\{\int (t-\theta)^2 \pi_n(\theta)\, d\theta\right\} = \int \frac{d}{dt}\left\{(t-\theta)^2\right\} \pi_n(\theta)\, d\theta$$

$$= \int 2\,(t-\theta)\, \pi_n(\theta)\, d\theta$$

and equating this to zero gives

$$t = \int \theta \pi_n(\theta)\, d\theta = \mathbb{E}_{\pi_n}[\theta]$$

and hence the optimal $t = \widehat{\theta}_n$ is the posterior expectation as stated.

Results for Different Loss Functions

(II) Under *absolute error loss*

$$L(\widehat{\theta}_n, \theta) = |\widehat{\theta}_n - \theta|$$

the Bayes estimate for θ is the solution of

$$\int_{-\infty}^{\widehat{\theta}_n} \pi_n(\theta)\, d\theta = \frac{1}{2}$$

that is, it is the *posterior median*.

Results for Different Loss Functions

The expected posterior loss is

$$\int L(\widehat{\theta}_n, \theta)\pi_n(\theta)\, d\theta = \int |\widehat{\theta}_n - \theta|\pi_n(\theta)\, d\theta$$

which needs to be minimized with respect to $\widehat{\theta}_n$. Let $t = \widehat{\theta}_n$. Then

$$\int |t - \theta|\, \pi_n(\theta)\, d\theta$$

$$= \int_{-\infty}^{t} (t - \theta)\, \pi_n(\theta)\, d\theta + \int_{t}^{\infty} (\theta - t)\, \pi_n(\theta)\, d\theta$$

Results for Different Loss Functions

Differentiating with respect to t the first term using the product rule yields

$$\begin{aligned}
&\frac{d}{dt}\left\{\int_{-\infty}^{t}(t-\theta)\,\pi_n(\theta)\,d\theta\right\} \\
&\quad=\frac{d}{dt}\left\{t\int_{-\infty}^{t}\pi_n(\theta)\,d\theta-\int_{-\infty}^{t}\theta\pi_n(\theta)\,d\theta\right\} \\
&\quad=t\pi_n(t)+\int_{-\infty}^{t}\pi_n(\theta)\,d\theta-t\pi_n(t).
\end{aligned}$$

Results for Different Loss Functions

Similarly

$$\frac{d}{dt}\left\{\int_t^{\infty}(\theta - t)\,\pi_n(\theta)\,d\theta\right\} = -t\pi_n(t) - \int_t^{\infty}\pi_n(\theta)\,d\theta + t\pi_n(t)$$

Thus, equating the original derivative to zero yields

$$\int_{-\infty}^{t}\pi_n(\theta)\,d\theta - \int_t^{\infty}\pi_n(\theta)\,d\theta = 0$$

so that

$$\int_{-\infty}^{t}\pi_n(\theta)\,d\theta = \int_t^{\infty}\pi_n(\theta)\,d\theta = \frac{1}{2}$$

and hence the optimal $t = \widehat{\theta}_n$ is the *posterior median*.

Results for Different Loss Functions

(III) Under *zero-one loss*

$$L(\mathsf{d}(\mathbf{y}), \theta) = \begin{cases} 0 & \mathsf{d}(\mathbf{y}) = \theta \\ 1 & \mathsf{d}(\mathbf{y}) \neq \theta \end{cases}$$

the Bayes rule for estimating θ is

$$\widehat{\mathsf{d}}_B(\mathbf{y}) = \widehat{\theta}_{nB}(\mathbf{y}) = \arg\max_{\theta \in \Theta} \pi_n(\theta)$$

that is, the *posterior mode*.

Results for Different Loss Functions

To see this, note that the expected posterior loss is

$$\int L(\widehat{\theta}_n, \theta)\pi_n(\theta)\, d\theta = \int_{\Theta \setminus \widehat{\theta}_n} \pi_n(\theta)\, d\theta$$

which needs to be minimized with respect to the choice of $\widehat{\theta}_n$. Consider the loss function

$$L_\delta(\widehat{\theta}_n, \theta) = \begin{cases} 0 & \widehat{\theta}_n \in (\theta - \delta, \theta + \delta) \\ 1 & \widehat{\theta}_n \notin (\theta - \delta, \theta + \delta) \end{cases}$$

for $\delta \geqslant 0$. That is, the loss is zero if $\left|\theta_n - \theta\right| < \delta$, and one otherwise.

Results for Different Loss Functions

The expected loss is therefore

$$\int L_\delta(\widehat{\theta}_n, \theta)\pi_n(\theta)\, d\theta = \int_{\Theta\setminus(\widehat{\theta}_n-\delta,\widehat{\theta}_n+\delta)} \pi_n(\theta)\, d\theta$$

$$= 1 - \Pr[\theta \in (\widehat{\theta}_n - \delta, \widehat{\theta}_n + \delta)|\mathbf{y}].$$

Thus we need to choose $\widehat{\theta}_n$ so that

$$\Pr[\theta \in (\widehat{\theta}_n - \delta, \widehat{\theta}_n + \delta)|\mathbf{y}]$$

is as large as possible, that is, we need to choose $\widehat{\theta}_n$ as the centre of the highest posterior probability region of width 2δ. As $\delta \longrightarrow 0$, this interval shrinks to be the posterior mode, as stated.

1.4 Likelihood Considerations

We have seen in the Bayesian calculation that the posterior distribution is highly dependent on the *likelihood* for its properties; on the log scale, we have in the iid case

$$\log \pi_n(\theta) = \sum_{i=1}^{n} \log f_Y(y_i;\theta) + \log \pi_0(\theta) + \text{constant}$$

and so as n grows, we expect the log-likelihood

$$\ell_n(\theta) = \sum_{i=1}^{n} \log f_Y(y_i;\theta)$$

to be the dominant term. Because of this it is useful to study the properties of the likelihood as n gets larger.

Asymptotic Theory of the Likelihood

Suppose that

- data $y_{1:n} = (y_1, \ldots, y_n)$ are realizations of iid random variables $Y_1, \ldots, Y_n$ drawn from distribution with pdf $f_0(y)$. We term this model the *true* model.

- we wish to represent the data using a parametric pdf $f_Y(y; \theta)$, where θ is d dimensional parameter. We term this model the *working* model.

Asymptotic Theory of the Likelihood

Typically, the analysis assumes that, for some θ_0,

$$f_0(y) \equiv f_Y(y; \theta_0)$$

that is, the parametric model is *correctly specified*.

However, if $f_0(y) \neq f_Y(y; \theta)$ for any θ, the model is *incorrectly specified*, and the theory needs to be reconsidered.

1. **Interpreting θ_0 in the working model:** We define the 'true' value of θ_0 as

$$\theta_0 = \arg\min_{\theta} KL(f_0, f_Y(.;\theta)) \tag{3}$$

Note that

$$KL(f_0, f_Y(.;\theta)) = \int \log f_0(y) f_0(y)\, dy - \int \log f_Y(y;\theta) f_0(y)\, dy$$

or equivalently, denoting $\log f_Y(y;\theta)$ by $\ell(y;\theta)$,

$$\theta_0 = \arg\max_{\theta} \mathbb{E}_{f_0}\left[\ell(Y;\theta)\right]. \tag{4}$$

2. **Maximum likelihood:** We maximize the sample-based expectation (or sample mean) to produce an estimator. Specifically, the estimator based on (4) will be

$$\widehat{\theta}_n = \arg\max_{\theta} \frac{1}{n} \sum_{i=1}^{n} \ell(Y_i; \theta).$$

This follows by the *weak law of large numbers*:

$$\frac{1}{n} \sum_{i=1}^{n} \ell(Y_i; \theta) \xrightarrow{p} \mathbb{E}_{f_0} \left[\ell(Y; \theta) \right] \tag{5}$$

as $n \longrightarrow \infty$ for any fixed θ, if the expectation exists.

We will assume that the log density $\ell(y;\theta)$ is at least three times differentiable with respect to θ; under this assumption, the estimate is defined as the solution to the *score equations*, the system of d equations given by

$$\frac{\partial}{\partial\theta}\left\{\frac{1}{n}\sum_{i=1}^{n}\ell(y_i;\theta)\right\} = \mathbf{0}_d$$

or equivalently,

$$\frac{1}{n}\sum_{i=1}^{n}\frac{\partial}{\partial\theta}\{\ell(y_i;\theta)\} = \frac{1}{n}\sum_{i=1}^{n}S(y_i;\theta) = \mathbf{0}_d \qquad (6)$$

say, where $S(y;\theta) = \dot{\ell}(y;\theta) = \partial\ell_1(y;\theta)/\partial\theta$. Denote the solution of (6) by $\widehat{\theta}_n \equiv \widehat{\theta}_n(y_{1:n})$.

3. **Taylor expansion:** We consider a Taylor expansion of the function $\ell(y;\theta)$ with respect to θ around θ_0.

$$\ell(y;\theta) = \ell(y;\theta_0) + \dot{\ell}(y;\theta_0)(\theta-\theta_0) + \frac{1}{2}(\theta-\theta_0)^\top \ddot{\ell}(y;\theta_0)(\theta-\theta_0) + \mathcal{R}_3(y;\theta^*) \quad (7)$$

where

$$\ddot{\ell}(y;\theta) = \frac{\partial^2 \ell(y;\theta)}{\partial\theta\partial\theta^\top} \qquad (d \times d).$$

and $\mathcal{R}_3(y;\theta^*)$ is a remainder term, for some θ^* such that $\|\theta_0 - \theta^*\| \leqslant \|\theta_0 - \theta\|$.

Evaluating (7) for each of $y_1, \ldots, y_n$ and summing the result, we have

$$\ell_n(\theta) = \ell_n(\theta_0) + \dot{\ell}_n(\theta_0)^\top(\theta - \theta_0) + \frac{1}{2}(\theta - \theta_0)^\top \ddot{\ell}_n(\theta_0)(\theta - \theta_0) + \mathcal{R}_3. \tag{8}$$

where $\mathcal{R}_3 \equiv \mathcal{R}_3(y_{1:n}; \theta^*)$ for $\|\theta_0 - \theta^*\| \leqslant \|\theta_0 - \theta\|$.

Asymptotic Theory of the Likelihood

At $\theta = \widehat{\theta}_n$ and rearranging we have

$$\ell_n(\widehat{\theta}_n) - \ell_n(\theta_0) = \dot{\ell}_n(\theta_0)^\top(\widehat{\theta}_n - \theta_0) + \frac{1}{2}(\widehat{\theta}_n - \theta_0)^\top \ddot{\ell}_n(\theta_0)(\widehat{\theta}_n - \theta_0) + \mathcal{R}_3 \tag{9}$$

4. **Asymptotic behaviour:** Consider (9) written in terms of random variables, with $\widehat{\theta}_n = \widehat{\theta}_n(Y_{1:n})$:

$$\ell_n(\widehat{\theta}_n) - \ell_n(\theta_0) = \dot{\ell}_n(\theta_0)^\top(\widehat{\theta}_n - \theta_0) + \frac{1}{2}(\widehat{\theta}_n - \theta_0)^\top \ddot{\ell}_n(\theta_0)(\widehat{\theta}_n - \theta_0) + \mathcal{R}_3 \tag{10}$$

First consider for arbitrary θ, the quantity

$$\frac{1}{n}\left(\ell_n(\theta) - \ell_n(\theta_0)\right) = \frac{1}{n}\sum_{i=1}^{n}\left(\ell(Y_i;\theta) - \ell(Y_i;\theta_0)\right).$$

We may rewrite this expression with terms involving the true density f_0 that cancel :

$$\frac{1}{n}\sum_{i=1}^{n}(\ell(Y_i;\theta) - \ell_0(Y_i)) - \frac{1}{n}\sum_{i=1}^{n}(\ell(Y_i;\theta_0) - \ell_0(Y_i)) \quad (11)$$

where $\ell_0(x) = \log f_0(y)$.

Asymptotic Theory of the Likelihood

For any θ, as $n \longrightarrow \infty$, we have by the weak law of large numbers that

$$\frac{1}{n}\sum_{i=1}^{n}(\ell(Y_i;\theta) - \ell_0(Y_i)) \xrightarrow{p} \mathbb{E}_{f_0}\left[\log\left(\frac{f_Y(Y;\theta)}{f_0(Y)}\right)\right]$$

$$= -KL(f_0, f_Y(.;\theta))$$

as $Y_1, \ldots, Y_n \sim f_0$.

Asymptotic Theory of the Likelihood

Therefore

$$\frac{1}{n}\sum_{i=1}^{n}\ell(Y_i;\theta)-\frac{1}{n}\sum_{i=1}^{n}\ell(Y_i;\theta_0)$$

converges in probability to

$$KL(f_0,f_Y(.;\theta_0))-KL(f_0,f_Y(.;\theta))$$

By definition of θ_0 via (3), $KL(f_0, f_Y(\theta))$ attains its minimum value at $\theta = \theta_0$, so

$$KL(f_0, f_Y(.;\theta_0)) - KL(f_0, f_Y(.;\theta)) \leqslant 0$$

and hence

$$\frac{1}{n}\sum_{i=1}^{n} \ell(Y_i;\theta) - \frac{1}{n}\sum_{i=1}^{n} \ell(Y_i;\theta_0)$$

converges in probability to a non-positive constant.

Therefore, we have that

$$\Pr_{f_0}[\ell_n(\theta_0) \geqslant \ell_n(\theta)] \longrightarrow 1 \tag{12}$$

as $n \longrightarrow \infty$. That is, with probability tending to 1, the log likelihood $\ell_n(\theta_0)$ is not less than $\ell_n(\theta)$ for any other θ.

Asymptotic Theory of the Likelihood

If we make an *identifiability* assumption, this statement may be strengthened: the model $f_Y(y;\theta)$ is *identifiable* if, for two parameter values $\theta^\dagger = \theta^\ddagger$,

$$f_Y(y;\theta^\dagger) = f_Y(y;\theta^\ddagger) \text{ for all } y \quad \Longrightarrow \quad \theta^\dagger = \theta^\ddagger.$$

If the model is identifiable, then the "true" value θ_0 is uniquely defined, and we have

$$\Pr_{f_0}[\ell_n(\theta_0) > \ell_n(\theta)] \longrightarrow 1 \qquad \theta \neq \theta_0. \tag{13}$$

Asymptotic Theory of the Likelihood

This theory holds for fixed θ_0 in the expression

$$\frac{1}{n}\left(\ell_n(\theta) - \ell_n(\theta_0)\right)$$

However, we need to study $\ell_n(\widehat{\theta}_n(Y_{1:n}))$, that is, where the parameter at which the log-likelihood is evaluated is itself a random variable, namely the estimator $\widehat{\theta}_n(Y_{1:n})$.

Asymptotic Theory of the Likelihood

It can be shown that $\widehat{\theta}_n(Y_{1:n}) \xrightarrow{p} \theta_0$ and $\widehat{\theta}_n(Y_{1:n})$ is *consistent* for θ_0, and by "continuous mapping" (as $\ell_n(\theta)$ is a continuous function in θ)

$$\left| \frac{1}{n} \left\{ \ell_n(\widehat{\theta}_n(Y_{1:n})) - \ell_n(\theta_0) \right\} \right| \xrightarrow{p} 0$$

so that, from (5), as $n \longrightarrow \infty$

$$\frac{1}{n} \sum_{i=1}^{n} \ell(Y_i; \widehat{\theta}_n(Y_{1:n})) \xrightarrow{p} \mathbb{E}_{f_0} \left[\ell(Y; \theta_0) \right] \tag{14}$$

5. **Asymptotic Normality:** For a continuous function such as $\dot{\ell}_n(\theta)$, with defined second derivative $\ddot{\ell}_n(\theta)$, it is guaranteed by the Mean Value Theorem that there exists an 'intermediate value'

$$\widetilde{\theta} = c\widehat{\theta}_n + (1-c)\theta_0$$

for some c, $0 < c < 1$, such that

$$\dot{\ell}_n(\widehat{\theta}_n) = \dot{\ell}_n(\theta_0) + \ddot{\ell}_n(\widetilde{\theta})(\widehat{\theta}_n - \theta_0)$$

- The left hand side is zero as $\widehat{\theta}_n$ is the mle.

Asymptotic Theory of the Likelihood

- Provided $\ddot{\ell}_n(\widetilde{\theta})$ is non-singular, we may write after rescaling and rearrangement that

$$\sqrt{n}(\widehat{\theta}_n - \theta_0) = \left\{ -\frac{1}{n}\ddot{\ell}_n(\widetilde{\theta}) \right\}^{-1} \left\{ \sqrt{n}\left(\frac{1}{n}\dot{\ell}_n(\theta_0) \right) \right\} \qquad (15)$$

Asymptotic Theory of the Likelihood

- In its random variable form, second term on the right hand side of (15) is

$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n} S(Y_i;\theta_0)\right)$$

that is, a sample average quantity scaled by $\sqrt{n}$. But by definition of θ_0,

$$\mathbb{E}_{f_0}[S(Y_i;\theta_0)] = \int \dot{\ell}(y;\theta_0) f_0(y)\, dy = \mathbf{0}_d$$

as, by definition θ_0 minimizes $KL(f_0, f_Y(;\theta))$, and therefore must be a solution of this equation.

Asymptotic Theory of the Likelihood

Therefore, by the Central Limit Theorem

$$\sqrt{n}\left(\frac{1}{n}\sum_{i=1}^{n} S(Y_i;\theta_0)\right) \xrightarrow{d} Normal_d(\mathbf{0}_d, \mathcal{J}_{f_0}(\theta_0)) \qquad (16)$$

where

$$\mathcal{J}_{f_0}(\theta_0) = \mathbb{E}_{f_0}[S(Y;\theta_0)S(Y;\theta_0)^\top] \equiv \mathrm{Var}_{f_0}[S(Y;\theta_0)]$$

is a $(d \times d \times d)$ quantity.

Asymptotic Theory of the Likelihood

- As $\widehat{\theta}_n \xrightarrow{p} \theta_0$, we have that

$$-\frac{1}{n}\ddot{\ell}_n(\widetilde{\theta}) \xrightarrow{\text{a.s.}} \mathcal{I}_{f_0}(\theta_0).$$

Therefore we write for an asymptotic approximation to (15)

$$\sqrt{n}(\widehat{\theta}_n - \theta_0) = \left\{-\frac{1}{n}\ddot{\ell}_n(\theta_0)\right\}\left\{\frac{1}{\sqrt{n}}\dot{\ell}_n(\theta_0)\right\} + \mathrm{o}_p(1)$$

where the distribution of the second term given by (16), and where $\mathrm{o}_p(1)$ denotes a term that converges in probability to zero.

Asymptotic Theory of the Likelihood

We therefore have that

$$\sqrt{n}(\widehat{\theta}_n - \theta_0) \xrightarrow{d} Normal_d(\mathbf{0}_d, \Sigma(\theta_0))$$

where

$$\Sigma(\theta_0) = \{\mathcal{I}_{f_0}(\theta_0)\}^{-1}\mathcal{J}_{f_0}(\theta_0)\{\mathcal{I}_{f_0}(\theta_0)\}^{-1}$$

6. **Correct specification:** Under *correct specification*

$$f_0(y) \equiv f_Y(y; \theta_0),$$

and we have from earlier results that

$$\mathcal{J}_{\theta_0}(\theta_0) = \mathcal{I}_{\theta_0}(\theta_0)$$

and hence from the general result we deduce that

$$\sqrt{n}(\widehat{\theta}_n - \theta_0) \xrightarrow{d} Normal_d(\mathbf{0}_d, \{\mathcal{I}_{\theta_0}(\theta_0)\}^{-1}).$$

Implications for Bayesian analysis

Using the same quadratic approximation for the likelihood at θ around $\widehat{\theta}_n$ we have

$$\ell_n(\theta) \doteq \ell_n(\widehat{\theta}_n) + \dot{\ell}_n(\widehat{\theta}_n)^\top(\widehat{\theta}_n - \theta) + \frac{1}{2}(\widehat{\theta}_n - \theta)^\top \ddot{\ell}_n(\widehat{\theta}_n)(\widehat{\theta}_n - \theta)$$

but noting that $\dot{\ell}_n(\widehat{\theta}_n) = 0$, we have that

$$\exp\{\ell_n(\theta)\} \doteq \exp\{\ell_n(\widehat{\theta}_n)\} \exp\left\{\frac{1}{2}(\widehat{\theta}_n - \theta)^\top \ddot{\ell}_n(\widehat{\theta}_n)(\widehat{\theta}_n - \theta)\right\}$$

$$\propto \exp\left\{-\frac{1}{2}(\theta - \widehat{\theta}_n)^\top \{-\ddot{\ell}_n(\widehat{\theta}_n)\}(\theta - \widehat{\theta}_n)\right\}.$$

Implications for Bayesian analysis

Thus, when the regularity conditions apply, the likelihood can be approximated by one arising from a Normal distribution

$$Normal_d\left(\widehat{\theta}_n, \left\{-\ddot{\ell}_n(\widehat{\theta}_n)\right\}^{-1}\right).$$

This approximation can be used in a wide variety of models.

1.5 Modelling Extensions

Beyond the iid case, Bayesian methods can be used for

- regression models (linear, non-linear, generalized linear);
- latent variable models;
- hierarchical models.

Regression models

We consider the infinite sequence $\{(X_n, Y_n), n = 1, 2, \ldots\}$ such that for any $n \geqslant 1$

$$f_{X_1,\ldots,X_n,Y_1,\ldots,Y_n}(x_1, \ldots, x_n, y_1, \ldots, y_n)$$

is factorized

$$f_{X_1,\ldots,X_n}(x_1, \ldots, x_n) f_{Y_1,\ldots,Y_n|X_1,\ldots,X_n}(y_1, \ldots, y_n | x_1, \ldots, x_n)$$

where each term has a de Finetti representation.

Regression models

$$f_{X_1,\ldots,X_n}(x_1,\ldots,x_n)$$

$$= \int \left\{ \prod_{i=1}^{n} f_X(x_i;\phi) \right\} \pi_0(d\phi)$$

$$f_{Y_1,\ldots,Y_n|X_1,\ldots,X_n}(y_1,\ldots,y_n|x_1,\ldots,x_n)$$

$$= \int \left\{ \prod_{i=1}^{n} f_{Y|X}(y_i|x_i;\theta) \right\} \pi_0(d\theta)$$

Regression models

Inference for (ϕ, θ) is required:

- inference for ϕ via the *marginal model* for the X variables;
- inference for θ via the *conditional model* for Y given that $X = x$ was observed.

In the latter case, the fact that X is random is immaterial as we perform a conditional on x analysis.

When considering the statistical behaviour of Bayesian (or frequentist) procedures, we must remember that X and Y have *joint* structure.

Example: Prediction

To predict Y_{n+1},

$$f_{Y_{n+1}|X_{1:n},Y_{1:n}}(y_{n+1}|x_{1:n},y_{1:n})$$

$$= \int f_{X_{n+1},Y_{n+1}|X_{1:n},Y_{1:n}}(x_{n+1},y_{n+1}|x_{1:n},y_{1:n})dx_{n+1}$$

$$= \int f_{Y_{n+1}|X_{1:n},X_{n+1},Y_{1:n}}(y_{n+1}|x_{1:n},x_{n+1},y_{1:n})$$

$$f_{X_{n+1}|X_{1:n},Y_{1:n}}(x_{n+1}|x_{1:n},y_{1:n})\ dx_{n+1}$$

Linear regression

Suppose that we have the linear regression model

$$Y_i = \mathbf{x}_i \beta + \varepsilon_i$$

where for $i = 1, \ldots, n$

- Y_i is a scalar
- $\mathbf{x}_i$ is $(1 \times d)$
- β is $(d \times 1)$
- $\varepsilon_i \sim Normal(0, \sigma^2)$, independently.

This describes the model for the partially exchangeable Y_i conditional on the $\mathbf{X}_i = \mathbf{x}_i$.

- There may or not be a need to model the distribution of the $\mathbf{X}_i$.

Linear regression

In vector form

$$\mathbf{Y} = \mathbf{X}\beta + \varepsilon$$

where $\mathbf{Y}$ and ε are $(n \times 1)$, $\mathbf{X}$ is $(n \times d)$.

We then have that in the conditional model

$$f_{Y_1,\ldots,Y_n|X_1,\ldots,X_n}(y_1,\ldots,y_n|x_1,\ldots,x_n;\beta,\sigma^2) \equiv Normal_n(\mathbf{X}\beta,\sigma^2\mathbf{I}_n)$$

where $\mathbf{I}_n$ is the $(n \times n)$ identity matrix.

Linear regression

Therefore the likelihood is

$$\mathcal{L}_n(\beta, \sigma^2) = \left(\frac{1}{2\pi\sigma^2}\right)^{n/2} \exp\left\{-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\beta)^\top(\mathbf{y} - \mathbf{X}\beta)\right\}.$$

A conjugate prior in this setting can be factorized

$$\pi_0(\beta, \sigma^2) = \pi_0(\sigma^2)\pi_0(\beta|\sigma^2)$$

where

$$\pi_0(\sigma^2) \equiv \mathit{InvGamma}(a_0/2, b_0/2)$$

$$\pi_0(\beta|\sigma^2) \equiv \mathit{Normal}_d(\mathbf{m}_0, \sigma^2\mathbf{M}_0)$$

where $a_0, b_0, \mathbf{m}_0$ and $\mathbf{M}_0$ are fixed constant *hyperparameters*.

$$\pi_0(\sigma^2) = \frac{(b_0/2)^{a_0/2}}{\Gamma(a_0/2)} \left(\frac{1}{\sigma^2}\right)^{a_0/2+1} \exp\left\{-\frac{b_0}{2\sigma^2}\right\}$$

$$\pi_0(\beta|\sigma^2) = \left(\frac{1}{2\pi\sigma^2}\right)^{d/2} \frac{1}{|\mathbf{M}_0|^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(\beta-\mathbf{m}_0)^\top \mathbf{M}_0^{-1}(\beta-\mathbf{m}_0)\right\}$$

To compute the joint posterior $\pi_n(\beta, \sigma^2)$ up to proportionality

$$\mathcal{L}_n(\beta, \sigma^2)\pi_0(\beta, \sigma^2)$$

we need to examine the exponent as a quadratic form.

Linear regression

The expression

$$(\mathbf{y} - \mathbf{X}\beta)^\top(\mathbf{y} - \mathbf{X}\beta) + (\beta - \mathbf{m}_0)^\top \mathbf{M}_0^{-1}(\beta - \mathbf{m}_0)$$

equates to

$$(\beta - \mathbf{m}_n)^\top \mathbf{M}_n^{-1}(\beta - \mathbf{m}_n) + c_n$$

where we need to find expressions for $\mathbf{m}_n$, $\mathbf{M}_n$ and c_n.

- Quadratic term:

$$\beta^\top \mathbf{M}_n^{-1}\beta = \beta^\top \mathbf{X}^\top \mathbf{X}\beta + \beta^\top \mathbf{M}_0^{-1}\beta$$

  so therefore

$$\mathbf{M}_n^{-1} = \mathbf{X}^\top \mathbf{X} + \mathbf{M}_0^{-1} \qquad \therefore \qquad \mathbf{M}_n = (\mathbf{X}^\top \mathbf{X} + \mathbf{M}_0^{-1})^{-1}$$

Linear regression

- Linear term:

$$\beta^\top \mathbf{M}_n^{-1} \mathbf{m}_n = \beta^\top \mathbf{X}^\top \mathbf{y} + \beta^\top \mathbf{M}_0^{-1} \mathbf{m}_0$$

  so therefore

$$\begin{aligned} \mathbf{m}_n &= \mathbf{M}_n(\mathbf{X}^\top \mathbf{y} + \mathbf{M}_0^{-1} \mathbf{m}_0) \\ &= (\mathbf{X}^\top \mathbf{X} + \mathbf{M}_0^{-1})^{-1}(\mathbf{X}^\top \mathbf{y} + \mathbf{M}_0^{-1} \mathbf{m}_0) \end{aligned}$$

Linear regression

- Constant term:

$$\mathbf{m}_n^\top \mathbf{M}_n^{-1} \mathbf{m}_n + c_n = \mathbf{y}^\top \mathbf{y} + \mathbf{m}_0^\top \mathbf{M}_0^{-1} \mathbf{m}_0$$

  so therefore

$$c_n = \mathbf{y}^\top \mathbf{y} + \mathbf{m}_0^\top \mathbf{M}_0^{-1} \mathbf{m}_0 - \mathbf{m}_n^\top \mathbf{M}_n^{-1} \mathbf{m}_n$$

Therefore for the joint posterior up to proportionality is

$$\left(\frac{1}{\sigma^2}\right)^{\frac{(n+a_0+d)}{2}+1} \exp\left\{-\frac{(c_n+b_0)}{2\sigma^2}\right\} \times \exp\left\{-\frac{1}{2\sigma^2}(\beta-\mathbf{m}_n)^\top \mathbf{M}_n^{-1}(\beta-\mathbf{m}_n)\right\}$$

from which we can conclude directly that for the conditional posterior

$$\pi_n(\beta|\sigma^2) \equiv Normal_d(\mathbf{m}_n, \sigma^2\mathbf{M}_n)$$

Integrating out β from the joint posterior, we obtain that up to proportionality

$$\pi_n(\sigma^2) \propto \left(\frac{1}{\sigma^2}\right)^{\frac{(n+a_0)}{2}+1} \exp\left\{-\frac{(c_n+b_0)}{2\sigma^2}\right\}$$

that is

$$\pi_n(\sigma^2) \equiv InvGamma(a_n/2, b_n/2)$$

where

$$a_n = n + a_0 \qquad b_n = c_n + b_0$$

Finally, we can compute the marginal posterior for β. From the arguments above we have that the joint posterior takes the form

$$\pi_n(\beta|\sigma^2)\pi_n(\sigma^2)$$

which equates to

$$\frac{(b_n/2)^{a_n/2}}{\Gamma(a_n/2)}\left(\frac{1}{\sigma^2}\right)^{a_n/2+1}\exp\left\{-\frac{b_n}{2\sigma^2}\right\}$$

$$\times\left(\frac{1}{2\pi\sigma^2}\right)^{d/2}\frac{1}{|\mathbf{M}_n|^{1/2}}\exp\left\{-\frac{1}{2\sigma^2}(\beta-\mathbf{m}_n)^\top\mathbf{M}_n^{-1}(\beta-\mathbf{m}_n)\right\}$$

The constant term is

$$\frac{(b_n/2)^{a_n/2}}{\Gamma(a_n/2)} \left(\frac{1}{2\pi}\right)^{d/2} \frac{1}{|\mathbf{M}_n|^{1/2}}$$

and to marginalize we must compute

$$\int_0^\infty \left(\frac{1}{\sigma^2}\right)^{\frac{a_n+d}{2}+1} \left\{-\frac{1}{2\sigma^2}\left[b_n + (\beta-\mathbf{m}_n)^\top \mathbf{M}_n^{-1}(\beta-\mathbf{m}_n)\right]\right\} d\sigma^2$$

The integrand is the kernel of an Inverse Gamma pdf so therefore we have that the integral equates to

$$\frac{\Gamma((a_n + d)/2)}{\left\{\frac{1}{2}\left[b_n + (\beta - \mathbf{m}_n)^\top \mathbf{M}_n^{-1}(\beta - \mathbf{m}_n)\right]\right\}^{\frac{a_n+d}{2}}}$$

Linear regression

Combining terms together, we have that

$$\pi_n(\beta) =$$

$$\frac{b_n^{a_n/2}}{\Gamma(a_n/2)\pi^{d/2}} \frac{1}{|\mathbf{M}_n|^{1/2}} \frac{\Gamma((a_n+d)/2)}{\left\{b_n + (\beta - \mathbf{m}_n)^\top \mathbf{M}_n^{-1}(\beta - \mathbf{m}_n)\right\}^{\frac{a_n+d}{2}}}$$

which is a *multivariate Student-t distribution*.

Note that we may rewrite this form as

$$\pi_n(\beta) =$$

$$\frac{\Gamma((a_n+d)/2)}{\Gamma(a_n/2)a_n^{d/2}\pi^{d/2}}\frac{1}{|\Sigma_n|^{1/2}}\frac{1}{\left\{1+a_n^{-1}(\beta-\mathbf{m}_n)^\top\Sigma_n^{-1}(\beta-\mathbf{m}_n)\right\}^{\frac{a_n+d}{2}}}$$

which is the typical representation[1], where we have written

$$a_n\Sigma_n = b_nM_n$$

[1] (https://en.wikipedia.org/wiki/Multivariate_t-distribution, as adopted in the R package mvnfast)

Note

We may express prior ignorance concerning β by considering $\mathbf{M}_0^{-1} \longrightarrow \mathbf{0}$, in which case

$$\mathbf{m}_n \longrightarrow (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

and

$$\mathbf{M}_n \longrightarrow (\mathbf{X}^\top \mathbf{X})^{-1}$$

yielding results equivalent to those of maximum likelihood.

This 'uniform' prior for β is in line with the earlier non-informative constructions.

Note

An alternative is the *g-prior*: for hyperparameter $\lambda > 0$

$$\mathbf{M}_0 = \lambda^{-1}(\mathbf{X}^\top \mathbf{X})^{-1}$$

in which case

$$\mathbf{M}_n = (1+\lambda)^{-1}(\mathbf{X}^\top \mathbf{X})^{-1}$$

Note

If, for hyperparameter $\lambda > 0$

$$\mathbf{m}_0 = \mathbf{0}_d \qquad \mathbf{M}_0 = \lambda \mathbf{I}_d$$

then

$$\mathbf{m}_n = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_d)^{-1} \mathbf{X}^\top \mathbf{y}$$

and

$$\mathbf{M}_n = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_d)^{-1}$$

yields the *ridge regression* procedure

Note

The log density is

$$\ell(\beta, \sigma^2) = -\frac{1}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(y - \mathbf{x}\beta)^2 + \text{constant}$$

so therefore

$$\frac{\partial \ell(\beta, \sigma^2)}{\partial \beta} = \frac{1}{\sigma^2}\mathbf{x}^\top(y - \mathbf{x}\beta)$$

$$\frac{\partial^2 \ell(\beta, \sigma^2)}{\partial \beta \partial \beta^\top} = -\frac{1}{\sigma^2}\mathbf{x}^\top\mathbf{x}$$

Note

Also

$$\frac{\partial \ell(\beta, \sigma^2)}{\partial \sigma^2} = -\frac{1}{2\sigma^2} + \frac{1}{2\sigma^4}(y - \mathbf{x}\beta)^2$$

$$\frac{\partial^2 \ell(\beta, \sigma^2)}{\partial (\sigma^2)^2} = \frac{1}{2\sigma^4} - \frac{1}{\sigma^6}(y - \mathbf{x}\beta)^2$$

and

$$\frac{\partial^2 \ell(\beta, \sigma^2)}{\partial \beta \partial \sigma^2} = -\frac{1}{\sigma^4}\mathbf{x}^\top (y - \mathbf{x}\beta)$$

Note

Hence the (unit) Fisher information is

$$\mathcal{I}(\beta, \sigma^2) = \left| - \begin{bmatrix} -\frac{1}{\sigma^2}\mathbf{x}^\top\mathbf{x} & 0 \\ 0 & -\frac{1}{2\sigma^4} \end{bmatrix} \right| = \frac{1}{2}\left(\frac{1}{\sigma^2}\right)^{d+2} \left|\mathbf{x}^\top\mathbf{x}\right|$$

which implies that Jeffreys's prior for linear regression is

$$\pi_0(\beta, \sigma^2) \propto \left(\frac{1}{\sigma^2}\right)^{d/2+1}$$

Note

This prior depends on dimension d. It is common instead to use the prior

$$\pi_0(\beta, \sigma^2) \propto \frac{1}{\sigma^2}$$

as an invariant prior for linear regression.

Non-linear regression

- **Generalized Linear Models:** $f_{Y|X}(y|x;\beta)$ follows an Exponential Family Model with

$$\mathbb{E}_{Y|X}[Y|\mathbf{X}=\mathbf{x};\beta] = g^{-1}(\mathbf{x}\beta) \equiv \mu$$

$$\mathrm{Var}_{Y|X}[Y|\mathbf{X}=\mathbf{x};\beta] = V(\mu)$$

that is

$$g(\mu) = \mathbf{x}\beta$$

for some *link function*, g.

Example: Poisson regression

$$Y_i|\mathbf{X}_i = \mathbf{x}_i \sim \textit{Poisson}(\mu_i)$$

$$\mathbb{E}_{Y|X}[Y_i|\mathbf{X}_i = \mathbf{x}_i; \beta] = \exp(\mathbf{x}_i\beta) \equiv \mu_i$$

$$\text{Var}_{Y|X}[Y|\mathbf{X}_i = \mathbf{x}_i; \beta] = \mu_i$$

so that

$$\mathcal{L}_n(\beta) = \prod_{i=1}^{n} \frac{\exp\{y_i \log \mu_i - \mu_i\}}{y_i!} = \prod_{i=1}^{n} \frac{\exp\{y_i \mathbf{x}_i\beta - \exp\{\mathbf{x}_i\beta\}\}}{y_i!}$$

Non-linear regression

Example: Poisson regression

$$\ell_n(\beta) = \sum_{i=1}^{n} (y_i \mathbf{x}_i \beta - \exp\{\mathbf{x}_i \beta\}) + \text{const.}$$

$$\dot{\ell}_n(\beta) = \sum_{i=1}^{n} \left(y_i \mathbf{x}_i^\top - \exp\{\mathbf{x}_i \beta\} \mathbf{x}_i^\top \right) = \sum_{i=1}^{n} \mathbf{x}_i^\top \left(y_i - \exp\{\mathbf{x}_i \beta\} \right)$$

$$\ddot{\ell}_n(\beta) = -\sum_{i=1}^{n} \exp\{\mathbf{x}_i \beta\} \mathbf{x}_i^\top \mathbf{x}_i$$

that is, writing $\mathbf{D}(\mathbf{X}\beta) = \text{diag}(\exp\{\mathbf{x}_1 \beta\}, \ldots, \exp\{\mathbf{x}_n \beta\})$.

$$\dot{\ell}_n(\beta) = \mathbf{X}^\top (\mathbf{y} - \boldsymbol{\mu}) \qquad \ddot{\ell}_n(\beta) = -\mathbf{X}^\top \mathbf{D}(\mathbf{X}\beta) \mathbf{X}$$

Non-linear regression

Example: Binary regression

$$Y_i|\mathbf{X}_i = \mathbf{x}_i \sim \textit{Bernoulli}(\mu_i)$$

$$\mathbb{E}_{Y|X}[Y_i|\mathbf{X} = \mathbf{x}_i; \beta] = \frac{\exp(\mathbf{x}_i\beta)}{1 + \exp(\mathbf{x}_i\beta)} \equiv \mu_i$$

$$\text{Var}_{Y|X}[Y_i|\mathbf{X}_i = \mathbf{x}_i; \beta] = \mu_i(1 - \mu_i)$$

Example: Binary regression

$$\begin{aligned}
\mathcal{L}_n(\beta) &= \prod_{i=1}^{n} \exp\left\{y_i \log \mu_i + (1-y_i)\log(1-\mu_i)\right\} \\
&= \prod_{i=1}^{n} \exp\left\{y_i \log\left(\frac{\mu_i}{1-\mu_i}\right) + \log(1-\mu_i)\right\} \\
&= \prod_{i=1}^{n} \exp\left\{y_i \mathbf{x}_i \beta - \log(1+\exp\{\mathbf{x}_i\beta\})\right\}
\end{aligned}$$

Example: Binary regression

$$\ell_n(\beta) = \sum_{i=1}^{n} \left(y_i \mathbf{x}_i \beta - \log(1 + \exp\{\mathbf{x}_i \beta\}) \right)$$

$$\dot{\ell}_n(\beta) = \sum_{i=1}^{n} \mathbf{x}_i^\top \left(y_i - \frac{\exp\{\mathbf{x}_i \beta\}}{1 + \exp\{\mathbf{x}_i \beta\}} \right)$$

$$\ddot{\ell}_n(\beta) = -\sum_{i=1}^{n} \frac{\exp\{\mathbf{x}_i \beta\}}{(1 + \exp\{\mathbf{x}_i \beta\})^2} \mathbf{x}_i^\top \mathbf{x}_i = -\sum_{i=1}^{n} \mu_i (1 - \mu_i) \mathbf{x}_i^\top \mathbf{x}_i$$

that is, now writing $\mathbf{D}(\mathbf{X}\beta) = \text{diag}(\mu_1(1-\mu_1), \ldots, \mu_n(1-\mu_n))$.

$$\dot{\ell}_n(\beta) = \mathbf{X}^\top (\mathbf{y} - \boldsymbol{\mu}) \qquad \ddot{\ell}_n(\beta) = -\mathbf{X}^\top \mathbf{D}(\mathbf{X}\beta) \mathbf{X}$$

Non-linear regression

Using the quadratic approximation theory, we have that

$$\mathcal{L}_n(\beta) \doteq c_n(\widehat{\beta}_n) \exp\left\{-\frac{1}{2}(\beta - \widehat{\beta}_n)^\top \Sigma_n^{-1}(\widehat{\beta}_n)(\beta - \widehat{\beta}_n)\right\}$$

where

$$\Sigma_n(\widehat{\beta}_n) = \left(\mathbf{X}^\top \mathbf{D}(\mathbf{X}\widehat{\beta}_n)\mathbf{X}\right)^{-1}$$

This approximate likelihood can be combined with a Normal prior on β.

Non-linear regression

Example: GLM

See `knitr 3`.

Non-linear regression

- **Non-linear regression:**

$$Y_i = g(\mathbf{x}_i; \theta) + \varepsilon_i$$

where $g(.;.)$ is some non-linear function of its arguments, and $\varepsilon_i \sim Normal(0, \sigma^2)$.

$$\mathcal{L}_n(\theta, \sigma^2) = \left(\frac{1}{2\pi\sigma^2}\right)^{n/2} \exp\left\{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - g(\mathbf{x}_i; \theta))^2\right\}.$$

Non-linear regression

Example: Exponential decay models

For $\theta = (\theta_0, \theta_1, \theta_3, \theta_4)^\top$ with $\theta_j > 0$ for $j = 1, 2, 3, 4$

$$g(\mathrm{x}_i; \theta) = \theta_1 e^{-\theta_2 \mathrm{x}_i} + \theta_3 e^{-(\theta_2 + \theta_4)\mathrm{x}_i}$$

where $x_i > 0$ is a scalar quantity.

- $\widehat{\theta}_n$ found numerically;
- $\dot{\ell}(\theta, \sigma^2)$ and $\ddot{\ell}(\theta, \sigma^2)$ straightforward to compute;
- similar $Normal(\widehat{\theta}_n, \Sigma_n(\widehat{\theta}_n)$ approximation available.

Latent variable models

Latent (or *auxiliary*) variables can be introduced to simplify calculations in a model.

Suppose $f_Y(y;\theta)$ is intractable, but

$$f_Y(y;\theta) = \int f_{Y,Z}(y,z;\theta)\, dz$$

for some other variable Z, where the augmented joint distribution

$$f_{Y,Z}(y,z;\theta)$$

is tractable.

Example: Mixture model

Suppose

$$f_Y(y;\theta) = (1-\omega) f_0(y;\theta_0) + \omega f_1(y;\theta_1)$$

so that $\theta = (\omega, \theta_0, \theta_1)$, so that $0 < \omega < 1$. Then

$$f_Y(y;\theta) = \sum_{z=0}^{1} f_{Y,Z}(y,z;\theta) = \sum_{z=0}^{1} f_{Y|Z}(y|z;\theta) p_Z(z;\theta)$$

where

$$p_Z(z;\theta) = \Pr[Z=z] = \begin{cases} 1-\omega & z=0 \\ \omega & z=1 \end{cases}$$

and

$$f_{Y|Z}(y|z;\theta) = f_z(y;\theta_z) \qquad z = 0, 1.$$

Example: Mixture model

Then

$$f_{Y,Z}(y_i, z_i; \theta) = \omega^{z_i}(1-\omega)^{1-z_i} f_0(y_i; \theta_0)^{1-z_i} f_1(y_i; \theta_1)^{z_i}$$

and the *sum* in the original pdf $f_Y(y; \theta)$ has become a *product*.

Example: Mixture model

Then

$$\prod_{i=1}^{n} f_Y(y_i;\theta) = \prod_{i=1}^{n} \{(1-\omega) f_0(y_i;\theta_0) + \omega f_1(y_i;\theta_1)\}$$

which is not very tractable, but

$$\prod_{i=1}^{n} f_{Y,Z}(y_i, z_i;\theta) = \prod_{i=1}^{n} \prod_{z=0}^{1} \{\omega_z f_z(y;\theta_z)\}^{\mathbb{1}_z(z_i)}$$

where $\omega_0 = (1-\omega)$ and $\omega_1 = \omega$, which is more tractable.

Latent variable models

Example: see also

- data with *censoring*;
- *state space* models.

Hierarchical models

Hierarchical or *multi-level* models are built by 'stacking' levels of variables.

- *random effects* (or *mixed*) models;
- *multi-level* models
  - hospital/physician or school *league tables*;
  - *multi-arm* clinical studies;

Example: Multi-centre models

K centres, labelled $1, 2, \ldots, K$.

- **STAGE 3:** For centre k, data $Y_{k1}, \ldots, Y_{kn_k}$ partially exchangeable, and conditionally independent given centre parameter θ_k. For each k

$$\prod_{i=1}^{n_k} f_k(y_{ki}; \theta_k).$$

- **STAGE 2:** Parameters $\theta_1, \ldots, \theta_K$ exchangeable,

$$\prod_{k=1}^{K} \pi_0^{(2)}(\theta_k | \phi).$$

- **STAGE 1:** Prior on ϕ, $\pi_0^{(1)}(\phi)$.

Hierarchical models

Example: Multi-centre models

Data generating model:

- Pick $\phi \sim \pi_0^{(1)}(\phi)$
- Pick $\theta_1, \ldots, \theta_K \sim \pi_0^{(2)}(\theta_k|\phi)$
- For each $k = 1, \ldots, K$, pick

$$Y_{k1}, \ldots, Y_{kn_k} \sim f_k(.; \theta_k)$$

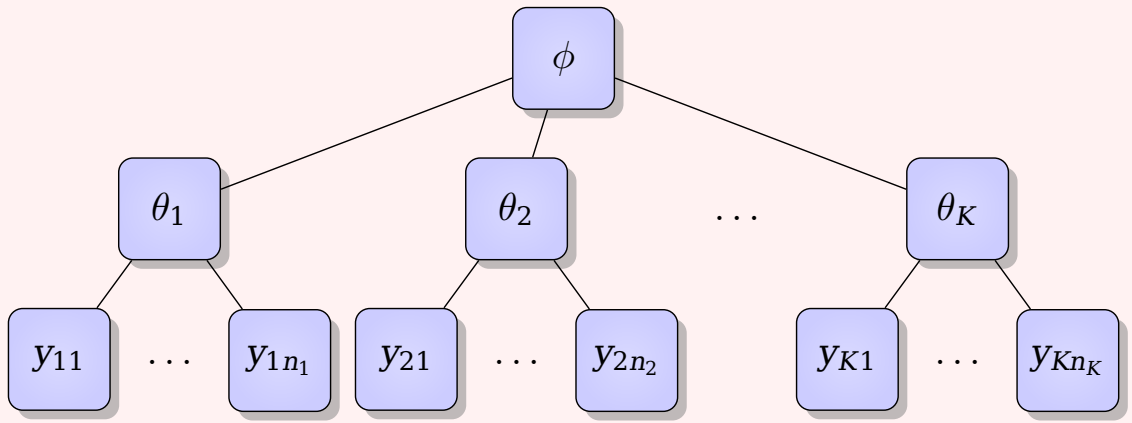
Hierarchical models

Example: Multi-centre models

STAGE 1 $\pi_0^{(1)}(\phi)$

STAGE 2 $\pi_2^{(2)}(\theta_k|\phi)$

STAGE 3 $f_k(y_{ki};\theta_k)$

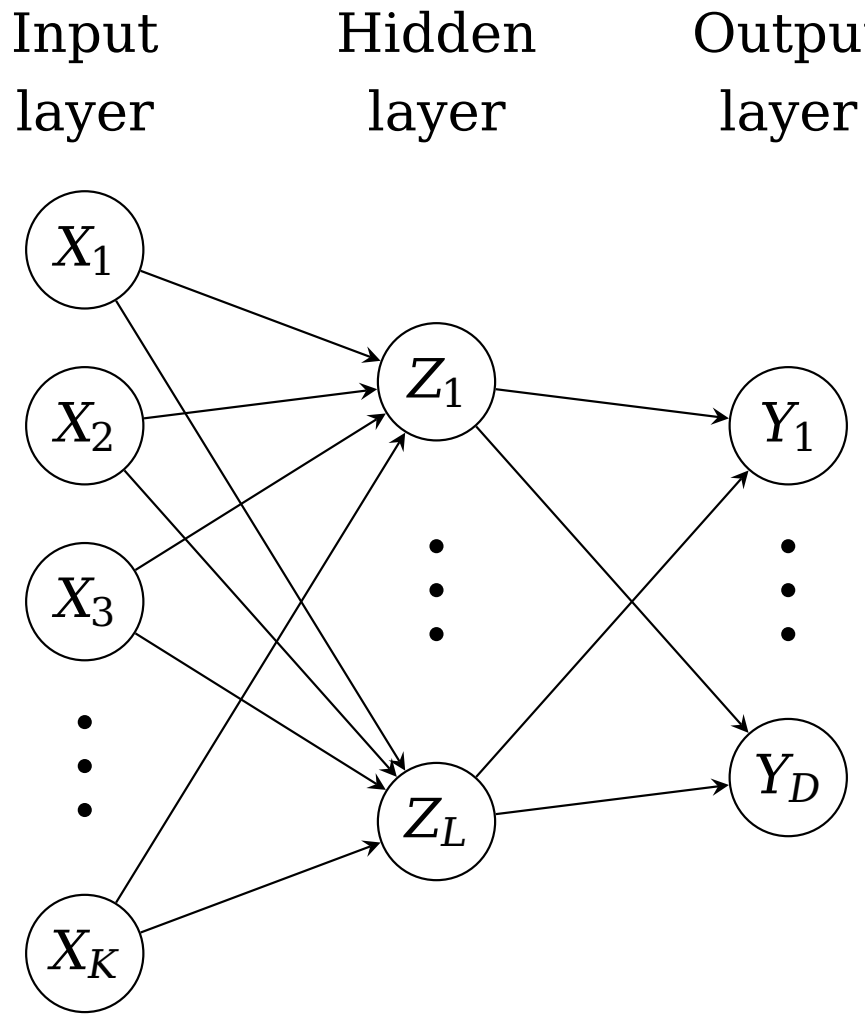


Hierarchical models

The posterior distribution $\pi_n(\phi, \theta_1, \ldots, \theta_K)$ is given, up to proportionality, by

$$\pi_n(\phi, \theta_1, \ldots, \theta_K) \propto \left\{ \prod_{k=1}^{K} \left\{ \prod_{i=1}^{n_k} f_k(y_{ki}; \theta_k) \right\} \pi_0^{(2)}(\theta_k | \phi) \right\} \pi_0^{(1)}(\phi)$$

Neural network models



Neural network models

Hidden Layer:

$$Z_l = g_{1l}\left(\sum_{k=1}^{K} w_{lk}^{(1)} X_k + b_l^{(1)}, \epsilon_l\right) \qquad l = 1, \ldots, L$$

with $\epsilon_1, \ldots, \epsilon_L$ residual errors.

Output Layer:

$$Y_d = g_{2d}\left(\sum_{l=1}^{L} w_{dl}^{(2)} Z_l + b_d^{(2)}, \varepsilon_d\right) \qquad d = 1, \ldots, D$$

with $\varepsilon_1, \ldots, \varepsilon_D$ residual errors.

Neural network models

- Data on $X_1, \ldots, X_K$ and $Y_1, \ldots, Y_D$ observed;
- Parameters are

$$\textit{Weights} : w_{lk}^{(1)}, l = 1, \ldots, L, k = 1, \ldots, K$$

$$: w_{dl}^{(2)}, d = 1, \ldots, D, l = 1, \ldots, L$$

$$\textit{Biases} : b_1^{(1)}, l = 1, \ldots, L$$

$$: b_d^{(2)}, d = 1, \ldots, D$$

- Link functions $g_{1l}(.), l = 1, \ldots, L$ and $g_{2d}(.), d = 1, \ldots, D$.

Neural network models

The *complete data* likelihood $\mathcal{L}_n(\mathbf{w}, \mathbf{b})$ is given, up to proportionality, by

$$\mathcal{L}_n(\mathbf{w}, \mathbf{b}) = \prod_{i=1}^{n} \left\{ \prod_{l=1}^{L} \left\{ f_{Z_{li}|\mathbf{x}_i}(z_{li}|\mathbf{x}_i; \mathbf{w}^{(1)}, \mathbf{b}^{(1)}) \right\} \right. \qquad (\textit{hidden})$$

$$\left. \times \prod_{d=1}^{D} \left\{ f_{Y_{di}|\mathbf{z}_i}(y_{di}|\mathbf{z}_i; \mathbf{w}^{(2)}, \mathbf{b}^{(2)}) \right\} \right\} \qquad (\textit{output})$$

where the hidden variables

$$Z_{li}, l = 1, \ldots, L, i = 1, \ldots, n$$

are treated as auxiliary quantities.

1.6 Model selection approaches

It is often necessary to consider model selection and evaluation approaches

- *in-sample* validity;
- *generalization*;

Assumptions

Consider the exchangeable, continuous case.

- For the *inference* model
  - $\theta \in \mathbb{R}^d$,
  - likelihood model $f_Y(y;\theta)$,
  - prior $\pi_0(\theta)$.
  - posterior $\pi_n(\theta)$.
- Suppose that the *data-generating* model is

$$f^*(y) \equiv f^*(y;\varphi)$$

with φ a fixed (but *unknown* to the *modeller*) value, so that exchangeability reduces to *independence*.

Predictive performance

The predictive distribution for the 'next' data point is

$$p_n(y) \equiv p_{Y_{n+1}|Y_1,\ldots,Y_n}(y|y_1,\ldots,y_n) = \int f_Y(y;\theta)\pi_n(\theta)\, d\theta$$

and is the usual Bayesian estimator of $f^*(y)$. It is used to assess the quality of a proposed model.

Predictive performance

If we consider instead

$$\widetilde{p}_n(y) = p_{Y_{n+1}|Y_1,\ldots,Y_n}\left(y|Y_1,\ldots,Y_n\right)$$

then the predictive distribution itself is a *random function*, as it is a function of the random variables $Y_1,\ldots,Y_n$, not the data $y_1,\ldots,y_n$.

We may similarly consider the *random* posterior $\widetilde{\pi}_n(\theta)$, a function of θ that is random because its inputs are $Y_1,\ldots,Y_n$ instead of $y_1,\ldots,y_n$.

Predictive performance

The KL divergence between $f^*(y)$ and $p_n(y)$ is

$$KL(f^*, p_n) = \int \log\left(\frac{f^*(y)}{p_n(y)}\right) f^*(y)\, dy$$

$$= \int \log(f^*(y)) f^*(y)\, dy - \int \log(p_n(y)) f^*(y)\, dy. \qquad (\diamondsuit)$$

The first term in $(\diamondsuit)$ is a constant which does not depend on the inference model.

A random variable version $KL(f^*, \widetilde{p}_n)$ can also be considered.

Predictive performance

- **Training loss:** The *training loss*, T_n, is a measure that approximates the KL divergence based on the sample

$$T_n \equiv T(Y_1, \ldots, Y_n) = -\frac{1}{n} \sum_{i=1}^{n} \log \tilde{p}_n(Y_i)$$

  which can be regarded as a sample-based estimator of the second term in ($\diamondsuit$), with the data drawn independently from f^*.

  In this form, T_n is random variable as it depends on $\tilde{p}_n$.

Predictive performance

- **Generalization loss:** The *generalization loss*, G_n, is the second term in ($\diamondsuit$):

$$G_n \equiv G(Y_1, \ldots, Y_n) = -\int \log \widetilde{p}_n(y) f^*(y)\, dy.$$

This can only be computed precisely if $f^*(y)$ is known. However, we can interpret G_n as a measure of proximity of the predictive model to the data-generating distribution.

Predictive performance

Note

The first term in ($\diamondsuit$) is often denoted $-S$

$$S = -\int \log(f^*(y)) f^*(y)\, dy$$

and is termed the *entropy* of f^*. The quantity

$$G_n - S$$

is termed the *generalization error*: note that $G_n \geqslant S$ as the KL divergence is non-negative.

Predictive performance

- **Cross-validation loss:** The *cross-validation* loss, C_n, is defined by

$$C_n = -\frac{1}{n}\sum_{i=1}^{n} \log \widetilde{p}_n^{(-i)}(Y_i)$$

where $\widetilde{p}_n^{(-i)}(y)$ is the posterior predictive distribution derived from the random variables

$$Y_{1:n}^{(-i)} = (Y_1, \ldots, Y_{i-1}, Y_{i+1}, \ldots, Y_n)$$

that is, the original collection with Y_i removed.

Predictive performance

Taking expectations of G_n and C_n with respect to the joint pdf of $Y_1, \ldots, Y_n$, which by independence reduces to

$$\prod_{i=1}^{n} f^*(y_i)$$

we can establish connections between the losses.

Predictive performance

Provided all expectations are finite

$$\begin{aligned}
\mathbb{E}[C_n] &= \mathbb{E}_{Y_1,\ldots,Y_n}\left[-\frac{1}{n}\sum_{i=1}^{n}\log \widetilde{p}_n^{(-i)}(Y_i)\right] \\
&= -\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_{Y_{1:n}^{(-i)}}\left[\mathbb{E}_{Y_i}\left[\log \widetilde{p}_n^{(-i)}(Y_i)\right]\right] \\
&= -\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_{Y_{1:n}^{(-i)}}\left[\int \log \widetilde{p}_n^{(-i)}(y) f^*(y)\ dy\right]
\end{aligned}$$

where the second line follows using iterated expectation.

Predictive performance

But for $i = 1, 2, \ldots, n$ the terms

$$\int \log \widetilde{p}_n^{(-i)}(y) f^*(y)\, dy$$

are *identically distributed* random variables, so

$$-\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{Y_{1:n}^{(-i)}} \left[\int \log \widetilde{p}_n^{(-i)}(y) f^*(y)\, dy \right]$$

is equal to

$$\mathbb{E}_{Y_{1:n}^{(-1)}} \left[- \int \log \widetilde{p}_n^{(-1)}(y) f^*(y)\, dy \right] \equiv \mathbb{E}[G_{n-1}]$$

again as $Y_1, \ldots, Y_n$ are iid from f^*.

Predictive performance

Note also that

$$p_n^{(-i)}(y) = \int f_Y(y;\theta)\pi_n^{(-i)}(\theta)\ d\theta$$

$$= \int f_Y(y;\theta)\frac{\prod_{j\neq i} f_Y(y_j;\theta)\pi_0(\theta)}{\int \prod_{j\neq i} f_Y(y_j;t)\pi_0(t)\ dt}\ d\theta$$

so therefore

$$\widetilde{p}_n^{(-i)}(Y_i) = \frac{\int f_Y(Y_i;\theta)\prod_{j\neq i} f_Y(Y_j;\theta)\pi_0(\theta)\ d\theta}{\int \prod_{j\neq i} f_Y(Y_j;t)\pi_0(t)\ dt}$$

Predictive performance

Numerator:

$$\int f_Y(Y_i;\theta)\prod_{j\neq i} f_Y(Y_j;\theta)\pi_0(\theta)\ d\theta = \int \prod_{j=1}^{n} f_Y(Y_j;\theta)\pi_0(\theta)\ d\theta$$

Denominator:

$$\int \prod_{j\neq i} f_Y(Y_j;t)\pi_0(t)\ dt = \int \frac{1}{f_Y(Y_i;t)} \prod_{j=1}^{n} f_Y(Y_j;t)\pi_0(t)\ dt$$

Predictive performance

Therefore

$$C_n = -\frac{1}{n}\sum_{i=1}^{n} \log \widetilde{p}_n^{(-i)}(Y_i)$$

$$= \frac{1}{n}\sum_{i=1}^{n} \log \frac{\displaystyle\int \frac{1}{f_Y(Y_i;t)} \prod_{j=1}^{n} f_Y(Y_j;t)\pi_0(t)\, dt}{\displaystyle\int \prod_{j=1}^{n} f_Y(Y_j;\theta)\pi_0(\theta)\, d\theta}$$

$$= \frac{1}{n}\sum_{i=1}^{n} \log \int \frac{1}{f_Y(Y_i;t)} \frac{\displaystyle\prod_{j=1}^{n} f_Y(Y_j;t)\pi_0(t)}{\displaystyle\int \prod_{j=1}^{n} f_Y(Y_j;\theta)\pi_0(\theta)\, d\theta}\, dt$$

Predictive performance

But t and θ are merely dummy integrating variables, so we may exchange them and write

$$C_n = \frac{1}{n}\sum_{i=1}^{n} \log \int \frac{1}{f_Y(Y_i;\theta)} \frac{\prod_{j=1}^{n} f_Y(Y_j;\theta)\pi_0(\theta)}{\int \prod_{j=1}^{n} f_Y(Y_j;t)\pi_0(t)\ dt}\, d\theta$$

$$= \frac{1}{n}\sum_{i=1}^{n} \log \mathbb{E}_{\widetilde{\pi}_n}\left[\frac{1}{f_Y(Y_i;\theta)}\right]$$

as the *term in red* is merely the random variable version of the posterior $\widetilde{\pi}_n(\theta)$.

Predictive performance

This identity may be useful as it gives an expression for computing the numerical value of C_n which does not depend on the *leave-one-out* posterior distributions:

- the original formula requires n separate posterior calculations of the quantities $p_n^{(-i)}(y)$;
- the new formula requires only the computation of $\pi_n(\theta)$, the full posterior;
- the new formula does require the computation of

$$\mathbb{E}_{\pi_n}\left[\frac{1}{f_Y(y_i;\theta)}\right]$$

for $i = 1, \ldots, n$.

Predictive performance

- **WAIC:** The *widely applicable information criterion* (or WAIC), W_n, is defined by

$$W_n = T_n + \frac{1}{n}\sum_{i=1}^{n} \mathrm{Var}_{\tilde{\pi}_n}[\log f_Y(Y_i;\theta)]$$

where, recall, T_n is the training loss

$$T_n = -\frac{1}{n}\sum_{i=1}^{n} \log \tilde{p}_n(Y_i)$$

Predictive performance

Note

It can be shown that if $Y_1, \ldots, Y_n$ are independently drawn, then

$$W_n = C_n + \mathrm{O}_p\left(\frac{1}{n^2}\right)$$

and so W_n provides a tractable approximation strategy.

Predictive performance

- **Marginal likelihood (or prior predictive):** The normalizing constant that appears in the denominator of the (random) posterior $\widetilde{\pi}_n(\theta)$ is

$$Z_n \equiv Z(Y_1, \ldots, Y_n) = \int \prod_{i=1}^{n} f_Y(Y_i; \theta) \pi_0(\theta) \, d\theta.$$

  and, by de Finetti, this can be interpreted as the value of the (random) joint pdf

$$f_{Y_{1:n}}(Y_{1:n}) \equiv f_{Y_1,\ldots,Y_n}(Y_1, \ldots, Y_n).$$

Predictive performance

The quantity Z_n is termed the

- *marginal likelihood*,
- *prior predictive* distribution.

In this form, $Z_n = Z(Y_1, \ldots, Y_n)$ is a random variable:

$$z_n = Z(y_1, \ldots, y_n)$$

can also be computed.

Predictive performance

Note that

$$KL(f^*_{Y_{1:n}}, f_{Y_{1:n}}) = \int \log\left(\frac{f^*_{Y_{1:n}}(y_{1:n})}{f_{Y_{1:n}}(y_{1:n})}\right) f^*_{Y_{1:n}}(y_{1:n})\, dy_{1:n}$$

measures the divergence between the data-generating joint pdf

$$f^*_{Y_{1:n}}(y_{1:n}) = \prod_{i=1}^{n} f^*_Y(y_i)$$

and the modelled joint pdf $f_{Y_{1:n}}(y_{1:n})$.

Predictive performance

Thus

$$KL(f^*_{Y_{1:n}}, f_{Y_{1:n}}) = \int \log f^*_{Y_{1:n}}(y_{1:n}) f^*_{Y_{1:n}}(y_{1:n})\, dy_{1:n} - \int \log f_{Y_{1:n}}(y_{1:n}) f^*_{Y_{1:n}}(y_{1:n})\, dy_{1:n}$$

for which the term being subtracted is

$$\mathbb{E}_{f^*_{Y_{1:n}}}[\log f_{Y_{1:n}}(Y_{1:n})] = \mathbb{E}[\log Z_n].$$

Predictive performance

The random variable

$$F_n = -\log Z_n$$

that is, minus the log marginal likelihood, is sometimes termed the *free energy*.

Predictive performance

We have that

$$p_n(y_{n+1}) = \int f_Y(y_{n+1};\theta) \frac{\prod_{i=1}^{n} f_Y(y_i;\theta)\pi_0(\theta)}{\int \prod_{i=1}^{n} f_Y(y_i;t)\pi_0(t)\ dt}\ d\theta$$

$$= \frac{\int \prod_{i=1}^{n+1} f_Y(y_i;\theta)\pi_0(\theta)\ d\theta}{\int \prod_{i=1}^{n} f_Y(y_i;t)\pi_0(t)\ dt}$$

$$= \frac{z_{n+1}}{z_n}$$

Predictive performance

Therefore

$$\log \widetilde{p}_n(Y_{n+1}) = \log Z_{n+1} - \log Z_n = F_n - F_{n+1}.$$

Predictive performance

Note

Note that by direct calculation, we have

$$\mathbb{E}[G_n] = \mathbb{E}[F_{n+1}] - \mathbb{E}[F_n]$$

or equivalently

$$\mathbb{E}[F_n] = \mathbb{E}[F_1] + \sum_{i=1}^{n-1} \mathbb{E}[G_i]$$

Predictive performance

The quantities

- T_n
- G_n
- C_n
- W_n
- F_n

can all be used for model evaluation and comparison.