

Mattias Villani

Bayesian Learning [rough draft]

A GENTLE INTRODUCTION

Some publisher

Copyright © 2020 Mattias Villani

PUBLISHED BY SOME PUBLISHER

TYPESET BY L^AT_EX USING TEMPLATE FROM TUFTE-LATEX.GITHUB.IO

I will have to figure out how to license this work. For the moment the license is restrictive.

First edition, December 2020

Contents

<i>The Bayesics</i>	9
<i>Single-parameter models</i>	19
<i>Multi-parameter models</i>	39
<i>Priors</i>	57
<i>Regression</i>	67
<i>Prediction and Decision making</i>	75
<i>Classification</i>	89
<i>Posterior simulation</i>	91
<i>Variational inference</i>	93
<i>Regularization</i>	95
<i>Model comparison</i>	97
<i>Variable selection</i>	99
<i>Gaussian processes</i>	101
<i>Mixture models</i>	103
<i>Dynamic models and sequential inference</i>	105
<i>Bibliography</i>	107
<i>Index</i>	109

Preface

Who is this book for?

This book can be used as a first book in Bayesian statistics at the advanced undergraduate or master level. The book is written so that it can accommodate also students in engineering and computer science who are interested in Bayesian learning for applications in the field of Machine Learning, but may not be heavily trained in probability and statistics.

In fact, the book grew out of a Bayesian course that I taught for groups of heterogeneous students with roughly half of students from statistics and the other half from engineering and computer science, often with an interest in machine learning. To my surprise, I found that it was indeed possible to teach the same material to all students, even if half the class had a much more extensive background in statistics. The course had always very favorable reviews from the students and not a single student has complained over the years on it being too easy or too hard. There are two main explanations for this. First, since most bachelor level Statistics are non-Bayesian in methods and thinking, taking a first course in Bayesian inference is in some way like starting from scratch. Sure, there are several overlapping concepts and probability is of course the underlying technical language (although with highly different interpretations), but there are nevertheless a lot of effort spent in basic statistics courses that are not needed prerequisites for a Bayesian course. Second, my courses are very computational, as is most of the Bayesian field, with a lot of computer labs and also a partly computerized exam. Engineering and particularly computer science students tend to have a comparative advantage in computing and programming. So the additional time that students from statistics had to spend on programming, computer science students could spend on catching up on statistical concepts. In the end, everyone seemed put in the same number of hours and everyone was happy with the learning experience. In order to accommodate both groups of students, my lectures covers also some rather elementary concepts, especially in the early part of the course,

but then rather quickly moves over to territory unknown to all students. This book is written in the same style using Tufte style margin notes and figures to fill in potential missing gaps in probability and statistics, without breaking the flow of the main text.

Programming is useful for the exercises, or at least basic familiarity with R, Python or Julia or a similar datacentric language. I will use pseudo code for certain smaller algorithms and Julia for real code; Julia is used to present algorithms in the book since the ability to use mathematical symbols in Julia (via unicode) makes the code easy to read, almost like pseudo code. All graphs were made in Julia using the Plots package with GR as backend.

Why the term Bayesian learning?

I have used the term Bayesian *learning* in the book's title instead of Bayesian *inference* or Bayesian *statistics*. There are several reasons for this.

First, I want my courses and this book to be welcoming to students in fields neighboring statistics, such as machine learning, computer science, and parts of engineering. This reflects my strong belief that a modern statistician or machine learner should be a little of a renaissance person that understands both probability and statistical modelling, and computing. The ideal class is therefore a mix of students from nearby disciplines that learn for each others competences as much as they learn from my classes or this book.

Second, the term learning instead of inference was chosen since Bayesian statistics is about learning from data, often in a very sequential way where incrementally collected information updates our knowledge about the world.

Finally, the title is meant to convey the message that this is not a traditional book in statistics. The approach taken here, especially in later chapters, is very computationally driven with many algorithms for real-world data analysis. It is also inspired by machine learning in that much of the focus is given to prediction and decision making, and almost none to hypothesis testing.

Acknowledgment

This section will be much more complete when the book is finished, but I want to note already now that this book has been influenced by many other excellent textbooks on Bayesian methods. This is particularly true for two books that I have used as course literature over the years. I taught my first Bayes course in the year of 2000 using the book *Statistical Inference - An Integrated Approach* by Migon and Gamerman. Second, I have used the book *Bayesian Data Analysis*

by Gelman et al. for a number of years while teaching. I imagine that I have been more influenced by these two books than I know, and I thank the authors for taking the time to write them. I now appreciate them even more: it takes a lot of time to write a book!

The Bayesics

TODO! write proper intro text.

Learning probability models

Throughout this book we will exclusively work with probability models. Probability models have the advantage of giving a precise quantification of uncertainty that can be directly used for decision making in the real world.

A central task in statistics and machine learning is to infer an unknown parameter $\theta \in \Theta$ in a probability model $p(X_1, \dots, X_n | \theta)$ from a dataset of n observations x_1, \dots, x_n . The **parameter space** Θ is the set of allowed parameter values. Some examples of problems with a single parameter are learning the voting share of a political party from exit polls, predicting the number of bugs in a software release and inferring a one-dimensional measure of a persons intelligence from IQ tests.

While the initial chapters focus on learning parameters in models, it is important to remember that parameter inference is usually an intermediate step toward the final aim of prediction or decision making under uncertainty. For example, the predictions and decisions of a robot are based on a probability model with network weights learned from training data; authorities need to learn the basic reproduction number R_0 in probabilistic models to predict disease spreading and for making decisions about interventions. The Bayesian approach to predictions and decisions will be presented in the chapter [Prediction and Decision making](#), and used in many places throughout the book.

Most problems require models with more than one parameter. A prominent example with an extremely large number of parameters are the deep neural network models widely used in artificial intelligence (AI); such models often have millions of network weights that have to be learned from training data. However, to focus on ideas and easy derivations, we will keep things as simple as possible in the

parameter space



Figure 1: Artificial intelligence and infectious disease models are examples where Bayesian learning is often used for quantifying uncertainty.

first two chapters and only consider models with a single parameter. Later chapters tackle more complex models and present methods specifically designed for models with many parameters.

We will initially assume that the observations X_1, \dots, X_n are *independent and identically distributed (iid)* conditional on θ so that we can write the joint distribution as a product

$$p(X_1, \dots, X_n | \theta) = \prod_{i=1}^n p(X_i | \theta).$$

We denote this by $X_1, \dots, X_n | \theta \stackrel{\text{iid}}{\sim} p(X | \theta)$. In this setting we can refer to 'the probability model' as the probability distribution $p(X | \theta)$ for a single observation.

EXAMPLE: A binary random variable $X \in \{0, 1\}$ follows a **Bernoulli distribution** if

$$\Pr(X = x | \theta) = \begin{cases} \theta & \text{for } x = 1 \\ 1 - \theta & \text{for } x = 0 \end{cases}$$

which can be written more compactly as

$$\Pr(X = x | \theta) = \theta^x (1 - \theta)^{1-x}. \quad (1)$$

A typical example of iid Bernoulli data occurs when a coin is flipped n times (also called **Bernoulli trials**) and the sequence of heads ($x = 1$) and tails ($x = 0$) are recorded. It is common to refer to the outcome $X = 1$ as a success, and $X = 0$ as a failure. The Bernoulli distribution is illustrated in Figure 2.

We make the usual distinction between *random variables* denoted by capital letters and their *realizations (data)*, so $X = x$ means a random variable X with outcome x . As we will see later on, this distinction will often be less relevant in a Bayesian world where all inferences are conditioned on the observed data; we will therefore be more sloppy with this distinction in later chapters, but no harm will come from this.

The likelihood function and maximum likelihood estimation

The likelihood function is a key component of Bayesian learning, and indeed in all of Statistics. Given a probability model $p(X_1, \dots, X_n | \theta)$, the **likelihood function** $p(x_1, \dots, x_n | \theta)$ is the joint probability of observing the data set x_1, \dots, x_n considered as a function of the parameter θ . If the data are iid we can express the likelihood in terms of the univariate distributions $p(X | \theta)$ as

$$p(x_1, \dots, x_n | \theta) = \prod_{i=1}^n p(x_i | \theta). \quad (2)$$

iid

Bernoulli distribution

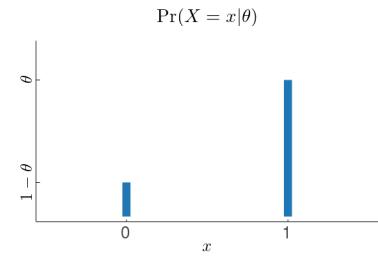


Figure 2: Bernoulli distribution with success probability $\theta = 0.8$.

Bernoulli trials

likelihood function

EXAMPLE: In the case of iid Bernoulli data the likelihood function is simply obtained by multiplying together the probability of success θ for the observations where $x_i = 1$ and probability of failure $1 - \theta$ when $x_i = 0$, giving the likelihood

$$p(x_1, \dots, x_n | \theta) = \theta^s(1 - \theta)^f, \quad (3)$$

where $s = \sum_{i=1}^n x_i$ is the number of successes in the sample, and $f = n - s$ is the number of failures.

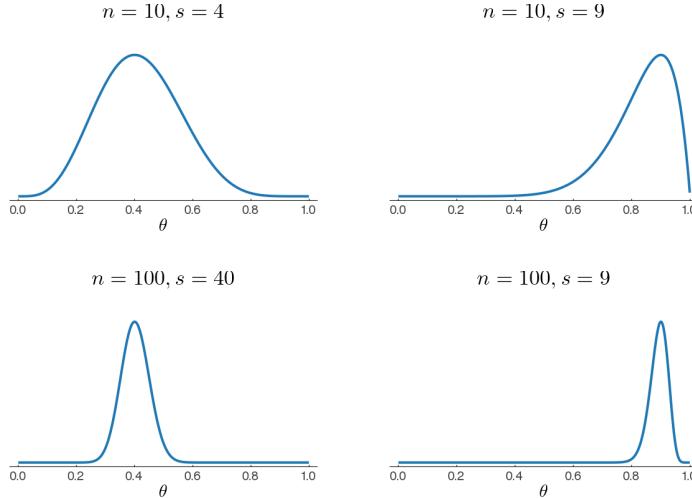


Figure 3: Bernoulli likelihood function for $n = 10$ and $s = 4$.

It is essential to have mental image of the likelihood function when thinking about statistical modeling. Figure 3 illustrates the likelihood function for Bernoulli model when $s = 4$ successes was obtained in $n = 10$ trials (top left) and when $s = 9$ successes was obtained in $n = 10$ trials (top right). The lower part of Figure 3 show results for $n = 100$ trials with the same success ratio s/n as in the upper part of the figure; the larger datasets make the likelihood more concentrated, i.e. more informative regarding the plausibility of different θ values.

Figure 3 nicely illustrates how the likelihood function can inform us about the plausibility of any given θ for any given dataset. If we want to select a single value, an **estimate** of θ , a natural candidate is the **maximum likelihood estimator**

$$\hat{\theta}_{\text{MLE}} = \arg \max_{\theta \in \Theta} p(x_1, \dots, x_n | \theta). \quad (4)$$

It makes some intuitive sense to estimate θ by the value that maximizes the probability of the observed data; the estimator $\hat{\theta}_{\text{MLE}}$ also enjoys several other attractive properties, particularly in large samples, i.e. when n is large.

It is quite easy to derive $\hat{\theta}_{\text{MLE}}$ for iid Bernoulli data. Rather than maximizing $p(x_1, \dots, x_n | \theta)$ directly with respect to θ it is often easier

estimate

maximum likelihood estimator

to maximize the *log-likelihood function*

$$\log p(x_1, \dots, x_n | \theta) = s \log \theta + f \log(1 - \theta).$$

Since the logarithm is a monotonically increasing function we obtain the same estimator if we maximize the likelihood or the log-likelihood function. We can now easily find $\hat{\theta}_{MLE}$ by taking the first derivative of the log-likelihood function with respect to θ , setting that derivative to zero and solving for θ . Solving

$$\frac{d \log p(x_1, \dots, x_n | \theta)}{d\theta} = \frac{s}{\theta} - \frac{f}{1-\theta} = 0,$$

gives the unique solution $\hat{\theta}_{MLE} = s/n$, the fraction of successes in the data. It is straightforward to show that this indeed a maximum by checking that the second derivative is negative at $\theta = \hat{\theta}_{MLE}$.

The maximum likelihood estimator is **unbiased** in this example, i.e. it is correct on average over all possible samples from the model:

$$\mathbb{E} [\hat{\theta}_{MLE}(X_1, \dots, X_n)] = \mathbb{E} \left(\frac{S}{n} \right) = \frac{n\theta}{n} = \theta,$$

where we have written out explicitly that an estimator is function of the sample. Note that the number of successes is random in this calculation as we are considering the variability over all possible samples, hence the use of capital letter S . We have also used that if $X_1, \dots, X_n | \theta \stackrel{iid}{\sim} \text{Bernoulli}$ then $S|\theta \sim \text{Binomial}(n, \theta)$ with mean $E(S) = n\theta$; see Figure 5 for an example of a **Binomial distribution**.

The **sampling variance** of an estimator is often used to assess the quality of an estimator. It is easily calculated for $\hat{\theta}_{MLE}$ in the Bernoulli example as

$$\mathbb{V} [\hat{\theta}_{MLE}(X_1, \dots, X_n)] = \mathbb{V} \left(\frac{S}{n} \right) = \frac{1}{n^2} \mathbb{V}(S) = \frac{\theta(1-\theta)}{n},$$

since $\mathbb{V}(S) = n\theta(1-\theta)$ when $S|\theta \sim \text{Binomial}(n, \theta)$.

It is important to understand that the above mean and variance of $\hat{\theta}_{MLE}$ are computed with respect to the **sampling distribution**, i.e. the distribution of the estimator as we repeatedly sample new datasets of size n from the assumed data generating process. They are **long run properties** of the estimation method, telling us how the estimator would perform on average over many repeatedly sampled datasets. Such long run properties play a very limited role in the Bayesian approach to inference where one can directly condition the inferences on the single dataset that we have observed. While sampling properties such as $\mathbb{E}(\hat{\theta}_{MLE})$ and $\mathbb{V}(\hat{\theta}_{MLE})$ are not used in the Bayesian approach, the likelihood function is at the core of Bayesian learning.

Binomial distribution

$$S \sim \text{Binom}(n, \theta)$$

Support: $S \in 0, 1, \dots, n$

$$p(s) = \binom{n}{s} \theta^s (1-\theta)^{n-s}$$

$$\mathbb{E}(X) = n\theta$$

$$\mathbb{V}(X) = n\theta(1-\theta)$$

Figure 4: The binomial distribution.

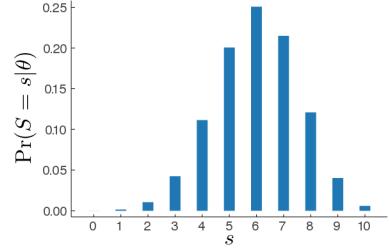


Figure 5: Binomial distribution with $n = 10$ and $\theta = 0.7$.

unbiased

Binomial distribution

sampling variance

sampling distribution

long run properties

The likelihood functions in Figure 3 look like a probability distribution for θ , and it is tempting to compute probabilities for θ , for example $\Pr(\theta \leq c | x_1, \dots, x_n)$ for some c . Of course, such probabilities only make sense if θ is a random variable, and we have so far considered θ to be a fixed unknown constant. So while $p(X_1, \dots, X_n | \theta)$ is a probability distribution for a random sample X_1, \dots, X_n for a fixed θ , the likelihood function is only the probability of a *fixed* sample x_1, \dots, x_n considered as function of θ ; the likelihood is therefore *not* a probability distribution for θ . Figure 6 reminds us of this error.

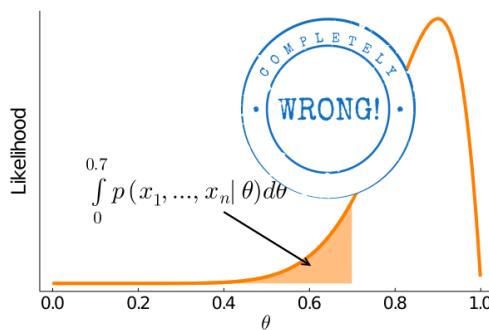


Figure 6: Areas under the likelihood function are **not** probabilities.

This is somewhat disappointing since having a probability distribution for θ would be very useful, for example when making a decision whose consequences depend on the unknown θ ; see Chapter [Prediction and Decision making](#). But again, it only makes sense to speak about probabilities for θ when θ is random. And this is where our Bayesian story begins.

Subjective Probability

What is the probability that the 10th decimal of π is 3? This may seem like a silly question since there is nothing intrinsically random about the 10th decimal of π ; it is a fixed quantity that does not vary. A Bayesian will however argue that if *you do not know its value* then you should express that uncertainty by a probability distribution. The Italian mathematician Bruno de Finetti, one of the founders of this school of probability, has expressed this well:

The only relevant thing is uncertainty - the extent of our knowledge and ignorance. The actual fact of whether or not the events considered are in some sense determined, or known by other people, and so on, is of no consequence.

Bruno de Finetti in his 1974 book 'A Theory of Probability' Vol 1.

Probability is the language of uncertainty and Bayesian learning is based on a **subjective probability**. A subjective probability measures

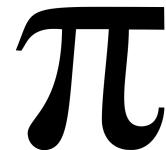


Figure 7: Bruno de Finetti, 1906-1985, a founder of subjective probability.

subjective probability

the **personal degree of belief** of a person. Since different persons have different knowledge and experience, such beliefs will vary between persons. A person that has no idea about the 10th decimal of π may use a uniform distribution on the integers 0-9. Someone else may however know this decimal with certainty and assigns a probability of 1 to that outcome. Again, whether or not the event is in some sense intrinsically random or not is of no consequence; the only relevant thing is *your* uncertainty. Einstein's famous statement "God does not play dice with the universe" may be interesting to ponder about, but has not bearing on subjective probability and Bayesian learning.

The notion of probability in Bayesian learning is therefore radically different from the frequentist interpretation of probability taught in most basic statistics classes. The **frequentist probability** of an event A is defined as the limiting proportion of times that event A occurs in an (imagined) infinite number of repetitions of an experiment; for example the tossing of a coin with the event of interest $A = \{\text{Heads}\}$. A subjective probability measure is instead defined as the personal degree of belief in the event A for a person. Note that subjective probabilities can be used to quantify uncertainties also for events that are unrepeatable, for example the probability of a nuclear disaster at a particular location. A subjective probability distribution can also contain useful information that may not directly come from observed data. As we will see, the Bayesian approach combines such subjective information with objective data in a natural way.

Luckily, the computational rules for probabilities are the same for both frequentist and subjective interpretations of probability; for example $0 \leq \Pr(A) \leq 1$ and $\Pr(A \cap B) = \Pr(A) + \Pr(B)$ when A and B are disjoint events. The rules can be motivated by considering subjective probabilities as the result of pricing of bets. Imagine that you are given the chance to enter a bet where you win \$1 if event A occurs. How much would you be willing to pay that bet? Surely not more than \$1 as then you would lose money with certainty. If you strongly believe that A will occur you would probably be willing to pay closer to \$1, but if you believe that A is nearly impossible your price for the bet would be close to \$0. The highest price that you would be willing to pay for the bet is your subjective probability in the event A . Given this setup one can easily show that your subjective probabilities must satisfy the axioms for probabilities otherwise you would be willing to enter a sequence of bets where you would lose an infinite amount with certainty; this is the so called **dutch book argument**. Objections have been raised against this argument, for example that the utility from the bet may not linearly increase with the monetary gain, and some people may even get utility just by

personal degree of belief

frequentist probability

dutch book argument

the excitement in gambling; subsequent refinements of this argument have therefore completely disposed with the notion of money in favor of a more general notion of utility; see the chapter [Prediction and Decision making](#).

Bayesian Learning

The general recipe for Bayesian learning about an event A is:

- Formulate your subjective *prior beliefs* $\Pr(A)$ about A .
- *Collect data* that inform you about A .
- *Update* your prior beliefs with the observed data.

The big question is *how* to update prior beliefs with data. Bayesian learning gets its name from using Bayes' theorem for this updating. The most basic version of **Bayes' theorem** computes the probability of an event A given the known occurrence of some other event B as

$$\Pr(A|B) = \frac{\Pr(B|A)\Pr(A)}{\Pr(B)}$$

One way to think about this result is that it 'reverses the conditioning', i.e. it computes $\Pr(A|B)$ from $\Pr(B|A)$.

Bayes' theorem will be used to infer an unknown parameter θ in a probability model, but let us first use the theorem to solve a simple problem. Imagine that you have taken a test for a specific latent disease and that the test was unfortunately positive. The doctor tells you that $\Pr(B|A) = 0.9$ where $A = \{\text{'Have disease'}\}$ and $B = \{\text{'Positive test'}\}$ and also $\Pr(B|A^c) = 0.05$, where A^c is the complement to A , i.e. the event that you do not have the disease. Hence, a positive test is very unlikely if you do not have the disease, so you start to worry. But what you really want to know is the probability of having the disease given a positive test, i.e. $\Pr(A|B)$. To compute this you need to know the so called *prior* probability of A before you took the test. The doctor tells you that only one in ten thousand has the disease and you set $\Pr(A) = 0.0001$. Given no other information (e.g. that you feel sick or have other symptoms) Bayes' theorem gives

$$\Pr(A|B) = \frac{\Pr(B|A)\Pr(A)}{\Pr(B)} = \frac{\Pr(B|A)\Pr(A)}{\Pr(B|A)\Pr(A) + \Pr(B|A^c)\Pr(A^c)} \approx 0.0018,$$

where we have expressed $\Pr(B)$ in the numerator using a version of the **law of total probability**. Hence, even though the test has increased the probability of having the disease by a factor of 18 from the initial $\Pr(A) = 0.0001$, the probability of actually having the disease is still tiny. The lesson here is that prior probabilities matter.

Bayes' theorem



Figure 8: Reverend Thomas Bayes, ca 1701-1761, whose famous theorem was published posthumously. Interestingly, we are not quite sure that the man in the photo actually is Thomas Bayes. Probably not.

law of total probability

To see how Bayes' theorem can be used for Bayesian learning from data, let us consider the event $B = \{\text{'Data } x_1, \dots, x_n \text{ was observed'}\}$ which we write simply as $B = \{x_1, \dots, x_n\}$. We can now use Bayes' theorem to update the initial beliefs $\Pr(A)$ about some event A with data $B = \{x_1, \dots, x_n\}$ by the formula

$$\Pr(A|x_1, \dots, x_n) = \frac{\Pr(x_1, \dots, x_n|A)\Pr(A)}{\Pr(x_1, \dots, x_n)}.$$

The initial belief $\Pr(A)$ is called a **prior** since it refers to beliefs about A *before* the data x_1, \dots, x_n was observed. Likewise $\Pr(A|x_1, \dots, x_n)$ is referred to as the **posterior** since it is the probability of A *after* data was observed.

Let us now show how Bayes' theorem can be used to infer a parameter in a probability model $p(X_1, \dots, X_n|\theta)$. We first take a simplified approach where the only possible parameter values are on a grid of values $\theta_1, \theta_2, \dots, \theta_K$. Let $B = \{x_1, \dots, x_n\}$ be the event of observing a specific dataset and $A_k = \{\theta_k\}$ be the event that $\theta = \theta_k$. The posterior probability for each $A_k = \{\theta_k\}$ is then

$$\Pr(\theta_k|x_1, \dots, x_n) = \frac{\Pr(x_1, \dots, x_n|\theta_k)\Pr(\theta_k)}{\sum_{j=1}^K \Pr(x_1, \dots, x_n|\theta_j)\Pr(\theta_j)}. \quad (5)$$

Note how we again used the law of total probability in the denominator to express $\Pr(B) = \Pr(x_1, \dots, x_n)$. This denominator is only there to guarantee that the posterior is a probability distribution, i.e. that $\sum_{j=1}^K \Pr(\theta_j|x_1, \dots, x_n) = 1$.

The really interesting stuff is however in the numerator of (5) and we will therefore often write Bayes' theorem in proportional form

$$\Pr(\theta_k|x_1, \dots, x_n) \propto \Pr(x_1, \dots, x_n|\theta_k)\Pr(\theta_k), \quad (6)$$

where the symbol \propto is read as 'is proportional to', i.e. a multiplicative normalizing constant is missing in the expression. Now here is the really crucial thing: the factor $\Pr(x_1, \dots, x_n|\theta_k)$ in Equation (6) is the *likelihood function* evaluated in the point θ_k . Equation (6) therefore expresses the fundamental idea in Bayesian learning:

$$\text{Posterior} \propto \text{Likelihood} \times \text{Prior}.$$

Figure 10 illustrates the updating from prior to posterior for the Bernoulli model with data $n = 10$ and $s = 9$ over a grid of θ values. Note how the posterior is a compromise between the prior information and the data information (likelihood).

Finally, taking a finer and finer grid in Equation 5 we get the following Bayes' theorem for a continuous parameter θ in the limit

$$p(\theta|x_1, \dots, x_n) = \frac{p(x_1, \dots, x_n|\theta)p(\theta)}{\int p(x_1, \dots, x_n|\theta)p(\theta)d\theta}, \quad (7)$$

prior

posterior

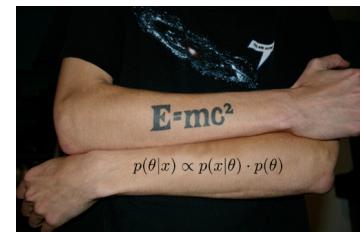


Figure 9: Great theorems make great tattoos.

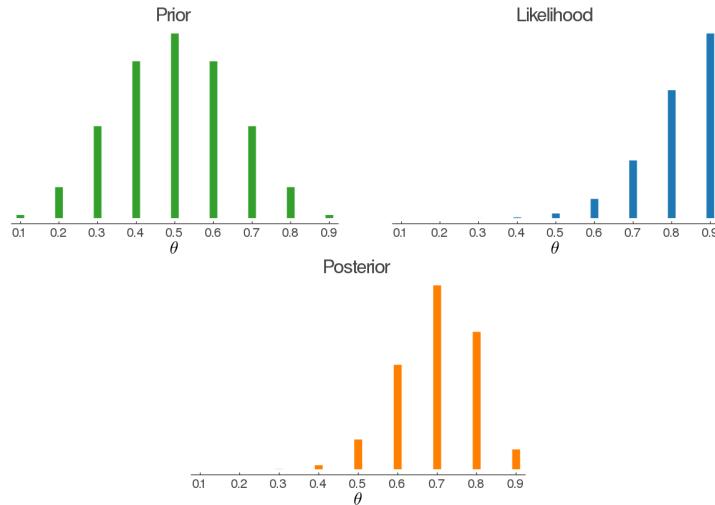


Figure 10: Prior, likelihood and posterior for Bernoulli model with $n = 10$ and $s = 9$.

where $p(\theta)$ is now a continuous **prior density** that gets updated with new data via the likelihood function $p(x_1, \dots, x_n | \theta)$ to a **posterior density** $p(\theta | x_1, \dots, x_n)$. The normalizing constant is now given by an integral over θ and is a continuous version of the law of total probability. We can again hide the unimportant normalizing constant to get the nicer form

$$p(\theta | x_1, \dots, x_n) \propto p(x_1, \dots, x_n | \theta) p(\theta). \quad (8)$$

It is important to note that the posterior distribution $p(\theta | x_1, \dots, x_n)$ is a probability distribution for the parameter θ ; it completely describes the knowledge about θ for a person with the prior $p(\theta)$ after having observed the data x_1, \dots, x_n . Remember that the likelihood can not be used to compute probabilities for θ . With a posterior distribution we actually *can* compute $\Pr(\theta \leq c | x_1, \dots, x_n) = \int p(\theta \leq c | x_1, \dots, x_n) d\theta$ or any other probability of interest. It is the prior $p(\theta)$ that makes it possible to use Bayes' theorem to revert the conditioning in the likelihood $p(x_1, \dots, x_n | \theta)$ into the conditional probability that we really care about, the posterior $p(\theta | x_1, \dots, x_n)$; but you need the prior to get the posterior. As Leonard Jimmie Savage, a founder of Bayesian analysis, has famously said:

You can't cook the Bayesian omelette without breaking the Bayesian eggs.

Leonard Jimmy Savage

The ability to use prior information is a strength, especially when one has to make a decision based by very weak data. Later in the book we will see how priors can be used to convey the idea that a functional relationship between two variables is in some sense

prior density

posterior density



Figure 11: Making a Bayesian omelette.

smooth, and how this can prevent models from overfitting the data. Nevertheless, the subjective elements of a Bayesian analysis can complicate the reporting of scientific evidence, where objectivity is the ideal. One can argue that objectivity is simply unattainable, and that the supposedly objective alternatives to Bayesian learning just sweeps the subjective elements under the carpet. A more pragmatic Bayesian approach for scientific communication is presented in Section [Noninformative priors](#) where priors are intentionally chosen to be neutral or minimally informative. Section [Invariant priors](#) gives an alternative approach to so called objective priors using invariance arguments.

There are also two aspects of a Bayesian approach that gives it a clear scientific character. The prior distribution is subjective, and therefore varies from person to person, but the rule that updates the beliefs with new data is objective: we *should* use Bayes' theorem and the data *should* enter the updating *only through the likelihood function*. The word 'should' is emphasized here since one can mathematically derive this result from some simple axioms, and it can be proved to be the optimal way to process information; see [Bernardo and Smith \[2009\]](#) and Section [Bayesian learning and the likelihood principle](#). Second, one can prove that the effect of the prior vanishes asymptotically as the sample size n grows large; objectivity is attained by a **subjective consensus**: persons with wildly different priors will eventually reach the same posterior distribution as we collect more data. This result is given in chapter [Classification](#) and we will see an empirical demonstration of this effect already in the next chapter.

subjective consensus

EXERCISES

1. This is the first problem.
2. **Computer exercise.** This is the first computer exercise.

Single-parameter models

Now that we know the basics of Bayesian updating of prior beliefs with new data, we can start to analyze models with a single parameter. This will allow to practice on deriving the posterior distribution in simple settings. The drawback of simple models is that they do not show anywhere near the full potential of Bayesian methods. But you need to crawl before you can walk, and some patience is required before we come to more useful models, such as regression and classification models in later chapters.

Bernoulli data

Let us return to iid Bernoulli data:

$$x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} \text{Bern}(\theta). \quad (9)$$

We first need a prior distribution $p(\theta)$ for θ . There are a number of ways to do **prior elicitation**, i.e. to extract a prior distribution from a person, for example an expert. Such methods involve ideas from psychology and usually consist of asking a series of questions to the expert, followed by checks for internal consistency of the elicited prior beliefs. One can in principle elicit any distribution, e.g. in the form of a histogram, but the most common approach is to first settle on a distributional family and then elicit the hyperparameters within the family. Since $\theta \in [0, 1]$, the **Beta distribution** is a suitable two-parameter family with quite a lot of flexibility; Figure 13 plots a few members of the Beta family. Note that $\text{Beta}(1, 1)$ is the **uniform distribution**. We will now show that the Beta family is particularly convenient as a prior for the iid Bernoulli model.

A nice feature of Bayesian inference is that one always know where to start. To derive the posterior distribution of a parameter θ we start with Bayes' theorem (8):

$$p(\theta | x_1, \dots, x_n) \propto p(x_1, \dots, x_n | \theta) p(\theta),$$

where $p(x_1, \dots, x_n | \theta) = \theta^s (1 - \theta)^f$ is the likelihood for iid Bernoulli

Beta distribution

$X \sim \text{Beta}(\alpha, \beta)$ for $X \in [0, 1]$.

$$p(x) = \frac{x^{\alpha-1} (1-x)^{\beta-1}}{B(\alpha, \beta)}$$

$$\mathbb{E}(X) = \frac{\alpha}{\alpha + \beta}$$

$$\mathbb{V}(X) = \frac{\alpha\beta}{(\alpha + \beta)^2 (\alpha + \beta + 1)}$$

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}, \text{ where } \Gamma(\alpha) \text{ is the Gamma function.}$$

Figure 12: The beta distribution.

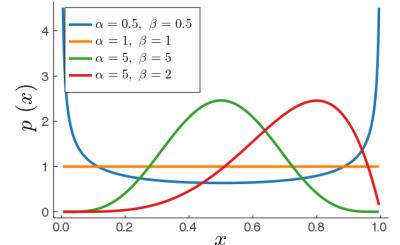


Figure 13: Some Beta distributions.

prior elicitation

Beta distribution

uniform distribution

Uniform distribution

$X \sim \text{Uniform}(a, b)$, $X \in [a, b]$.

$$p(x) = \frac{1}{b-a}$$

$$\mathbb{E}(X) = \frac{a+b}{2}$$

$$\mathbb{V}(X) = \frac{(b-a)^2}{12}$$

Figure 14: The uniform distribution.

data and $p(\theta)$ is the $\theta \sim \text{Beta}(\alpha, \beta)$ prior. So,

$$p(\theta|x_1, \dots, x_n) \propto \theta^s (1-\theta)^f \frac{\theta^{\alpha-1} (1-\theta)^{\beta-1}}{B(\alpha, \beta)} \quad (10)$$

$$\propto \theta^{\alpha+s-1} (1-\theta)^{\beta+f-1}, \quad (11)$$

where the second line puts the Beta function $B(\alpha, \beta)$ into the missing proportionality constant. Note that $1/B(\alpha, \beta)$ is a multiplicative constant and *not* a function of θ and will therefore not affect the shape of the posterior distribution, just scale it vertically. In the final step will recover the normalizing constant so that $p(\theta|x_1, \dots, x_n)$ integrates to one over its support, as required. Now, from the pdf of the Beta distribution we see that the expression in (10) can be recognized as proportional to a Beta distribution. We see this as the expression is of the form $\theta^{a-1} (1-\theta)^{b-1}$ where $a = \alpha + s$ and $b = \beta + f$. The posterior for θ is therefore the $\text{Beta}(\alpha + s, \beta + f)$ distribution and the missing proportionality constant in (10) is then known to be $1/B(\alpha + s, \beta + f)$. The prior-to-posterior updating for the Bernoulli model is summarized in Figure 15. Note that the random variables in the model are written with lowercase letters for simplicity.

Conjugate analysis - Bernoulli model

Model: $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} \text{Bern}(\theta)$

Prior: $\theta \sim \text{Beta}(\alpha, \beta)$

Posterior: $\theta|x_1, \dots, x_n \sim \text{Beta}(\alpha + s, \beta + f)$

where $s = \sum_{i=1}^n x_i$ and $f = n - s$.

Figure 15: Prior-to-Posterior updating for the Bernoulli data with a Beta prior.

Using a Beta prior for the Bernoulli parameter is convenient since the posterior distribution then belongs to the *same distributional family* as the prior distribution; the posterior is also a Beta distribution. The beta family is said to be *conjugate* to the Bernoulli model, or that the beta distribution is the **conjugate prior** for the Bernoulli model. Conjugate priors are easy to use since all we have to do when updating a Beta prior with Bernoulli data is to add the number of successes s to α and the number of failures f to β . The way that α and β enter the posterior also shows that the information in a $\text{Beta}(\alpha, \beta)$ prior corresponds to a prior dataset with α successes and β failures. We usually do not have an explicit prior sample at hand, and α and β need not even be integers, but we can nevertheless think about the prior information as being equivalent to an **imaginary prior sample**.

conjugate prior

Similar conjugate results for several other models will be presented in this book, but there are many models for which a known conjugate prior do not exist. For such models, the posterior is often

imaginary prior sample

not available in closed form, but several easy-to-use approximation or simulation methods are presented in later chapters.

It is interesting to compare a Bayesian analysis of Bernoulli data with the maximum likelihood estimator $\hat{\theta}_{MLE} = s/n$. A common **Bayes estimator**, or Bayesian point estimator, is the posterior mean $E(\theta|x_1, \dots, x_n) = \frac{\alpha+s}{\alpha+\beta+n}$, which follows directly from the formula for the mean of a Beta distribution. Let us also assume a uniform prior for θ as some sort of non-informative prior, i.e. our prior is the Beta(1,1) distribution. Consider the case when we have observed no successes ($s = 0$) in a small number of trials n . We then have the quite unreasonable MLE of $\hat{\theta}_{MLE} = 0$, whereas the Bayes estimator is $E(\theta|x_1, \dots, x_n) = 1/(n+2) > 0$. We will return to this example and the idea of a non-informative prior in Sections [Noninformative priors](#) and [Invariant priors](#).

Bayes estimator

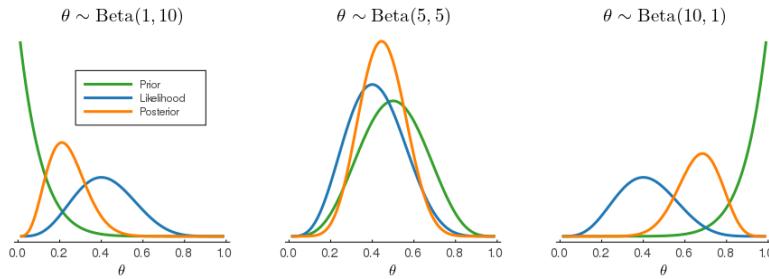


Figure 16: Bayesian analysis of $n = 10$ randomly chosen emails from the SpamBase data using three different priors. The likelihood is normalized.

EXAMPLE: SPAM EMAILS. The **SpamBase** dataset from the UCI repository¹ consists of 4601 emails that have been manually classified as *spam* (junk email) or *ham* (non-junk email). The dataset also contains a vector of covariates/features for each email, such as the number of capital letters or \$-signs; this information can be used to build a spam filter that automatically separates spam from ham. We will in this chapter only analyze the proportion of spam emails without using the covariates; we return to the more interesting case with features in the [Classification](#) chapter. So, let $x_1, \dots, x_n | \theta \stackrel{iid}{\sim} \text{Bern}(\theta)$ for the $n = 4601$ emails, where $x_i = 1$ if the email is spam and $x_i = 0$ for ham. The unknown quantity θ is the probability of spam.

SpamBase dataset

¹ Dheeru Dua and Casey Graff. UCI machine learning repository, 2017. URL <http://archive.ics.uci.edu/ml/datasets/Spambase/>

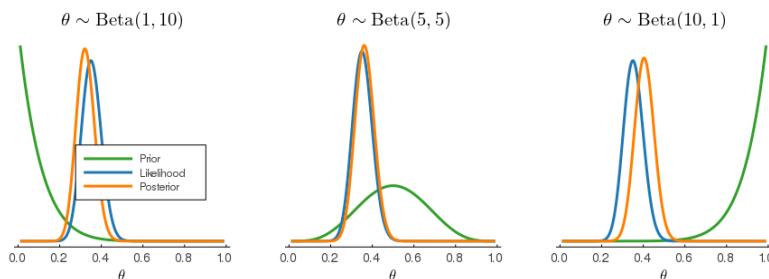


Figure 17: Bayesian analysis of $n = 100$ randomly chosen emails from the SpamBase data using three different priors. The likelihood is normalized.

To illustrate the incremental learning process in Bayesian learning we start off by analyzing only $n = 10$ randomly sampled emails, out of which $s = 4$ were spam. Figure 16 shows the posterior distribution of θ for three persons with very different priors. With only $n = 10$ data points, the three persons' posteriors are of course very different. The results in Figure 17 are based on $n = 100$ randomly sampled emails, including the 10 emails used in Figure 16. The posteriors are now in rather close but not perfect agreement. Finally, Figure 18 shows the posterior for the full dataset with $n = 4601$; here there is a complete subjective consensus between the three persons that initially had very different beliefs about the spam probability.

From this dataset we have thus learned that around 40% or all emails are spam, and we are also quite certain about this percentage as the posterior distribution is very concentrated around 0.4. This information is not useful for building a spam filter where one instead needs the spam probability for each email to be a function of the text in that specific email (e.g. the number of \$-signs). We will achieve this in chapter [Classification](#) when derive the posterior for a binary regression and use the methods in chapter [Prediction and Decision making](#) to construct Bayesian spam predictions from such a model.

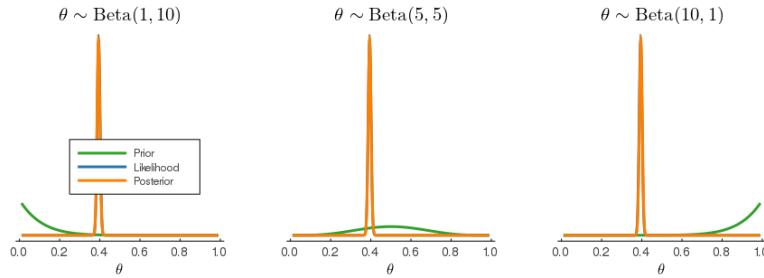


Figure 18: Bayesian analysis of all $n = 4601$ emails from the SpamBase data using three different priors. The likelihood is normalized.

Bayesian learning and the likelihood principle

We will use the Bernoulli example to demonstrate an important feature of Bayesian learning. Consider the following three experiments, all resulting in s successes in n trials:

- **Experiment 1:** sample data from $X_1, \dots, X_n | \theta \sim \text{Bern}(\theta)$, where n is a predetermined number of trials.
Data: the outcome in each trial: x_1, \dots, x_n .
- **Experiment 2:** sample data from $X_1, \dots, X_n | \theta \sim \text{Bern}(\theta)$, where n is a predetermined number of trials.
Data: the total number of successes: $s = \sum_{i=1}^n x_i$
- **Experiment 3:** sample data from $X_i | \theta \sim \text{Bern}(\theta)$ until exactly s , a predetermined number of successes, have been obtained.

Data: the number of trials, n , until s successes have been obtained.

The above three experiments show that we need to be careful in defining exactly *which* data to use in the likelihood function. We know from before that the likelihood from Experiment 1 is

$$p(x_1, \dots, x_n | \theta) = \theta^s (1 - \theta)^{n-s}, \quad (12)$$

In the second experiment we only get to observe that there were s successes in n trials, but the exact sequence x_1, \dots, x_n is not recorded. So the data is here represented as the outcome of a random variable $S = \sum_{i=1}^n X_i \sim \text{Binom}(n, \theta)$. The likelihood for experiment 2 is therefore given by the binomial distribution

$$p(s) = \binom{n}{s} \theta^s (1 - \theta)^{n-s}. \quad (13)$$

This is different from the likelihood in Experiment 1 since the outcome $S = s$ can be obtained from several different observed data sequences x_1, \dots, x_n , each with exactly s successes. The exact number of such possible sequences is given by the binomial factor $\binom{n}{s}$.

Finally, the random variable in Experiment 3 is the number of performed trials, which follows the **negative binomial distribution**. The likelihood from Experiment 3 is therefore

$$p(n) = \binom{n-1}{s-1} \theta^s (1 - \theta)^{n-s}. \quad (14)$$

The factor $\binom{n-1}{s-1}$ counts the number of ways we can order the $s-1$ successes in the first $n-1$ trials; we know that the n th trial must have been a success since the experiment terminated after n trials. Note that there are several versions of the negative binomial distribution depending on whether we count the number of trials or the number of failures until s successes.

Now, the likelihood functions in (12)-(14) differ only by a constant that does not depend on θ , i.e. the likelihoods are proportional. The likelihood for the j th experiment can therefore be written as $c_j f(\theta)$, where $f(\theta) = \theta^s (1 - \theta)^{n-s}$, $c_1 = 1$, $c_2 = \binom{n}{s}$ and $c_3 = \binom{n-1}{s-1}$. The posterior distribution of θ from the j th experiment is then by (7)

$$p_j(\theta | x_1, \dots, x_n) = \frac{c_j f(\theta) p(\theta)}{\int c_j f(\theta) p(\theta) d\theta} = \frac{f(\theta) p(\theta)}{\int f(\theta) p(\theta) d\theta}.$$

The posterior distribution for θ is therefore the same in all three experiments. It is now obvious that Bayesian inference always satisfies the following likelihood principle.

Definition. Likelihood principle. Two experiments that result in (proportionally) equal likelihood functions should give the same inferences.

negative binomial distribution

Likelihood principle

Informally, the likelihood principle says that all relevant information in an experiment about θ is contained in the likelihood function. The importance of the likelihood principle is that it can be mathematically derived from two simpler principles that everyone hold as self evident. Hence the word *should* in the principle; see Casella and Berger [2002, ch. 6.2] for a discussion of this famous **Birnbaum's theorem**.

Many frequentist methods violate the likelihood principle. The maximum likelihood *estimate* is easily seen to be $\hat{\theta}_{MLE} = s/n$ for all three experiments for a given data set. However, the sampling variability of the maximum likelihood *estimator*, $V(\hat{\theta}_{MLE})$, will be different in Experiment 3 from that in Experiment 1 and 2. This is a consequence of the estimator being S/n in Experiment 1 and 2, but s/N in Experiment 3; note the difference in random variables (capital letters) in these estimators.

In summary, Bayesian inference *conditions on the observed data* and does not rely on repeated sampling properties. The data only enters through the likelihood function and Bayesian inference respects the likelihood principle.

Gaussian data - known variance

In this section we derive the posterior distribution for the mean in the iid Gaussian model $x_1, \dots, x_n | \theta, \sigma^2 \stackrel{iid}{\sim} N(\theta, \sigma^2)$. Since this chapter is about models with a single parameter we will assume the variance σ^2 to be known; this is rarely the case in practise and we return to the Gaussian model with both parameters unknown in Chapter [Multi-parameter models](#).

Uniform prior

We will first derive the posterior for a so called non-informative prior, i.e. a prior that is supposed to contain no, or at least very little, prior information. The most common non-informative prior for θ is a uniform distribution $p(\theta) = c$ for $\theta \in \mathbb{R}$ where $c > 0$ is a constant; the idea is that this distribution does not favor any particular value for θ . A uniform distribution over an unbounded space is not a proper distribution since $\int_{-\infty}^{\infty} p(\theta) d\theta = \infty$. It is nevertheless possible to use this somewhat strange prior since the resulting posterior is proper after observing a single data point. We can also think about the uniform prior as a limiting normal distribution with a variance that tends to infinity.

By Bayes' theorem, the posterior distribution for θ under a uni-

Birnbaum's theorem

Normal distribution

$$X \sim N(\mu, \sigma^2)$$

Support: $X \in (-\infty, \infty)$

$$p(x) = \frac{\exp(-\frac{1}{2\sigma^2}(x - \mu)^2)}{\sqrt{2\pi\sigma^2}}$$

$$\mathbb{E}(X) = \mu$$

$$V(X) = \sigma^2$$

Figure 19: The Gaussian distribution.

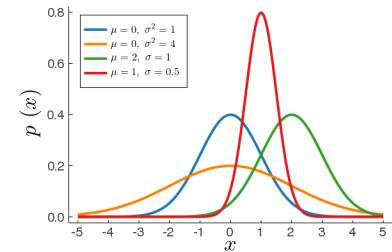


Figure 20: Some Normal distributions.

form prior is

$$\begin{aligned} p(\theta|x_1, \dots, x_n) &\propto p(x_1, \dots, x_n|\theta)p(\theta) \\ &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x_i - \theta)^2\right) \cdot c \\ &\propto \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \theta)^2\right). \end{aligned}$$

Let $\bar{x}_n = \sum_{i=1}^n x_i$ be the sample mean, then

$$\sum_{i=1}^n (x_i - \theta)^2 = \sum_{i=1}^n (x_i - \bar{x} - (\theta - \bar{x}))^2 = \sum_{i=1}^n (x_i - \bar{x})^2 + n(\theta - \bar{x})^2,$$

since the cross term $2(\theta - \bar{x}) \sum_{i=1}^n (x_i - \bar{x}) = 0$. Note that the term $\sum_{i=1}^n (x_i - \bar{x})^2$ does not depend on θ and we therefore get

$$p(\theta|x_1, \dots, x_n) \propto \exp\left(-\frac{n}{2\sigma^2}(\theta - \bar{x})^2\right), \quad (15)$$

and hence that the posterior for θ can be recognized as

$$\theta|x_1, \dots, x_n \sim N\left(\bar{x}, \frac{\sigma^2}{n}\right).$$

Normal prior

Consider now a normal prior, $\theta \sim N(\mu_0, \tau_0^2)$; following Gelman et al. [2013] the subscript 0 is used to denote that these are **hyperparameters** in the prior, i.e. based on 0 observations. The user must decide the most probable value for θ , μ_0 , and also how sure she is by setting the prior standard deviation, τ_0 . One way to elicit these prior hyperparameters is to ask the user for a 95% probability interval for θ and then back out μ_0 and τ_0 ; see Exercise 2.

hyperparameters

By Bayes' theorem and the rewrite of the likelihood in (15) we have

$$p(\theta|x_1, \dots, x_n) \propto \exp\left(-\frac{n}{2\sigma^2}(\theta - \bar{x})^2\right) \times \exp\left(-\frac{1}{2\tau_0^2}(\theta - \mu_0)^2\right)$$

In Exercise 4 you are asked to complete the squares in this expression to prove that this expression is proportional to a normal density of the form given in Figure 21.

The normal prior is therefore conjugate to the normal model with known variance (i.e. a normal prior gives a normal posterior). The interpretation of the posterior mean μ_n and τ_n^2 in Figure 21 are quite intuitive. Note first that the expression for the posterior variance τ_n^2 is written in terms of precision = 1/variance. The first term $n/\sigma^2 = 1/(\sigma^2/n)$ is the precision in the data. This can be seen in several

Conjugate analysis - Gaussian model with known variance

Model: $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$, σ^2 known

Prior: $\theta \sim N(\mu_0, \tau_0^2)$

Posterior: $\theta | x_1, \dots, x_n \sim N(\mu_n, \tau_n^2)$.

Posterior precision: $\frac{1}{\tau_n^2} = \frac{n}{\sigma^2} + \frac{1}{\tau_0^2}$

Posterior mean: $\mu_n = w\bar{x} + (1-w)\mu_0$, where $\bar{x} = \sum_{i=1}^n x_i$

Weight: $w = \frac{n/\sigma^2}{n/\sigma^2 + 1/\tau_0^2}$

Figure 21: Prior-to-Posterior updating for normal data with known variance and normal prior for the mean.

ways, for example by the sampling variance being $V(\bar{x}) = \sigma^2/n$.

Hence the formula for the posterior precision $\frac{1}{\tau_n^2} = \frac{n}{\sigma^2} + \frac{1}{\tau_0^2}$ can be read

$$\text{Posterior precision} = \text{Data precision} + \text{Prior precision}.$$

The posterior mean $\mu_n = w\bar{x} + (1-w)\mu_0$ is a weighted average of the data mean \bar{x} and the prior mean. The weight w on \bar{x} in Figure 21 is the data precision relative to the prior precision. The posterior therefore puts more emphasis on the data when n is large, σ small or τ_0 is large. It will not always be possible to get this clear a view of the prior-to-posterior updating in other models, but the same logic will apply also there.

Example: Internet connection speed

The maximum internet connection speed downstream in my home is 50 Mbit/sec. This maximum will typically never be reached, but my internet service provider (ISP) claims that the average speed is *at least* 20Mbit/sec. To test this, I collect a total of five measurements over the course of five consecutive using an speed testing internet service; I will call this the **Internet speed dataset**. The measurements are assumed to be $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$, where θ is the average speed; we ignore for simplicity that the measurements cannot be negative. The measurements are reported to have a standard deviation of $\sigma = 5$ by speed testing service. I will use a prior centered on the average claimed by the ISP, $\mu_0 = 20$, with a prior standard deviation of $\tau_0 = 5$. My prior beliefs are therefore that $\theta \in [10, 30]$ with approximately 95% probability.

Figure 22 (left) displays the prior, normalized likelihood and posterior of θ based on only the first measurement $x_1 = 15.770$ Mbit/sec; the probability of interest $\Pr(\theta \geq 20 | x_1, \dots, x_n) \approx 0.275$ is marked out by the shaded orange region. Since the prior precision happened to be equal to the data precision of a single obser-

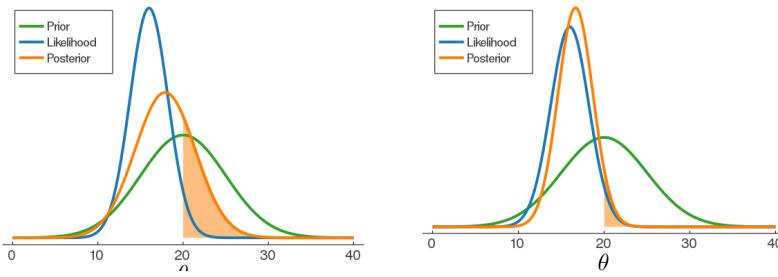


Figure 22: Internet speed data. Posterior updating based on $n = 1$ observation (left) and $n = 5$ observations (right). The orange shaded region marks out $\Pr(\theta > 20 | x_1, \dots, x_n)$.

vation, the weight on the data in the posterior mean μ_n is exactly $w = 0.5$. Figure 22 (left) shows the updated posterior using all $n = 5$ data points with $\bar{x} = 16.001$; we are beginning to be rather confident that the ISP's claim that $\theta \geq 20$ is false since we now have $\Pr(\theta \geq 20 | x_1, \dots, x_n) \approx 0.051$. The weight w is now 0.833 so that data is starting to dominate the prior.

Figure 22 illustrates a situation where the posterior is computed by combining the prior at day 0, $N(\mu_0, \tau_0^2)$, with the likelihood for all x_1, \dots, x_n data points; hence the posterior on day n is computed as

$$p(\theta | x_1, \dots, x_n) \propto p(x_1, \dots, x_n | \theta) p(\theta). \quad (16)$$

We can however equally well compute this posterior by updating yesterday's posterior $(\theta | x_1, \dots, x_{n-1})$ with today's measurement x_n by

$$p(\theta | x_1, \dots, x_n) \propto p(x_n | \theta) p(\theta | x_1, \dots, x_{n-1}). \quad (17)$$

The updating in (16) and (17) give the same result, but (17) can be used sequentially in what is often called **online learning**, where "yesterday's posterior becomes today's prior". This online learning is illustrated in Figure 23 for the internet speed data.

online learning

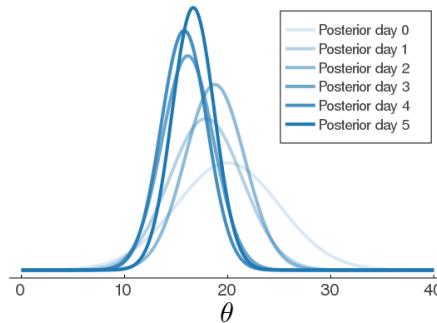


Figure 23: Internet speed data. Bayesian online learning.

The same online learning holds also for dependent data, e.g. time

series, as is easily proved as follows

$$\begin{aligned} p(\theta|x_1, \dots, x_n) &\propto p(x_1, \dots, x_n|\theta)p(\theta) \\ &= p(x_n|\theta, x_1, \dots, x_{n-1})p(x_1, \dots, x_{n-1}|\theta)p(\theta) \\ &\propto p(x_n|\theta, x_1, \dots, x_{n-1})p(\theta|x_1, \dots, x_{n-1}), \end{aligned} \quad (18)$$

where the second line follows from the decomposition results in Figure 24. For iid data we have the additional simplification $p(x_n|\theta, x_1, \dots, x_{n-1}) = p(x_n|\theta)$, hence showing the equivalence of (16) and (17).

By the same proof we also see that Bayesian methods are directly applicable in **batch learning**, where the posterior can be incrementally updated using batches of several observations, since for any $1 \leq m \leq n - 1$

$$p(\theta|x_1, \dots, x_n) \propto p(x_{m+1}, \dots, x_n|\theta)p(\theta|x_1, \dots, x_m). \quad (19)$$

Implementing online or batch learning is straightforward for conjugate models since:

- any intermediate posterior $p(\theta|x_1, \dots, x_m)$ belongs to the same distribution family as the original prior $p(\theta)$ and
- the prior is conjugate to the likelihood for any data, and therefore also to the likelihood of the new batch $p(x_{m+1}, \dots, x_n|\theta)$.

In the case of the iid normal model with known variance we have the recursions for observation $i = 1, 2, \dots$

$$\begin{aligned} \frac{1}{\tau_i^2} &= \frac{1}{\sigma^2} + \frac{1}{\tau_{i-1}^2} \\ w_i &= \frac{\sigma^{-2}}{\sigma^{-2} + \tau_{i-1}^{-2}} \\ \mu_i &= w_i x_i + (1 - w_i) \mu_{i-1}. \end{aligned}$$

When the prior is not conjugate one has to resort to numerical methods that can be more or less computationally attractive in online mode; see in the chapters [Posterior simulation](#) and [Variational inference](#).

Poisson data

Count data $X \in \{0, 1, 2, \dots\}$ is a quite frequently occurring data type in many applications; some examples are the number of software bugs, the number of lethal car accidents in a region, or the number of scooters available at a given pick-up station. The most commonly used model for count data is the **Poisson distribution**. The mean and variance of a Poisson variable are always equal, which can be

batch learning

Decomposing distributions

For two random variables X, Y

$$p(x, y) = p(y|x)p(x)$$

For n random variables

$$\begin{aligned} p(x_1, \dots, x_n) &= p(x_1)p(x_2|x_1) \times \\ &\dots \times p(x_n|x_1, \dots, x_{n-1}) \end{aligned}$$

and conditional on θ

$$\begin{aligned} p(x_1, \dots, x_n|\theta) &= p(x_1|\theta) \times \\ &\dots \times p(x_n|x_1, \dots, x_{n-1}, \theta) \end{aligned}$$

Figure 24: Marginal-Conditional decomposition of a joint distribution.

Poisson distribution

$X \sim \text{Pois}(\theta)$ for $X \in \{0, 1, 2, \dots\}$

$$p(x) = \frac{\theta^x e^{-\theta}}{x!}$$

$$\mathbb{E}(X) = \theta$$

$$\mathbb{V}(X) = \theta$$

Figure 25: The Poisson distribution.

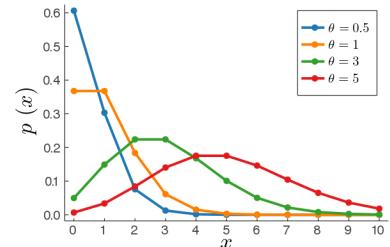


Figure 26: Some Poisson distributions.

Poisson distribution

restrictive in some application, but the model often fits many real datasets surprisingly well or can be extended to do so.

Figure 27.

The likelihood function for $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} \text{Pois}(\theta)$, is

$$p(x_1, \dots, x_n | \theta) = \prod_{i=1}^n \frac{\theta^{x_i} e^{-\theta}}{x_i!} \propto \theta^{\sum_{i=1}^n x_i} e^{-n\theta}. \quad (20)$$

Comparing the functional form of the likelihood in (20) with a list of common probability distributions we can see that the likelihood from iid Poisson data looks very much like a **Gamma distribution** in θ . Even more, the form of the Gamma distribution tells us that a Gamma prior may indeed combine nicely with this likelihood. So let us try if $\theta \sim \text{Gamma}(\alpha, \beta)$ is conjugate to the iid Poisson model:

$$\begin{aligned} p(\theta | x_1, \dots, x_n) &\propto p(x_1, \dots, x_n | \theta)p(\theta) \\ &\propto \theta^{\sum_{i=1}^n x_i} e^{-n\theta} \cdot \theta^{\alpha-1} e^{-\beta\theta} \\ &= \theta^{\alpha+\sum_{i=1}^n x_i - 1} e^{-(\beta+n)\theta}, \end{aligned}$$

where we have directly written up the $\text{Gamma}(\alpha, \beta)$ prior without normalization constant. This expression is indeed proportional to a Gamma distribution and we have the following result:

Conjugate analysis - Poisson model

Model: $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} \text{Pois}(\theta)$

Prior: $\theta \sim \text{Gamma}(\alpha, \beta)$

Posterior: $\theta | x_1, \dots, x_n \sim \text{Gamma}(\alpha + \sum_{i=1}^n x_i, \beta + n)$

Gamma distribution

$X \sim \text{Gamma}(\alpha, \beta)$ for $X > 0$.

$$p(x) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}$$

$$\mathbb{E}(X) = \frac{\alpha}{\beta}$$

$$\mathbb{V}(X) = \frac{\alpha}{\beta^2}$$

Figure 27: Gamma distribution.

Gamma distribution

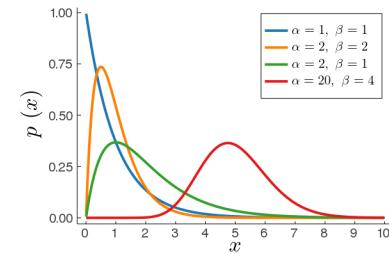


Figure 28: Some Gamma distributions.

Figure 29: Prior-to-Posterior updating for the Poisson data with a Gamma prior.

EXAMPLE: INTERNET AUCTION DATA. The **eBayCoin dataset** collected by [Wegmann and Villani \[2011\]](#) and made available in the UCI repository² consist of data from 1000 eBay auctions of collectors coins. For each auction, the dataset records the final price of the auctioned coin, the number of bidder in the auction and a number of covariates such as the quality of the sold coin, the lowest price that the seller would agree to sell for etc. We will here analyze the number of bidders using an iid Poisson model without covariates. We return to this dataset in Chapter [Classification](#) where we make use of the covariates in a Poisson regression model for predicting the number of bidders.

To compute the posterior distribution for θ , the average number of bidders in an auction we need the summary statistic $\sum_{i=1}^n x_i = 3635$. The sample mean in the $n = 1000$ auctions is therefore $\bar{x} = 3.635$

eBayCoin dataset

² <http://archive.ics.uci.edu/ml/datasets/eBayCoin/>

bidders per auction. I will use the gamma prior with $\alpha = 2$ and $\beta = 1/2$ since this implies a prior mean of $\mathbb{E}(\theta) = 4$ and prior standard deviation of $S(\theta) = 2.283$, which I find matches quite well with my prior beliefs. This prior and the posterior updated with data from $n = 1000$ auctions are shown in Figure 30. Note the different scales on the horizontal axis. We are now more or less certain that the average number of bidders is in the interval $\theta \in [3.4, 3.9]$.

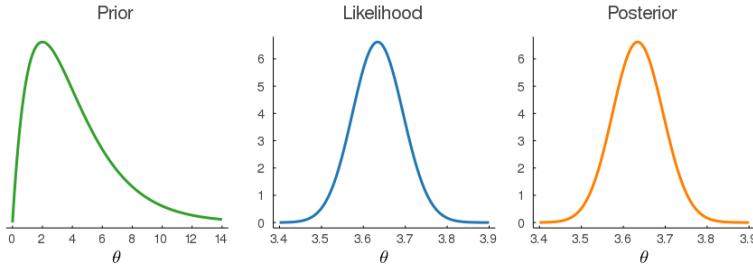


Figure 30: Bayesian analysis of the numbers of bidders in $n = 1000$ eBay coin auctions.

Figure 31 a) plots the fitted Poisson distribution with θ set equal to the posterior mean against the observed data. It is obvious that the Poisson distribution is too restrictive as the fit is terrible.

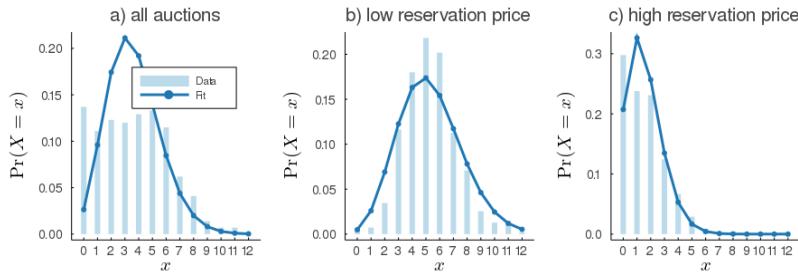


Figure 31: Assessing the fit of the Poisson model with the posterior mean estimate of θ .

The poor fit can be attributed to the heterogeneity of the auctions. For example, some of the auctions had a high so called reservation price, i.e. the lowest price that the seller is willing to sell for, while other auctions had a very low reservation price. It is expected that a high reservation price discourages bidders from entering the auction.

To explore the effect of the reservation price we split the data into low and high reservation price auctions, and analyze the two auction types separately. The prior-to-posterior updating is shown in Figure 32; the priors now reflect that θ is likely to be larger for the auctions with low reservation prices. The posteriors are clearly different in the two subpopulations. The Poisson model fits better on the two subpopulations as shown in Figure 31 b) and c), but it is not perfect. We will return to this dataset in Chapter Regression using a Poisson regression with the reservation price as covariate as well as other auction specific covariates.

We have now seen that:

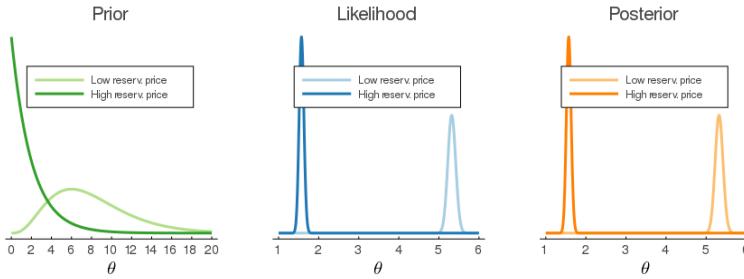


Figure 32: eBay auctions. Bayesian analysis of the numbers of bidders in $n = 550$ auctions with a low reservation price and $n = 450$ auctions with a high reservation price.

- the beta prior is conjugate to the Bernoulli likelihood
- the normal prior is conjugate to the normal likelihood
- the gamma prior is conjugate to the Poisson likelihood.

Here is a formal definition of a conjugate prior.

Definition (Conjugate prior). A family of prior distributions \mathcal{P} is conjugate to a family of likelihoods $\mathcal{L} = \{p(\mathbf{x}|\theta), \theta \in \Theta\}$ if

$$p(\theta) \in \mathcal{P} \Rightarrow p(\theta|\mathbf{x}) \in \mathcal{P} \quad \text{for all } p(\mathbf{x}|\theta) \in \mathcal{L}.$$

Summarizing a posterior distribution

The posterior distribution for models with a single parameter are easily plotted and gives a complete visual quantification of uncertainty. Starting from the next chapter, our models will typically contain more than one parameter, and not seldom quite many. It is then impractical to plot the whole posterior distribution and we will now explore some commonly used numerical summaries of the posterior, for example a point estimate and posterior probability intervals.

A point estimate of θ summarizes the posterior with a single point. The three most commonly used Bayesian point estimates are:

- The posterior mean $\hat{\theta}_{\text{mean}} \equiv \mathbb{E}(\theta|x_1, \dots, x_n)$.
- The posterior median $\hat{\theta}_{\text{med}}$, i.e. the 50th quantile of $p(\theta|x_1, \dots, x_n)$.
- The posterior mode $\hat{\theta}_{\text{mode}} \equiv \arg \max_{\theta \in \Theta} p(\theta|x_1, \dots, x_n)$.

We will see in chapter [Prediction and Decision making](#) that the choice of point estimate can be formalized as a decision problem.

A point estimate says nothing about the variability in the posterior. One way to quantify the uncertainty is the posterior standard deviation $S(\theta|x_1, \dots, x_n) = \sqrt{\text{V}(\theta|x_1, \dots, x_n)}$.

EXAMPLE: INTERNET AUCTION DATA. As we saw earlier the posterior for the mean θ of a Poisson distribution with a $\theta \sim \text{Gamma}(\alpha, \beta)$

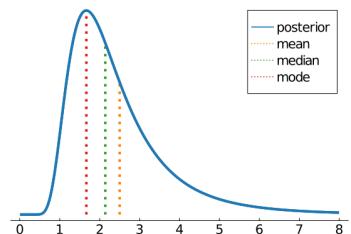


Figure 33: Three common point estimates for summarizing a posterior.

prior is $\theta|x_1, \dots, x_n \sim \text{Gamma}(\alpha + \sum_{i=1}^n x_i, \beta + n)$. From properties of the Gamma distribution, the posterior mean estimate is hence $(\alpha + \sum_{i=1}^n x_i)/(\beta + n)$ and the posterior variance is $(\alpha + \sum_{i=1}^n x_i)/(\beta + n)^2$. For the eBay data [Poisson data](#) we have $\mathbb{E}(\theta|x_1, \dots, x_n) = \frac{2+3635}{0.5+1000} \approx 3.635$ bidders and $S(\theta|x_1, \dots, x_n) = \sqrt{\frac{2+3635}{(0.5+1000)^2}} \approx 0.060$.

Before presenting how to summarize a posterior by an interval, let us first informally recall the definition of a frequentist confidence interval. A 95% *confidence interval* for a parameter θ is a random interval $[l(X_1, \dots, X_n), u(X_1, \dots, X_n)]$ that contains the true θ in 95% of all possible datasets X_1, \dots, X_n from the data generating process. As usual with frequentist methods we are guaranteed a long run performance over all possible datasets, but the realized interval $[l(x_1, \dots, x_n), u(x_1, \dots, x_n)]$ either does or does not cover the true θ .

A Bayesian interval is defined in a much more direct way, and is conditional on the actually observed dataset. This simpler definition is possible since the posterior is a probability distribution; we have broken the Bayesian eggs and can enjoy the omelette. A 95% posterior **credibility interval** for $\theta \in \Theta \subset \mathbb{R}$ is an interval $[l, u] \subset \Theta$ such that $\Pr(\theta \in [l, u] | x_1, \dots, x_n) = 0.95$, i.e. an interval that contains 95% of the posterior probability mass. We can generalize this to a more general region than an interval, for example a union of disjoint intervals, and of course to other probability coverages than 95%.

There are many ways to construct a credibility interval with a certain coverage probability. An **equal tail credibility interval** is an interval that cuts off equal probability in the left and right tail; for example, a 95% interval sets l and u to the 2.5% and 97.5% posterior quantile, respectively. Another popular interval construction is the highest posterior density (HPD) region which, as the name suggest, is made up of the θ values with highest posterior density. We use the word *region* instead of interval here since HPD regions need not be intervals. Here is the definition.

Definition (HPD region). A **Highest Posterior Density (HPD) region** for $\theta \in \Theta$ with coverage probability γ is a region $R \subset \Theta$ such that:

- $\Pr(\theta \in R | x_1, \dots, x_n) = \gamma$ and
- $p(\theta_{\text{in}} | x_1, \dots, x_n) \geq p(\theta_{\text{out}} | x_1, \dots, x_n)$ for all $\theta_{\text{in}} \in R$ and $\theta_{\text{out}} \notin R$.

Figure 34 illustrates the difference between equal tail intervals and HPD regions for some example densities. Note how the equal tail interval construction can exclude θ values that actually have highest posterior density (middle graph) and how HPD regions can be disconnected (righthand graph).

credibility interval

equal tail credibility interval

Highest Posterior Density (HPD) region

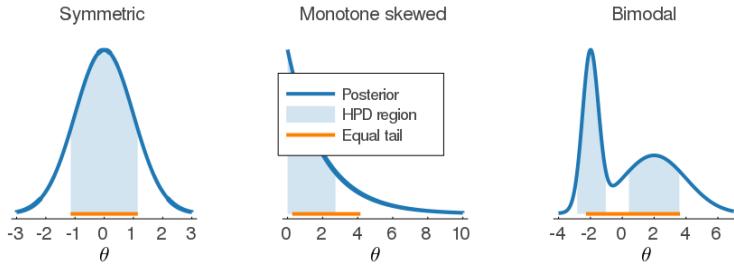


Figure 34: HPD regions vs equal tail intervals.

A disadvantage of HPD regions is that they are not invariant to reparametrization; the HPD for a transformed parameter $\eta(\theta)$ is typically not a direct map of the HPD for θ .

EXAMPLE: INTERNET AUCTION DATA The 95% equal tail interval for the mean number of bidders in the iid Poisson model is $[3.518, 3.754]$ which is virtually indistinguishable from the HPD interval $[3.517, 3.754]$ since the posterior is essentially symmetric, see Figure 35.

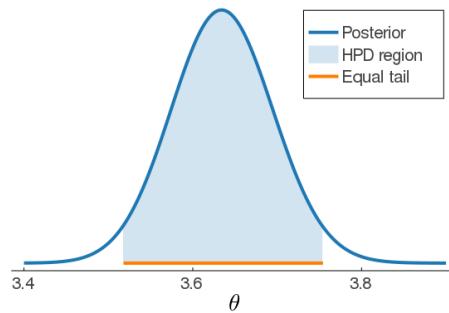


Figure 35: 95% credibility intervals for the Gamma posterior in the eBay auction data.

Exponential Family and Sufficiency*

This section presents the concept of sufficient statistics and the exponential family of distributions, with particular emphasis on their role in Bayesian learning. While these concepts are very important in statistics, this starred section can be skipped at first reading, but should be read before the generalized linear models in Chapter [Classification](#), where the exponential family plays a prominent role.

Sufficient statistics

In all models covered so far in this book, the dataset, (x_1, \dots, x_n) , has only entered the likelihood through some low-dimensional summary statistic; for example the number of successes $s = \sum_{i=1}^n x_i$ in the

Bernoulli model, the sample mean $\bar{x} = n^{-1} \sum_{i=1}^n x_i$ in the Gaussian model, and the sum of counts, $\sum_{i=1}^n x_i$, in the Poisson model. Note that we did not choose this data reduction, it just turned out that the likelihood only depended on the summarizing statistic; the statistic captured all the relevant information in the sample. In all of the above examples, the statistic was one-dimensional. In other models more than a single dimension is needed to compress the dataset, and we let the vector-valued function $\mathbf{t}(x_1, \dots, x_n) \rightarrow \mathbb{R}^k$ denote the statistic in general, where k is the dimension of reduction.

The following definition captures the idea that a statistic may contain *all* relevant information in the data about a parameter θ .

Definition. *Sufficient statistic.* A statistic $\mathbf{t}(X_1, \dots, X_n)$ is sufficient for θ if the conditional distribution of the sample X_1, \dots, X_n given the value of the statistic $\mathbf{t}(X_1, \dots, X_n)$ does not depend on θ .

Sufficient statistic

The sufficiency of a statistic can be checked by the following lemma; see [Casella and Berger \[2002\]](#) for a proof.

Lemma 1. *Factorization criterion.* A statistic $t(x_1, \dots, x_n)$ is sufficient for a parameter θ if and only if the likelihood can be factorized as

Factorization criterion

$$p(x_1, \dots, x_n | \theta) = h(x_1, \dots, x_n) f(\mathbf{t}(x_1, \dots, x_n); \theta), \quad (21)$$

where $h(x_1, \dots, x_n)$ does not depend on θ and $f(\mathbf{t}; \theta)$ is a function of the data only through the sufficient statistic $\mathbf{t}(x_1, \dots, x_n)$.

The idea behind sufficient statistics is so appealing that it is often formulated as a desired inference principle similar to the likelihood principle presented in the section [Bayesian learning and the likelihood principle](#).

Definition. *Sufficiency principle.* If $\mathbf{t}(X_1, \dots, X_n)$ is a sufficient statistic for θ then any inference about θ should depend on the sample x_1, \dots, x_n only through the value $\mathbf{t}(x_1, \dots, x_n)$.

Sufficiency principle

Theorem 1. Bayesian learning satisfies the sufficiency principle.

Proof. If $\mathbf{t}(x_1, \dots, x_n)$ is a sufficient statistic for θ then by Lemma 1

$$\begin{aligned} p(\theta | x_1, \dots, x_n) &= \frac{p(x_1, \dots, x_n | \theta) p(\theta)}{\int p(x_1, \dots, x_n | \theta) p(\theta) d\theta} \\ &= \frac{h(x_1, \dots, x_n) f(\mathbf{t}(x_1, \dots, x_n); \theta) p(\theta)}{\int h(x_1, \dots, x_n) f(\mathbf{t}(x_1, \dots, x_n); \theta) p(\theta) d\theta} \\ &= \frac{f(\mathbf{t}(x_1, \dots, x_n); \theta) p(\theta)}{\int f(\mathbf{t}(x_1, \dots, x_n); \theta) p(\theta) d\theta'} \end{aligned}$$

which only depends on the data through the sufficient statistic $\mathbf{t}(x_1, \dots, x_n)$. □

Exponential family

All models considered so far are part of the large and important exponential family of distributions. A random variable X follows a distribution in the (one-parameter) **exponential family** if its density can be written in the form

$$p(x|\theta) = h(x) \exp\left(\eta(\theta)t(x) - A(\theta)\right), \text{ for } x \in \mathcal{X}, \quad (22)$$

where $h(x)$ is a function of only x and $A(\theta)$ is a function of only θ . The support \mathcal{X} is not allowed to depend on θ , so that for example the $\text{Uniform}(0, \theta)$ distribution does not belong to the exponential family. The function $\eta(\theta)$ is called the **natural parameter** and is an invertible transformation of the parameter θ . Here are some examples.

EXAMPLE: POISSON DISTRIBUTION. The $\text{Pois}(\theta)$ distribution can be rewritten as follows

$$p(x|\theta) = \frac{\theta^x e^{-\theta}}{x!} = \frac{e^{x \ln \theta} e^{-\theta}}{x!} = \frac{1}{x!} \exp(x \ln \theta - \theta),$$

which is in the exponential family with $h(x) = (x!)^{-1}$, $A(\theta) = \theta$, $\eta(\theta) = \ln \theta$ and $t(x) = x$. Note in particular that the natural parameter is the logarithm of the Poisson mean, $\eta(\theta) = \ln \theta$.

EXAMPLE: BERNOULLI DISTRIBUTION. The $\text{Bern}(\theta)$ distribution can also be written as an exponential family:

$$p(x|\theta) = \theta^x (1-\theta)^{1-x} = \left(\frac{\theta}{1-\theta}\right)^x (1-\theta) = \exp\left(\eta(\theta)x - A(\theta)\right),$$

where $\eta(\theta) = \ln(\frac{\theta}{1-\theta})$, $A(\theta) = \ln(\frac{1}{1-\theta})$, $t(x) = x$ and $h(x) = 1$. The natural parameter for the Bernoulli distribution is therefore the log-odds, $\ln(\frac{\theta}{1-\theta})$.

The normal distribution and many other distributions can similarly be shown to belong to the exponential family; but not all do, for example the **student-t distribution**. We will use $\text{ExpFam}(\theta)$ as a generic notation for a distribution in the exponential family, leaving the specific $h(x)$, $A(\theta)$, $\eta(\theta)$ and $t(x)$ functions implicit.

The likelihood function for iid data from an $\text{ExpFam}(\theta)$ distribution is

$$p(x_1, \dots, x_n|\theta) = \left[\prod_{i=1}^n h(x_i) \right] \exp\left(\eta(\theta) \sum_{i=1}^n t(x_i) - nA(\theta)\right). \quad (23)$$

Lemma 1 can be directly used to show that $\sum_{i=1}^n t(x_i)$ is a sufficient statistic for θ . In the next chapter we will see a multiparameter version of the exponential family with a vector of k sufficient statistics.

exponential family

natural parameter

Student-t distribution

$X \sim t(\mu, \sigma, \nu)$ for $X \in (-\infty, \infty)$

$$\begin{aligned} p(x) &= \frac{\Gamma((\nu+1)/2)}{\Gamma(\nu/2)\sqrt{\pi\nu\sigma^2}} \\ &\times \left(1 + \frac{1}{\nu}\left(\frac{x-\mu}{\sigma}\right)^2\right)^{-\nu/2} \\ \mathbb{E}(X) &= \mu \text{ if } \nu > 1 \\ \mathbb{V}(X) &= \sigma^2 \frac{\nu}{\nu-2} \text{ if } \nu > 2 \end{aligned}$$

Figure 36: The student-t distributions.

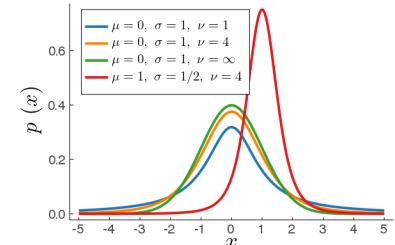


Figure 37: Some Student-t distributions.

student-t distribution

The Pitman–Koopman–Darmois theorem [Bernardo and Smith, 2009] proves that among distributions whose support does not depend on θ , only the exponential family have sufficient statistics of fixed dimension, i.e the dimension k does not depend on the size of the data, n (or at least is bounded).

The exponential family has several other attractive properties [Sundberg, 2019]. One property of particular interest here is that a conjugate prior always exists for models in the exponential family. In fact, the following family of priors is conjugate to the exponential family likelihood in (23)

$$p(\theta) = H(\tau_0, \nu_0) \exp \left(\eta(\theta)\tau_0 - \nu_0 A(\theta) \right), \quad (24)$$

where $H(\tau_0, \nu_0)$ is the normalizing constant. Note that this prior has two hyperparameter τ_0 and ν_0 that needs to be set by the user. We will use the symbol $\theta \sim \text{ExpFamConj}(\tau_0, \nu_0)$ for this prior distribution, where it must be remembered that the form of the prior depends on which specific exponential family member the prior is conjugate to, i.e. it depends on $\eta(\theta)$ and $A(\theta)$.

EXAMPLE: BERNOUlli MODEL. It was shown above that $\eta(\theta) = \ln \left(\frac{\theta}{1-\theta} \right)$ and $A(\theta) = \ln \left(\frac{1}{1-\theta} \right)$, for Bernoulli data. The prior in (24) is therefore

$$\begin{aligned} p(\theta) &\propto \exp \left(\eta(\theta)\tau_0 - \nu_0 A(\theta) \right) \\ &= \exp \left(\ln \left(\frac{\theta}{1-\theta} \right) \tau_0 - \nu_0 \ln \left(\frac{1}{1-\theta} \right) \right) \\ &\propto \theta^{\tau_0} (1-\theta)^{\nu_0 - \tau_0}, \end{aligned}$$

which is proportional to the Beta($\tau_0, \nu_0 - \tau_0$) distribution. The parametrization in (24) is hence interpreted as the information from a (imaginary) prior sample of τ_0 success in ν_0 trials. The Beta(α, β) prior from before expresses instead the prior information as a sample of α success and β failures.

Conjugate analysis from iid exponential family data

Model: $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} \text{ExpFam}(\theta)$

Prior: $\theta \sim \text{ExpFamConj}(\tau_0, \nu_0)$

Posterior: $\theta | x_1, \dots, x_n \sim \text{ExpFamConj}(\tau_0 + \sum_{i=1}^n t(x_i), \nu_0 + n)$

Figure 38: Prior-to-Posterior updating for iid exponential family data with a conjugate prior.

The posterior distribution for θ in the exponential family with a conjugate prior is obtained by multiplying the likelihood in (23) with

prior (24)

$$p(\theta|x_1, \dots, x_n) \propto \exp \left[\eta(\theta) \left(\tau_0 + \sum_{i=1}^n t(x_i) \right) - (\nu_0 + n) A(\theta) \right],$$

which is of the form ExpFamConj, but with updated hyperparameters: $\tau_0 \Rightarrow \tau_0 + \sum_{i=1}^n t(x_i)$ and $\nu_0 \Rightarrow \nu_0 + n$. We summarize this in Figure 38.

This result shows that we can think quite generally about ν_0 as the (imaginary) prior sample size and τ_0 as the prior data compressed by the sufficient statistic. For example, in the Poisson model the information in the conjugate prior equals a prior sample of ν_0 data points with a mean count of τ_0/ν_0 .

EXERCISES

1. Let $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} \text{Expon}(\theta)$ be exponentially distributed data. Show that the Gamma distribution is the conjugate prior for this model.
2. I determined my normal prior in the internet speed data example by specifying the prior mean θ_0 and standard deviation τ_0 . Assume that another person instead specified a 95% prior probability interval for θ as $[20, 30]$. Use this information to determine that persons normal prior, i.e. compute θ_0 and τ_0 for this person.
3. (a) Let x_1, \dots, x_{10} be a sample with $\bar{x} = 1.873$. Assume the model $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} N(\theta, 1)$ and the prior $\theta \sim N(0, 5)$. Compute the posterior distribution of θ .

 (b) You now get hold of a second sample $y_1, \dots, y_{10} | \theta \stackrel{\text{iid}}{\sim} N(\theta, 2)$, where θ is the same quantity as in (a) but the measurements have a larger variance. The sample mean in this second sample is $\bar{y} = 0.582$. Compute the posterior distribution of θ using both samples (the x 's and the y 's) under the assumption that the two samples are independent.

 (c) You finally obtain a third sample $z_1, \dots, z_{10} | \theta \stackrel{\text{iid}}{\sim} N(\theta, 3)$, with mean $\bar{z} = 1.221$. Unfortunately, the measuring device for this latter sample was defective and any measurement above 3 was recorded as exactly 3. There were two such measurements. Give an expression for the unnormalized posterior distribution (likelihood \times prior) for θ based on all three samples (x, y and z). If you have computer available you may plot this unnormalized posterior over a grid of θ values. Hint: the posterior distribution is not normal anymore when the measurements are truncated at 3.

4. Derive the posterior distribution for the normal model with a normal prior in Figure 21. *Hint: complete the square.*
5. (a) Let $x_1, \dots, x_n | \theta \sim \text{Uniform}(\theta - 1/2, \theta + 1/2)$. Let $\hat{\theta} = \bar{x}$ be an estimator of θ . Derive an expression for the sampling variance of $\hat{\theta}$.
(b) Derive the posterior distribution for θ assuming a uniform prior distribution. *Hint: once you have observed some data, some values for θ are no longer possible.*
(c) Assume that you have observed three data observations: $x_1 = 1.1, x_2 = 2.09, x_3 = 1.4$. What would a frequentist conclude about θ ? What would a Bayesian conclude? Discuss.
6. Show that the $N(\mu, 1)$ distribution belongs to the exponential family.

NOTEBOOKS

1. Analyzing Bernoulli data with Beta prior.

Multi-parameter models

Joint posterior distributions

Most models have more than one parameter, and many models are incredibly rich on parameters. Datasets are increasingly rapidly in size and makes it possible to estimate increasingly more complex models. To explore how Bayesian methods can be used in multiparameter models we first return in this chapter to the iid $N(\theta, \sigma^2)$, but now in the more realistic setting where both θ and σ^2 are unknown parameters. In later chapters we will tackle regression and classification models where each covariate (input) x_k affects the response (output) y through a regression coefficient β_k ; hence in a regression with K covariates we have K regression coefficients β_1, \dots, β_K .

Consider a general probability model $p(x_1, \dots, x_n | \theta_1, \dots, \theta_K)$ with K parameters for a dataset x_1, \dots, x_n ; for example the iid normal model where $\theta_1 = \mu$ and $\theta_2 = \sigma^2$. Bayesian learning proceeds exactly as with a single parameter, except that the prior and posterior distribution are now both multidimensional joint distributions. Figure 41 gives an illustration of a bivariate ($K = 2$) normal distribution.

Using Bayes' theorem in proportional form, the **joint posterior distribution** $p(\theta_1, \dots, \theta_K | x_1, \dots, x_n)$ is given by

$$p(\theta_1, \dots, \theta_K | x_1, \dots, x_n) \propto p(x_1, \dots, x_n | \theta_1, \dots, \theta_K) p(\theta_1, \dots, \theta_K),$$

where $p(\theta_1, \dots, \theta_K)$ is a multidimensional prior distribution and $p(x_1, \dots, x_n | \theta_1, \dots, \theta_K)$ is the likelihood function; Note that the likelihood function is now a **likelihood surface** in the sense that it is a function of several parameters, $\theta_1, \dots, \theta_K$.

To keep the notation simpler we often use vector notation and write $\boldsymbol{\theta} \equiv (\theta_1, \dots, \theta_n)$ and $\mathbf{x} \equiv (x_1, \dots, x_n)$. The multivariate Bayes' theorem can then be expressed as

$$p(\boldsymbol{\theta} | \mathbf{x}) \propto p(\mathbf{x} | \boldsymbol{\theta}) p(\boldsymbol{\theta}). \quad (25)$$

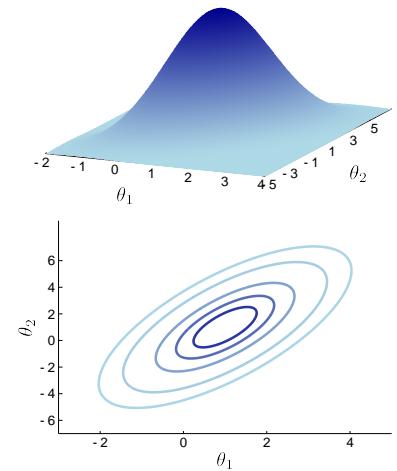


Figure 41: Surface and contour plot of the bivariate normal distribution. The contour levels contain 25, 50, 75, 95 and 99% of the probability mass, respectively.

joint posterior distribution

likelihood surface

Marginalization

The joint posterior distribution $p(\theta|x)$ contains all posterior information about θ , but is obviously hard to visualize in the same way as we did for single-parameter models. In many cases we are also most interested in a subset of parameters, and the other parameters are only needed to model the data well but are of no real interest. Such parameters are just a nuisance when presenting inferences and are therefore often called **nuisance parameters**. Getting rid of nuisance parameters is very difficult in a non-Bayesian setting, for example when using maximum likelihood estimation. So what is the Bayesian solution to this dilemma?

Nuisance parameters can be handled in a very natural way in a Bayesian approach since the posterior distribution is a probability distribution for θ . We can therefore just integrate out, or marginalize out, the nuisance parameters just as in ordinary probability calculus. Take a simple example where $\theta = (\theta_1, \theta_2)$ and assume that the parameter of interest is θ_1 whereas θ_2 is considered a nuisance parameter; θ_1 could for example be the mean of iid Gaussian model and θ_2 the variance. The marginal posterior of θ_1 is then

$$p(\theta_1) = \int p(\theta_1, \theta_2) d\theta_2,$$

where the integration is over the full support of θ_2 . Figure 42 illustrates the marginalization concept. Using the decomposition $p(\theta_1, \theta_2) = p(\theta_1|\theta_2)p(\theta_2)$ we can alternatively express this as

$$p(\theta_1) = \int p(\theta_1|\theta_2)p(\theta_2) d\theta_2,$$

which shows that marginalization is achieved by averaging over the values of θ_2 with weights given by $p(\theta_2)$.

More generally, with more than two parameters, partition the elements of θ into two vectors, θ_a and θ_b . The marginal posterior of θ_a is the obtained by marginalizing out θ_b from the joint posterior

$$p(\theta_a) = \int \cdots \int p(\theta_a, \theta_b) d\theta_b. \quad (26)$$

We will see examples of marginalization in the following sections.

Gaussian data with unknown variance

The previous chapter analyzed iid normal data $x_1, \dots, x_n | \theta, \sigma^2 \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$ under the usually unrealistic assumption that σ^2 is known. Let us now tackle the case where both parameters are unknown. It

nuisance parameters

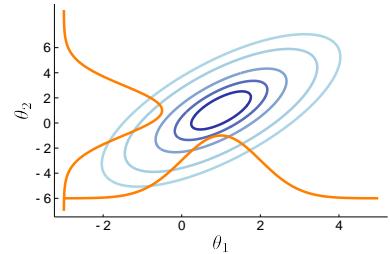


Figure 42: Contour plot of the bivariate normal distribution in Figure 41 along with the marginal distributions.

turns out that the conjugate prior for this model has dependence between θ and σ , so we will describe the prior using the decomposition $p(\theta|\sigma^2)p(\sigma^2)$ as follows

$$\theta|\sigma^2 \sim N(\mu_0, \sigma^2/\kappa_0) \quad (27)$$

$$\sigma^2 \sim \text{Inv}-\chi^2(\nu_0, \sigma_0^2). \quad (28)$$

The marginal conjugate prior for σ^2 involves a new distribution, the **scaled inverse chi-squared distribution**, denoted by $\text{Inv}-\chi^2(\nu_0, \sigma_0^2)$; see Figure 43. This distribution is a specific parametrization of the **inverse Gamma distribution**. The name comes from the characterization

$$X \sim \chi_\nu \Rightarrow Y = \nu\tau^2 \frac{1}{X} \sim \text{Inv}-\chi^2(\nu, \tau^2),$$

so that a $\text{Inv}-\chi^2(\nu, \tau^2)$ variable really is an inverted χ_ν^2 variable scaled by $\nu\tau^2$. Note that the parameter τ^2 is close to the mean when ν is large. The mode is $\nu\tau^2/(\nu + 2)$, so τ^2 is somewhere between the mode and the mean. We will therefore call τ^2 the location of $\text{Inv}-\chi^2(\nu, \tau^2)$, or sometimes just sloppily as "our best guess".

The conjugate prior in (27) is specified via the four prior hyperparameters:

- μ_0 - the prior mean for θ
- κ_0 - the number of prior data observations for θ
- σ_0^2 - the prior location of σ^2
- ν_0 - the prior degrees of freedom for σ^2 .

Note that, similar to the conjugate prior for the exponential family, we are only *interpreting* κ_0 as the number of prior observations. The prior may not actually be based on previous data, but the information in the prior $\theta|\sigma^2 \sim N(\mu_0, \sigma^2/\kappa_0)$ has the equivalent strength of an *imaginary* prior sample of κ_0 observations from a data generating process with variance σ^2 .

Figure 44 shows that the posterior is indeed in the same form as the prior in (27), as required for a conjugate prior. There is a lot of greek letters in Figure 44, but note that the same sort of intuition applies here as in the case with a known variance in Chapter Single-parameter models:

- the posterior mean μ_n is a weighted average of the data mean \bar{x} and the prior mean μ_0
- the weight on the data $w = n/(\kappa_0 + n)$ is close to one when either the data is informative (large n) or the prior is weak (small κ_0)

scaled inverse chi-squared distribution

inverse Gamma distribution

Inv- χ^2 distribution

$$X \sim \text{Inv}-\chi^2(\nu, \tau^2), X \in (0, \infty)$$

$$p(x) = \frac{(\tau^2\nu/2)^{\nu/2}}{\Gamma(\nu/2)} \frac{\exp\left(-\frac{\nu\tau^2}{2x}\right)}{x^{1+\nu/2}}$$

$$\mathbb{E}(X) = \frac{\nu}{\nu - 2}\tau^2$$

$$\mathbb{V}(X) = \frac{2\nu^2\tau^4}{(\nu - 2)^2(\nu - 4)}$$

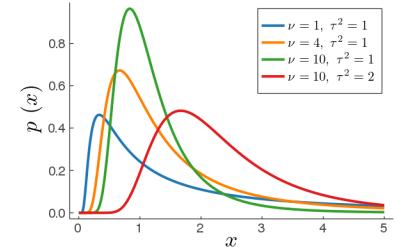


Figure 43: Some Scaled-Inv-Gamma distributions.

Gaussian iid data with conjugate prior

Model: $x_1, \dots, x_n | \theta, \sigma^2 \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$

Prior: $\theta | \sigma^2 \sim N(\mu_0, \sigma^2 / \kappa_0)$

$\sigma^2 \sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2)$

Posterior: $\theta | \sigma^2, \mathbf{x} \sim N(\mu_n, \sigma^2 / \kappa_n)$

$\sigma^2 | \mathbf{x} \sim \text{Inv-}\chi^2(\nu_n, \sigma_n^2)$

$$\mu_n = w\bar{x} + (1-w)\mu_0$$

$$w = \frac{n}{\kappa_0 + n}$$

$$\kappa_n = \kappa_0 + n$$

$$\nu_n = \nu_0 + n$$

$$\nu_n \sigma_n^2 = \nu_0 \sigma_0^2 + (n-1)s^2 + \frac{\kappa_0 n}{\kappa_0 + n} (\bar{x} - \mu_0)^2$$

where $\bar{x} = \sum_{i=1}^n x_i$ and $(n-1)s^2 = \sum_{i=1}^n (x_i - \bar{x})^2$

Marginal: $\theta | \mathbf{x} \sim t(\mu_n, \sigma_n^2 / \kappa_n, \nu_n)$

Figure 44: Prior-to-Posterior updating for the iid Gaussian model with unknown mean and variance using the conjugate prior.

- the reason why σ^2 does not appear in w is that the prior variance for θ is scaled by σ^2 in the conjugate prior, and σ^2 therefore cancels out in w .
- the posterior sample size $\kappa_n = \kappa_0 + n$ is the sum of the number of prior observations κ_0 and the sample size n .

Interest centers mainly on the average download speed, so we would like to obtain the marginal posterior distribution of θ . This distribution can be derived by marginalizing out the nuisance parameter σ^2 from the joint posterior

$$p(\theta | x_1, \dots, x_n) = \int p(\theta | \sigma^2, x_1, \dots, x_n) p(\sigma^2 | x_1, \dots, x_n) d\sigma^2,$$

where $p(\theta | \sigma^2, x_1, \dots, x_n)$ and $p(\sigma^2 | x_1, \dots, x_n)$ are given in Figure 44.

In Exercise 1 you are asked to show that the marginal posterior of θ is a student- t distribution; see Figure 36 and 37 for a definition and properties. Specifically, we have the following result

$$\theta | x_1, \dots, x_n \sim t(\mu_n, \sigma_n^2 / \kappa_n, \nu_n), \quad (29)$$

where μ_n , σ_n^2 , κ_n and ν_n are all defined as in Figure 44. Note that also the marginal prior for θ follows a student- t distribution of the form (29), but with hyperparameters naturally subscripted by 0 instead of n .

EXAMPLE: INTERNET SPEED DATA. Let us return to the example with the $n = 5$ download speeds with a mean of $\bar{x} = 15.998$ Mbit/s from the chapter Single-parameter models. This time we assume that

also σ^2 , the variability of the measurements from the speed testing service, is unknown. I will use the prior hyperparameters $\mu_0 = 20$, $\kappa_0 = 1$, $v_0 = 5$ and $\sigma_0^2 = 5^2$, which agrees in location with my previous prior when σ^2 was assumed known at $\sigma^2 = 5^2$; setting $v_0 = 5$ gives a prior equal to the green distribution in the right graph of Figure 46, which I find sensible.

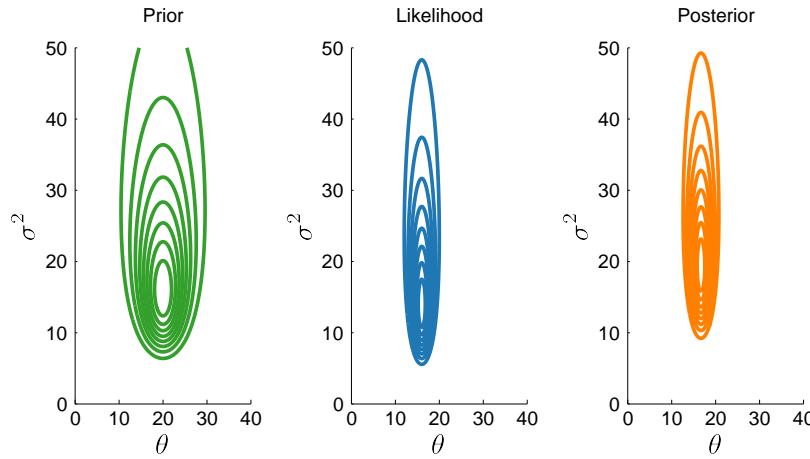


Figure 45: Prior-to-Posterior updating for the internet speed data in the iid Normal model. Contours of joint distributions of θ and σ^2 .

Figure 45 displays contours of the joint prior, likelihood and posterior for θ and σ^2 ; the posterior is more concentrated than the prior, especially for θ . The marginal priors and posterior for the two parameters are shown in Figure 46. The data have made both marginal posteriors more concentrated, but less so for σ^2 since we do not learn so much about a variance from only $n = 5$ observations. The probability of at least 20 Mbit download speed has decreased from the prior probability of 0.5 to 0.066 in the posterior.

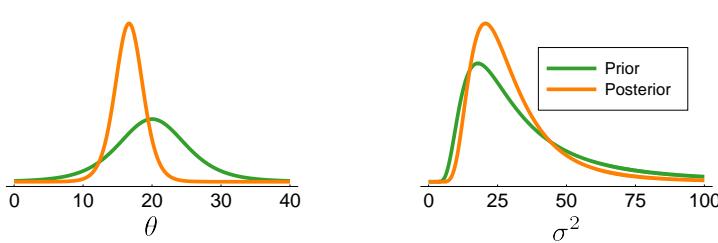


Figure 46: Marginal posteriors for the internet speed data in the iid Normal model.

A first look at Monte Carlo simulation

The iid Gaussian model with conjugate prior is an example of a model where we can obtain both the joint and the marginal posteriors in analytical form. This is rarely the case in more complex models or when non-conjugate priors are used. The idea with Monte Carlo methods is to simulate **posterior draws** of θ from $p(\theta|x_1, \dots, x_n)$ and approximate the posterior by for example a histogram. We will have much more to say about this in Chapter [Posterior simulation](#) where powerful simulation algorithms are presented, but we will already here introduce the most basic Monte Carlo simulation method.

posterior draws

Posterior simulation - iid Gaussian with conjugate prior.

```

Input: data  $x = (x_1, \dots, x_n)$ 
        number of posterior draws  $m$ .
compute  $\mu_n, \sigma_n^2, \kappa_n$  and  $\nu_n$  using Figure 44.
for  $i$  in  $1:m$  do
     $\sigma^2 \leftarrow \text{rINVCHI2}(\nu_n, \sigma_n^2)$ 
     $\theta \leftarrow \text{rNORMAL}(\mu_n, \sigma^2 / \kappa_n)$ 
end
Output:  $m$  draws for  $\theta$  and  $\sigma^2$  from joint posterior.

Function  $\text{rINVCHI2}(\nu, \tau^2)$ 
     $x = \text{rCHI2}(\nu)$ 
     $y = \nu \tau^2 / x$ 
    return  $y$ 
```

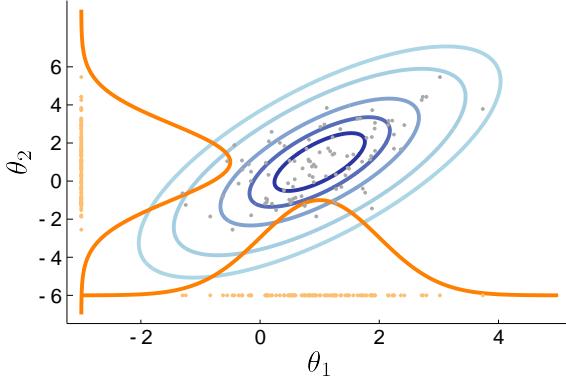
Figure 47: Algorithm for posterior simulation for the iid Normal model with conjugate prior. The `rNORMAL` and `rCHI2` random number generators are assumed to be part of the standard library. The variable σ^2 is highlighted in orange to indicate that the most recent draw of σ^2 is used in the call to the `rNORMAL` function.

The algorithm in Figure 47 gives pseudo-code for simulating from the $p(\theta, \sigma^2 | \mathbf{x})$ in the iid normal model by iteratively simulating from $p(\sigma^2 | \mathbf{x})$ followed by simulation from $p(\theta | \sigma^2, \mathbf{x})$. Note how this involves using the most recently simulated value of σ^2 when simulating θ . The algorithm includes the subfunction `rINVCHI2(ν_n, σ_n^2)` to draw from the Inv- χ^2 distribution. The algorithm implicitly assumes that the standard library of your programming language includes random number generators `rCHI2(ν)` and `rNORMAL($\mu_n, \sigma^2 / \kappa_n$)` for the χ^2 and normal distributions, respectively.

EXAMPLE: INTERNET SPEED DATA

Let us now simulate from the posterior of θ and σ^2 in the Internet speed data. The second and third columns in Table 1 show the output from generating $m = 10,000$ joint posterior draws with the algorithm in Figure 47.

draw	θ	σ^2	σ/θ	$\theta \geq 20$
1	18.165	18.451	0.236	0
2	20.431	29.943	0.267	1
3	15.565	29.094	0.346	0
:	:	:	:	:
10,000	16.400	21.668	0.283	0
Mean	16.645	30.813	0.330	0.066



One attractive feature of simulating from the joint posterior distribution is that all marginal posterior distributions are directly obtained by just selecting the column for the parameter in question; tedious integration is replaced by plotting a histogram of the selected column. This is illustrated in Figure 48.

Figure 51 shows the marginals for the internet speed data example obtained from simulation; the figure also plots the analytical marginal posteriors, which happen to be known in this simple example.

The histograms of the simulated draws in Figure 51 are clearly approximating the posteriors extremely well. Monte Carlo simulation is theoretically known to be **simulation consistent** in the sense that we are guaranteed to get arbitrary close to the true posterior if we simulate a large number of draws. For example, if we let $\theta^{(i)}$ denote the i th posterior draw of any of the parameters in a model, then

$$\bar{\theta}_{1:m} \equiv \frac{1}{m} \sum_{i=1}^m \theta^{(i)} \xrightarrow{p} \mathbb{E}(\theta|\mathbf{x}) \text{ as } m \rightarrow \infty,$$

where \xrightarrow{p} denotes **convergence in probability**, see Figure 49. The result says that the mean of the posterior draws will get closer and closer to the theoretical posterior mean $\mathbb{E}(\theta|\mathbf{x})$ as we increase the number of simulations, m . This is version of the **law of large numbers**, see Figure 50. The left side of Figure 52 illustrates this convergence by plotting the posterior mean estimates $\bar{\theta}_{1:m}$ for increasing m ; note that the figure shows the cumulative estimates only up to

Table 1: Posterior simulation output for the Internet speed dataset with computed functions of the parameters.

Figure 48: Illustrating marginalization by selection. The figure plots the contours of a joint distribution with the marginal distributions overlaid as orange curves. The gray points are 100 draws from joint distribution and the orange points are projections of the gray points on the two axes. The orange points correspond to the draws obtained by selecting out each parameter from the joint simulation and clearly represent the marginal posteriors.

Convergence in probability

A sequence of random variables X_1, \dots, X_n **converges in probability to a constant c** , if and only if for any $\epsilon > 0$

$$\Pr(|X_n - c| > \epsilon) \rightarrow 0 \text{ as } n \rightarrow \infty.$$

We then write $X_n \xrightarrow{p} c$.

X_1, \dots, X_n **converges in probability to a random variable X** if and only if for any $\epsilon > 0$

$$\Pr(|X_n - X| > \epsilon) \rightarrow 0 \text{ as } n \rightarrow \infty.$$

We write $X_n \xrightarrow{p} X$.

Figure 49: Convergence in probability.

Law of large numbers

Let X_1, X_2, \dots be iid random variables with finite mean μ . Then

$$\bar{X}_n \xrightarrow{p} \mu \text{ as } n \rightarrow \infty,$$

where \xrightarrow{p} denotes convergence in probability.

There is also a strong law of large numbers based on an alternative notion of probabilistic convergence called **almost sure convergence**, as well as laws for variables that are not iid.

Figure 50: Weak law of large numbers.
simulation consistent

$m = 1000$.

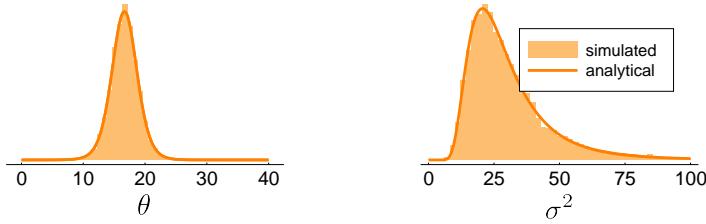


Figure 51: Histogram of simulated marginal posteriors for the internet speed data with analytical marginal posterior densities overlayed.

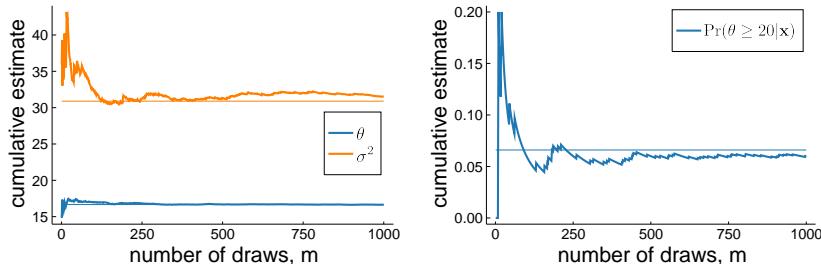


Figure 52: Convergence of the Monte Carlo estimate of the posterior expectation of θ and σ^2 (left) and $\Pr(\theta \geq 20|x)$ (right). The analytical posterior results are displayed as thin horizontal lines.

The **central limit theorem** (Figure 54) can be used to prove that $\bar{\theta}_{1:m}$ **converges in distribution** (Figure 53) to a normal distribution. Hence, the following approximation of the posterior estimate $\bar{\theta}_{1:m}$ is accurate when m is large:

$$\bar{\theta}_{1:m} \sim N \left(\mathbb{E}(\theta|x), \frac{\mathbb{V}(\theta|x)}{m} \right), \quad (30)$$

where $\mathbb{V}(\theta|x)$ is the posterior variance of θ ; note that we get the usual reduction in variance that comes from taking averages of m draws, i.e. the variance of $\bar{\theta}_{1:m}$ decreases with m . The result in (30) can be used to determine the required number of draws m needed for a given estimation precision. A multivariate version of the central limit theorem can be used to prove a similar result to (30) when θ is a vector; an interesting aspect is that $\text{Cov}(\bar{\theta}_{1:m})$ (a covariance matrix in the multiparameter case) still decreases at the rate $1/m$, regardless of the dimension of θ .

It is often the case that the quantities of interest are functions $f(\theta)$ of the parameters; for example the **coefficient of variation** σ/θ in the iid normal model. Even when the posterior for the model parameters θ is available analytically, deriving the posterior for $f(\theta)$ involves tedious multidimensional change-of-variables calculations. Here is a second attractive property of simulation: the posterior for $f(\theta)$ can be

Convergence in distribution

A sequence of random variables X_1, \dots, X_n **converges in distribution** to the random variable X , if and only if

$$F_n(x) \rightarrow F(x) \text{ as } n \rightarrow \infty,$$

for all x where $F(\cdot)$ is continuous, where $F_n(x)$ and $F(x)$ are the cumulative distribution function (CDF) of X_n and X , respectively.

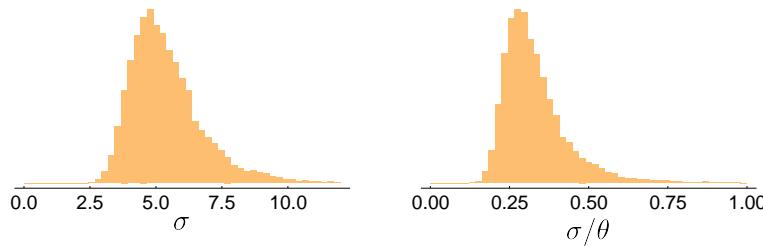
We then write $X_n \xrightarrow{d} X$.

Figure 53: Convergence in distribution.

coefficient of variation

directly obtained from a posterior sample of θ by simply computing the function $f(\theta)$ for each posterior draw. Provided the posterior variance of $f(\theta)$ exists, a central limit theorem of the form (30) exists also in this case, with the expected value and variance replaced by those of $f(\theta)$.

To illustrate how simulation immediately provides inference for any function of the parameters, Table 1 contains a fourth column named σ/θ with the computed coefficient of variation for each draw. We can now just plot a histogram of this new column to approximate the marginal posterior of the function $f(\theta, \sigma^2) = \sigma/\theta$. The results are presented in the right part of Figure 55; the left part of the figure shows the results for the standard deviation $f(\theta, \sigma^2) = \sqrt{\sigma^2}$.



The final column of Table 1 is a binary variable that records if θ was at least 20, i.e. it computes the indicator function $f(\theta, \sigma^2) = I(\theta \geq 20)$. The marginal posterior probability $\Pr(\theta \geq 20 | \mathbf{x})$ is then easily approximated by the mean of the final column; the right side of Figure 52 illustrates the Monte Carlo convergence of this estimate.

Multinomial data

Categorical data have observations that belong to one of C discrete classes. A computer bug can for example be allocated to C developing teams; an items sold in an auction may reported as: 'defective', 'normal quality', or 'new'; a continuous variable like age can recorded in age intervals: 0–18, 19–28, 29–49, 50–64 and 65+, which would then also be a categorical variable. The categories in the latter two situations are examples of **ordinal data** where the categories have a natural order. There are special models for ordinal data which we will not cover in this chapter; here we will consider categorical data without natural order. Categorical variables are often called **multi-class** in the machine learning literature.

A multi-class random variable X is often written in **one-hot encoding** as $\mathbf{x} = (x_1, \dots, x_C)$ where $X = c$ is encoded as $x_c = 1$ and

Central limit theorem (CLT)

Let X_1, X_2, \dots be iid random variables with finite mean μ and variance σ^2 . Then

$$\sqrt{n} (\bar{X}_n - \mu) \xrightarrow{d} N(0, 1),$$

as $n \rightarrow \infty$ where \xrightarrow{d} denotes convergence in distribution.

The CLT is often informally written as

$$\bar{X}_n \xrightarrow{d} N(\mu, \sigma^2) \text{ as } n \rightarrow \infty.$$

Figure 54: The central limit theorem.

Figure 55: Histogram of simulated marginal posteriors for σ (left) and the coefficient of variation σ/θ (right) for the internet speed data.

Categorical data

ordinal data

multi-class

one-hot encoding

$x_j = 0$ for $j \neq c$; hence when $C = 3$, $\mathbf{x} = (0, 1, 0)$ means that the observation belongs to the second class. The categorical random variable $X|\theta \sim \text{Cat}(\theta_1, \dots, \theta_C)$ has probability distribution

$$p(x) = \theta_1^{x_1} \cdots \theta_C^{x_C}, \quad (31)$$

where (x_1, \dots, x_C) is the one-hot encoding of x , $0 < \theta_c < 1$ is the probability of class c and $\sum_{c=1}^C \theta_c = 1$. Note how Bernoulli data is the special case with $C = 2$ categories 'success' and 'failure', so that the $\text{Cat}(\theta_1, \dots, \theta_C)$ distribution generalizes the Bernoulli distribution to the case $C > 2$. Figure 56 is an example of $\text{Cat}(\theta_1, \dots, \theta_C)$ for $C = 4$.

We saw in Section [The likelihood function and maximum likelihood estimation](#) that counting the number of successes s in n binary Bernoulli trials gave rise to $S \sim \text{Binomial}(n, \theta)$ data. In the same way we can count the number of observations in category c for $c = 1, \dots, C$ in multi-class data. This gives data as a count vector $\mathbf{y} = (y_1, \dots, y_C)$ where y_c is the number of observations in category c in $n = \sum_{c=1}^C y_c$ 'trials'. Here is an example:

MOBILE PHONE SURVEY DATA. A survey was conducted among $n = 513$ mobile phone users. Among other questions, the participants were asked: 'What kind of mobile phone do you mainly use?' with the four options: i) iPhone, ii) Android, iii) Windows and iv) Other/- Don't know. The number of responses in the four categories were: $\mathbf{y} = (180, 230, 62, 41)$.

The **multinomial distribution** generalizes the binomial distribution to $C > 2$ categories; its main properties are summarized in Figure 57. The Binomial distribution in Figure 4 is the special case with $C = 2$ categories, which is seen by defining $\theta = \theta_1$, $\theta_2 = 1 - \theta$, $x = x_1$, $x_2 = n - x$, and noting that

$$\frac{n!}{x_1!x_2!} = \frac{n!}{x!(n-x)!} = \binom{n}{x}. \quad (32)$$

The multinomial distribution is a multivariate distribution with convenient marginalization properties. For example, if we group the counts in one or more categories - for example turning the mobile phone dataset into three categories by merging 'Windows' and 'Other' - the distribution remains multinomial. The probability of a merged category is simply the sum of the probabilities of the merged categories. Hence

$$(x_1, x_2, x_3 + x_4) \sim \text{Multinomial}(\theta_1, \theta_2, \theta_3 + \theta_4).$$

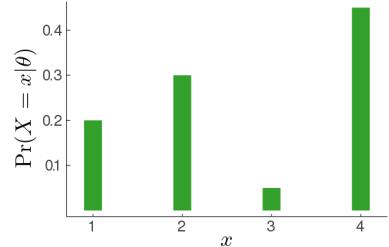


Figure 56: Categorical distribution with probabilities $\theta = (0.20, 0.30, 0.05, 0.45)$.

multinomial distribution

Multinomial distribution

$(X_1, \dots, X_C) \sim \text{MultiNom}(n, \theta)$
where $\sum_{c=1}^C X_c = n$,
 $\theta = (\theta_1, \dots, \theta_C)$ and $\sum_c \theta_c = 1$.

$$p(\mathbf{x}) = \frac{n!}{x_1! \cdots x_C!} \theta_1^{x_1} \cdots \theta_C^{x_C}$$

$$\mathbb{E}(X_c) = n\theta_c$$

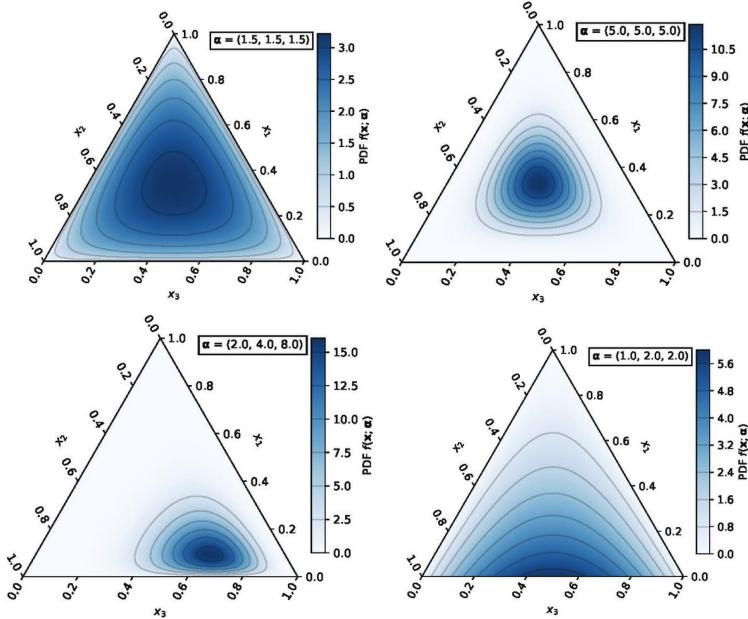
$$\mathbb{V}(X_c) = n\theta_c(1 - \theta_c)$$

Figure 57: The multinomial distribution.

In particular, merging to only two categories - for example 'iPhone' and 'not iPhone' - gives a binomial distribution where the probability of failure (not iPhone) is $\theta_2 + \theta_3 + \theta_4$.

A Bayesian analysis of multinomial data requires a prior distribution for the model parameters, $\theta = (\theta_1, \dots, \theta_C)$. Since each θ_c is a probability, the first distribution that comes to mind may be a Beta distribution; the Beta distribution is not appropriate here however since it does not enforce the constraint that the probabilities sum to one. Hence, the parameter space of the multinomial distribution is the **unit simplex**, i.e. the set $\theta = (\theta_1, \dots, \theta_C) : 0 < \theta_c < 1$ and $\sum_c \theta_c = 1$. Luckily, there is a very nice distribution on the unit simplex, the Dirichlet distribution, summarized in Figure 58.

The Dirichlet distribution is specified with the prior hyperparameters $\alpha_c > 0$, see Figure 59 for some examples. The *relative* sizes of the elements in α determine the prior means for elements of θ . For example, setting $\alpha_1 = \dots = \alpha_C = 1.5$, as in the upper left graph of Figure 59, gives equal prior mean for all categories: $\mathbb{E}(\theta_c) = 1/C$ for all c . The *absolute* size of α , measured by $\alpha_+ = \sum_{c=1}^C \alpha_c$, is inversely related to the variance, see Figure 58; hence, the prior hyperparameters $\alpha = (1.5, \dots, 1.5)$ and $\alpha = (5, \dots, 5)$ in the upper part of Figure 59 have the same mean, but the latter has smaller variance. Finally, the bottom part of Figure 59 shows examples where the prior mean is different over the categories.



The $\text{Dirichlet}(1, \dots, 1)$ has constant density and is therefore the **uniform distribution on the unit simplex**; this generalizes the re-

Dirichlet distribution

$\theta|\alpha \sim \text{Dirichlet}(\alpha)$ where
 $\theta = (\theta_1, \dots, \theta_C)$, $\sum_c \theta_c = 1$,
 $\alpha = (\alpha_1, \dots, \alpha_C)$ and $\alpha_c > 0$.

$$\begin{aligned} p(\theta) &= k \cdot \theta_1^{\alpha_1-1} \cdots \theta_C^{\alpha_C-1} \\ k &= \frac{\Gamma(\sum_{c=1}^C \alpha_c)}{\prod_{c=1}^C \Gamma(\alpha_c - 1)}. \\ \mathbb{E}(\theta_c) &= \frac{\alpha_c}{\sum_{j=1}^C \alpha_j} \\ \mathbb{V}(\theta_c) &= \frac{\tilde{\alpha}_c(1-\tilde{\alpha}_c)}{1+\alpha_+} \\ \alpha_+ &= \sum_{c=1}^C \alpha_c. \end{aligned}$$

Marginal distributions:

$$\theta_c \sim \text{Beta}(\alpha_c, \alpha_+ - \alpha_c).$$

Figure 58: The Dirichlet distribution.

unit simplex

Figure 59: Examples of Dirichlet distributions for $x = (x_1, x_2, x_3)$.
Source: Wikipedia.

uniform distribution on the unit simplex

sult that Beta(1,1) is uniform on the unit interval [0,1]. Finally, when $\alpha_c < 1$, the Dirichlet density becomes 'bathtub shaped' with probability mass piling up against the edges of the unit simplex.

The Dirichlet distribution is conjugate to the multinomial likelihood which is easily seen by computing the posterior

$$p(\boldsymbol{\theta}|\mathbf{y}) \propto p(\mathbf{y}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \quad (33)$$

$$= \frac{n!}{x_1! \cdots x_C!} \theta_1^{x_1} \cdots \theta_C^{x_C} \cdot \frac{\Gamma(\sum_{c=1}^C \alpha_c)}{\prod_{c=1}^C \Gamma(\alpha_c - 1)} \theta_1^{\alpha_1-1} \cdots \theta_C^{\alpha_C-1} \quad (34)$$

$$= \theta_1^{\alpha_1+x_1-1} \cdots \theta_C^{\alpha_C+x_C-1}, \quad (35)$$

which is proportional to the Dirichlet($\alpha_1 + x_1, \dots, \alpha_C + x_C$) density. This is a convenient result: the posterior is simply obtained by adding the data count x_c to the prior hyperparameter α_c in each category. This parallels and generalizes the binary case where a Beta(α, β) prior was updated to a posterior by adding the number of successes s to α and the number of failures f to β . Figure 6o summarizes the prior-to-posterior updating for multinomial data with a Dirichlet prior.

Multinomial data with Dirichlet prior

Model: $\mathbf{n}|\boldsymbol{\theta} \sim \text{Multinomial}(\boldsymbol{\theta})$, where

$\mathbf{n} = (n_1, \dots, n_C)$ are counts in C categories

$\boldsymbol{\theta} = (\theta_1, \dots, \theta_C)$ are category probabilities.

Prior: $\boldsymbol{\theta} \sim \text{Dirichlet}(\boldsymbol{\alpha})$, for $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_C)$

Posterior: $\boldsymbol{\theta} \sim \text{Dirichlet}(\boldsymbol{\alpha} + \mathbf{n})$

Figure 6o: Prior-to-Posterior updating for multinomial data with the Dirichlet prior.

MOBILE PHONE SURVEY DATA We are now ready to analyze the four market shares $\theta_1, \dots, \theta_4$ in the mobile phone data. We will determine the prior hyperparameters in the Dirichlet prior using data from a similar survey from four years ago. The proportions in the four categories back then were: 30%, 30%, 20% and 20%. This was a large survey, but since time has passed and user patterns most likely have changed, I value the information in this older survey as being equivalent to a survey with only 50 participants. This gives us the prior:

$$(\theta_1, \dots, \theta_4) \sim \text{Dirichlet}(\alpha_1 = 15, \alpha_2 = 15, \alpha_3 = 10, \alpha_4 = 10)$$

Note that $E(\theta_1) = 15/50 = 0.3$ and so on, so the prior mean is set equal to the proportions from the older survey. Also, $\sum_{k=1}^4 \alpha_k = 50$, so the prior information is equivalent to a survey based on 50 respondents, as required.

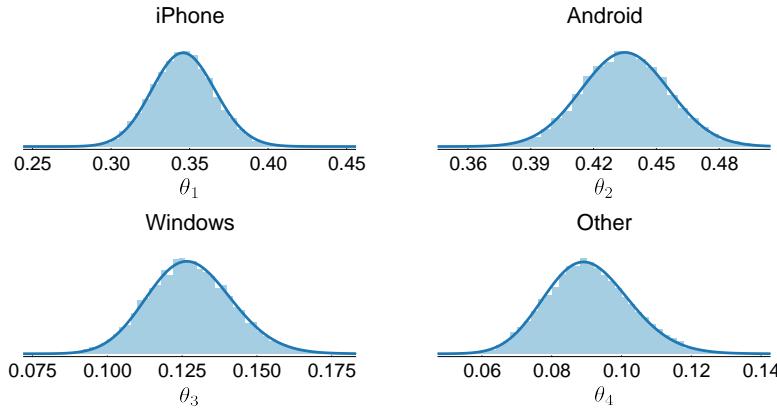


Figure 61: Marginal posteriors of the market shares for the mobile phone survey data. Simulated (histogram) draws and analytical density functions (solid curves).

The joint posterior distribution of all four shares is by Figure 60 equal to

$$(\theta_1, \dots, \theta_4) | \mathbf{y} \sim \text{Dirichlet}(15 + 180, 15 + 230, 10 + 62, 10 + 41)$$

The marginal posteriors are plotted in Figure 61 as histograms from Monte Carlo simulation (see the algorithm in Figure 62); the analytical posteriors from Figure 58 are overlayed.

draw	θ_1	θ_2	θ_3	θ_4	θ_2 largest
1	0.338	0.446	0.130	0.086	1
2	0.332	0.457	0.124	0.086	1
3	0.325	0.442	0.136	0.094	1
:	:	:	:	:	:
10,000	0.343	0.443	0.132	0.081	1
Mean	0.346	0.435	0.127	0.090	0.991

Table 2: Posterior simulation output for the multinomial model applied to the mobile phone survey data. The last column is a computed binary indicator for the event that Android has the largest market share, i.e. if $\theta_2 > \max(\theta_1, \theta_3, \theta_4)$.

Figure 61 indicates that Android may have the largest market share with a posterior mean around 0.44 versus iPhones posterior mean of 0.35. Computing the probability that Android has the largest market share involves integrating the joint posterior $\theta | \mathbf{y} \sim \text{Dirichlet}(\boldsymbol{\alpha} + \mathbf{y})$ over the region $\{\theta : \theta_2 > \max(\theta_1, \theta_3, \theta_4)\}$, a tedious calculation. The probability is however easily computed by simulation by recording for each posterior θ draw if the condition $\theta_2 > \max(\theta_1, \theta_3, \theta_4)$ is satisfied; see Table 2, which shows that

$$\Pr(\text{Android has largest market share} | \mathbf{y}) \approx 0.991.$$

We are almost certain that Android is the most popular mobile phone in the population targeted by the survey.

Posterior simulation - Multinomial data, Dirichlet prior.

Input: data $\mathbf{n} = (n_1, \dots, n_C)$
prior hyperparameters $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_C)$
the number of posterior draws m .

for i in $1:m$ **do**
| $\boldsymbol{\theta} \leftarrow \text{RDIRICHLET}(\boldsymbol{\alpha} + \mathbf{n})$
end

Output: m posterior draws of $\boldsymbol{\theta} = (\theta_1, \dots, \theta_C)$.

Function $\text{RDIRICHLET}(\boldsymbol{\alpha})$
for c in $1:C$ **do**
| $\mathbf{y}[c] \leftarrow \text{RGAMMA}(\boldsymbol{\alpha}[c], 1)$
end
return $\mathbf{y}/\text{SUM}(\mathbf{y})$

Figure 62: Algorithm for posterior simulation for the multinomial model with the conjugate Dirichlet prior. The `RGAMMA` random number generator is assumed to be part of the standard library.

Multivariate normal data with known covariance

This section considers the iid multivariate normal model for a p -dimensional data vector \mathbf{x} :

$$\mathbf{x}_1, \dots, \mathbf{x}_n | \boldsymbol{\theta}, \boldsymbol{\Sigma} \stackrel{\text{iid}}{\sim} N(\boldsymbol{\theta}, \boldsymbol{\Sigma}), \quad (36)$$

where $\boldsymbol{\theta}$ is the p -dimensional mean vector and $\boldsymbol{\Sigma}$ is a $p \times p$ positive definite covariance matrix. We will here take $\boldsymbol{\Sigma}$ to be known and derive the posterior for $\boldsymbol{\theta}$.

Presenting a Bayesian analysis of this model here gives us a chance to meet the important multivariate normal distribution and its properties relatively early in the book; see Figure 63 for the density and properties, and Figure 64 for contour plots of some example densities.

The likelihood for the multivariate model in (36) is the product of the individual densities for each vector observation \mathbf{x}_i

$$p(\mathbf{x}_1, \dots, \mathbf{x}_n | \boldsymbol{\theta}, \boldsymbol{\Sigma}) \propto |\boldsymbol{\Sigma}|^{-n/2} \exp \left(-\frac{1}{2} \sum_{i=1}^n (\mathbf{x}_i - \boldsymbol{\theta})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \boldsymbol{\theta}) \right),$$

A vector version of the argument leading up to (15) in the univariate case can be used to show that the likelihood can be written as the exponential of a quadratic (form):

$$p(\mathbf{x}_1, \dots, \mathbf{x}_n | \boldsymbol{\theta}, \boldsymbol{\Sigma}) \propto \exp \left(-\frac{n}{2} (\boldsymbol{\theta} - \bar{\mathbf{x}})^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{\theta} - \bar{\mathbf{x}}) \right), \quad (37)$$

where $\bar{\mathbf{x}} = n^{-1} \sum_{i=1}^n \mathbf{x}_i$ is the usual sample mean vector.

Multivariate normal

$\mathbf{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ where $\mathbf{x} \in \mathbb{R}^p$, $\boldsymbol{\mu} \in \mathbb{R}^p$ and $\boldsymbol{\Sigma}$ is a $p \times p$ positive definite covariance matrix.

$$\begin{aligned} p(\mathbf{x}) &= |2\pi\boldsymbol{\Sigma}|^{-\frac{1}{2}} \\ &\times \exp \left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right) \end{aligned}$$

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

$$\mathbb{V}(\mathbf{x}) = \boldsymbol{\Sigma}$$

Define the decomposition

$$\mathbf{x} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}$$

and similarly for $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$

$$\boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix} \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} \end{pmatrix}$$

Marginal distributions:

$$\mathbf{x}_k \sim N(\boldsymbol{\mu}_k, \sigma_k^2)$$

$$\mathbf{x}_1 \sim N(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_{11})$$

Conditional distributions:

$$\mathbf{x}_1 | \mathbf{x}_2 \sim N(\tilde{\boldsymbol{\mu}}_1, \tilde{\boldsymbol{\Sigma}}_1)$$

where

$$\tilde{\boldsymbol{\mu}}_1 = \boldsymbol{\mu}_1 + \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}(\mathbf{x}_2 - \boldsymbol{\mu}_2)$$

$$\tilde{\boldsymbol{\Sigma}}_1 = \boldsymbol{\Sigma}_{11} - \boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{22}^{-1}\boldsymbol{\Sigma}_{21}$$

Figure 63: The multivariate normal distribution.

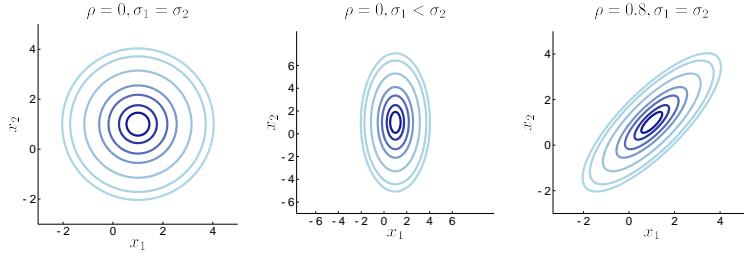


Figure 64: Contour plots of some bivariate normal distributions with correlation ρ .

Not too surprisingly, the multivariate normal prior

$$\boldsymbol{\theta} \sim N(\boldsymbol{\theta}_0, \boldsymbol{\Lambda}_0),$$

turns out to be conjugate for this model. The posterior can be derived by multiplying together the likelihood in (37) with the prior and completing the quadratic forms in the exponentials; see Figure 65 for a general result on quadratic form completion. The posterior can then be shown to indeed be a multivariate normal:

$$\boldsymbol{\theta} | \mathbf{x}_1, \dots, \mathbf{x}_n \sim N(\boldsymbol{\theta}_n, \boldsymbol{\Lambda}_n),$$

where

$$\begin{aligned}\boldsymbol{\theta}_n &= (\boldsymbol{\Lambda}_0^{-1} + n\boldsymbol{\Sigma}^{-1})^{-1}(\boldsymbol{\Lambda}_0^{-1}\boldsymbol{\theta}_0 + n\boldsymbol{\Sigma}^{-1}\bar{\mathbf{x}}) \\ \boldsymbol{\Lambda}_n^{-1} &= \boldsymbol{\Lambda}_0^{-1} + n\boldsymbol{\Sigma}^{-1}.\end{aligned}$$

Letting $\boldsymbol{\Lambda}_0^{-1} \rightarrow \mathbf{0}$ (in a matrix sense) we obtain a noninformative (uniform) prior and the posterior

$$\boldsymbol{\theta} | \mathbf{x}_1, \dots, \mathbf{x}_n \sim N(\bar{\mathbf{x}}, n^{-1}\boldsymbol{\Sigma}).$$

Likelihood and Information

A Taylor expansion of the log likelihood around the MLE $\hat{\boldsymbol{\theta}}$ gives

$$\begin{aligned}\ln p(\mathbf{x}|\boldsymbol{\theta}) &= \ln p(\mathbf{x}|\hat{\boldsymbol{\theta}}) + \frac{\partial \ln p(\mathbf{x}|\boldsymbol{\theta})}{\partial \boldsymbol{\theta}}|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) \\ &\quad + \frac{1}{2!} \frac{\partial^2 \ln p(\mathbf{x}|\boldsymbol{\theta})}{\partial \boldsymbol{\theta}^2}|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^2 + \dots\end{aligned}$$

The high order terms indicated by \dots can be shown to be small in large samples. From the definition of the MLE we know that

$$\frac{\partial \ln p(\boldsymbol{\theta}|\mathbf{x})}{\partial \boldsymbol{\theta}}|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} = 0$$

We therefore have the following approximation of the likelihood in large samples

$$p(\mathbf{x}|\boldsymbol{\theta}) \approx p(\mathbf{x}|\hat{\boldsymbol{\theta}}) \exp\left(-\frac{1}{2}J_{\mathbf{x}}(\hat{\boldsymbol{\theta}})(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^2\right)$$

Completing quadratic forms

This formula shows how to combine two quadratic forms in a vector of interest \mathbf{x} , to a single quadratic form in \mathbf{x} plus constant terms:

$$\begin{aligned}(\mathbf{x} - \mathbf{a})^\top \mathbf{A}(\mathbf{x} - \mathbf{a}) + (\mathbf{x} - \mathbf{b})^\top \mathbf{B}(\mathbf{x} - \mathbf{b}) \\ = (\mathbf{x} - \mathbf{d})^\top \mathbf{D}(\mathbf{x} - \mathbf{d}) \\ + (\mathbf{d} - \mathbf{a})^\top \mathbf{A}(\mathbf{d} - \mathbf{a}) \\ + (\mathbf{d} - \mathbf{b})^\top \mathbf{B}(\mathbf{d} - \mathbf{b}),\end{aligned}$$

where

$$\mathbf{D} = \mathbf{A} + \mathbf{B} \text{ and } \mathbf{d} = \mathbf{D}^{-1}(\mathbf{A}\mathbf{a} + \mathbf{B}\mathbf{b}).$$

Figure 65: Completing quadratic forms.

where

$$J_x(\tilde{\theta}) = -\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta^2} \Big|_{\theta=\hat{\theta}}.$$

Hence, the likelihood function will be proportional to the $N[\hat{\theta}, J_x^{-1}(\hat{\theta})]$ density in large samples. The quantity $J_x(\tilde{\theta})$ is clearly the precision in the likelihood and is a natural measure of the information in the data \mathbf{x} about the parameter θ :

Definition (Observed information - one-parameter case). *The observed information in a sample $\mathbf{x} = (x_1, \dots, x_n)$ is defined as*

$$J_{\theta,\mathbf{x}} = -\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta^2} \Big|_{\theta=\hat{\theta}_{MLE}} \quad (38)$$

Recall for calculus that the second derivative measures how fast the first derivative changes, i.e. $J_{\theta,\mathbf{x}}$ measures how peaked the log-likelihood is around the maximum. The negative sign in the definition makes sure the information is always positive, since we know from calculus that the second derivative is negative at the maximum.

The observed information $J_{\theta,\mathbf{x}}$ varies from sample to sample. The average, or expected, information is called the Fisher information:

Definition (Observed information). *The Fisher information is the expected information over all possible samples from the model*

observed information

$$I(\theta) = \mathbb{E}_{\mathbf{x}|\theta} (J_{\theta,\mathbf{x}}). \quad (39)$$

The observed and Fisher information can be extended to the multiparameter case as follows.

Definition (Observed information - multiparameter case). *The observed information matrix in a sample $\mathbf{x} = (x_1, \dots, x_n)$ from the model $p(\mathbf{x}|\theta)$ with a p -dimensional parameter vector θ is defined as*

Fisher information

$$J_{\theta,\mathbf{x}} = -\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta \partial \theta^\top} \Big|_{\theta=\hat{\theta}_{MLE}}, \quad (40)$$

where $\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta \partial \theta^\top}$ is the $p \times p$ matrix of second derivatives.

observed information matrix

Definition (Fisher information - multiparameter case). *The Fisher information matrix is the expected information matrix over all possible samples from the model*

Fisher information matrix

$$I(\theta) = \mathbb{E}_{\mathbf{x}|\theta} (J_{\theta,\mathbf{x}}). \quad (41)$$

The matrix $\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta \partial \theta^\top}$ in (40) may be a little intimidating. Writing out its elements explicitly in the case of two parameters, $\theta = (\theta_1, \theta_2)$,

$$\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta \partial \theta^\top} = \begin{pmatrix} \frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta_1^2} & \frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta_1 \partial \theta_2} \\ \frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta_1 \partial \theta_2} & \frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta_2^2} \end{pmatrix},$$

we see that calculating $\frac{\partial^2 \ln p(\mathbf{x}|\theta)}{\partial \theta \partial \theta^\top}$ is no harder than calculating a single second derivative, there are just more of them. Luckily, we will learn in the Chapter [Classification](#) that we can often let the computer do this job for us.

EXERCISES

1. Derive the marginal posterior of θ in (29) for the iid Gaussian model $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$.
2. Let $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$, where θ is assumed known. Show that the Inv- χ^2 distribution is a conjugate prior for σ^2 .

NOTEBOOKS

1. Analyzing mobile phone survey data with a multinomial model.

Priors

The secret sauce of Bayesian learning is the prior. Only with a prior can we turn a likelihood function into a probability distribution for the unknown parameters, and subsequently use this posterior distribution for decision making. Priors make it possible to fuse information from a variety of different sources. This chapter discusses some of these different types of prior information, and we will return to this issue in later chapters when we perform more serious modelling.

Eliciting a prior takes effort and there may be situations where one may want to use as little prior information as possible, or at least use a prior where the information added is transparent to everyone involved. One example is the reporting of scientific results to an unknown audience with potentially rather different prior opinions. The ideal would be to present the posterior distribution for a variety of different priors to contrast the different views and to examine the possibility of a subjective consensus. This is challenging however, particularly when the model contains many parameters and data is weak; Sections [Noninformative priors](#) and [Invariant priors](#) presents several ‘non-informative’ priors that may be appealing in such circumstances.

Time series

A time series model will be used to illustrate some ways in which priors can be specified. Time series data have **dependent observations**, and models for such data are therefore necessarily more complex; it is however worthwhile to spend a little time on it in this chapter as the particular model presented here will be used many times in this book.

A **time series** is a realization of a **stochastic process** observed over discrete number of time periods, here denoted by $t = 1, 2, \dots, T$. Time series are one of the most commonly occurring data types and are destined to play a large role in the future as time-stamped data are now collected by many electronic devices and at a rapid pace. Figure 66 shows a time series of Swedish inflation, Figure 67 display the

dependent observations

time series

stochastic process

daily number of rides with a bike sharing company, and Figure 68 illustrates a time series of electroencephalography (EEG) recordings of electrical activity at one brain location. Many timeseries consist of multivariate measurements at every time period, for example EEG recordings taken simultaneously at multiple locations, see Figure 69, or meteorological data collected at different spatial locations.

The **autoregressive model** of order p is a time series model of the form

$$y_t = \mu + \phi_1(y_{t-1} - \mu) + \dots + \phi_p(y_{t-p} - \mu) + \varepsilon_t, \quad \varepsilon_t \stackrel{iid}{\sim} N(0, \sigma^2), \quad (42)$$

where y_{t-k} is the k th **lagged value** of time series and ε_t are the disturbances, or innovations, that drives the process. Hence, an AR(p) process models today's value y_t as a linear function of the measurements at the p most recent days y_{t-1}, \dots, y_{t-p} plus a random disturbance ε_t . The time series may equally well be observed on another frequency than daily, for example monthly, with lags being past months. The effect of the k th lags is captured by the AR coefficients ϕ_k .

The AR(p) process in (42) is in **steady-state form** where the parameter μ is the unconditional mean $\mathbb{E}(y_t)$ of the process. We assume that the AR(p) process is **stationary**, meaning that the mean μ and variance $\mathbb{V}(y_t)$ remain unchanged over time, and also that the covariance between any two time points $\text{Cov}(y_t, y_s)$ is only a function of the time distance $|t - s|$. The assumption of a constant mean may seem restrictive, but often means stationary around a deterministic time trend. The unconditional mean μ is important since long horizon forecasts are guaranteed to end up at μ when the process is stationary, i.e.

$$\mathbb{E}(y_{T+h}|y_{1:T}) \rightarrow \mu \text{ as } h \rightarrow \infty,$$

where $y_{1:T}$ are all historical data available at the time of the forecast $t = T$. The convergence usually happens rather fast in applications; see Figure 70 where an AR(1) model estimated by maximum likelihood is used to predict Swedish inflation for the coming 60 months.

In later chapters we will learn how to obtain the joint posterior of all parameter $p(\mu, \phi_1, \dots, \phi_p, \sigma^2 | \mathbf{y})$ by approximation or simulation. In this chapter will only worry about how to elicit a prior distribution for all model parameters, i.e. the joint prior $p(\mu, \phi_1, \dots, \phi_p, \sigma^2)$. We make the simplifying assumption that all parameters are independent a priori; this is most likely not our true beliefs since properties like stationarity involves all ϕ parameters, but it is nevertheless what is most often used in applications. We will walk through a number of methods for prior elicitation and use different methods for different parameters.

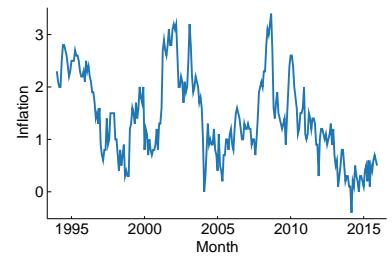


Figure 66: Swedish inflation 1995–2016 – annualized monthly observations.

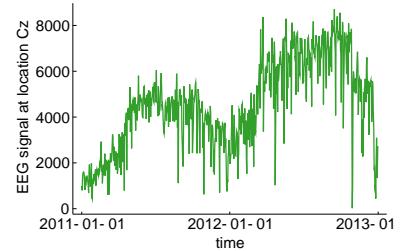


Figure 67: Daily number of rides with a bike sharing company.

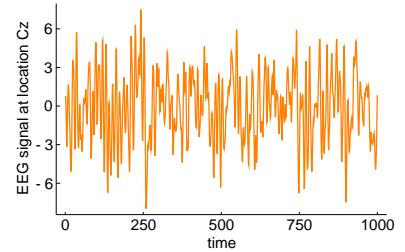


Figure 68: EEG recordings of electrical activity at one brain scalp location.

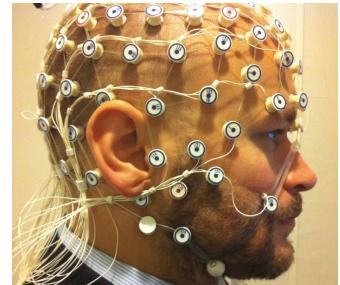


Figure 69: Positioning of EEG electrodes on a subject's brain scalp.

autoregressive model

lagged value

steady-state form

stationary

Past or other data

Bayes' theorem dictates that we are not allowed to use the same data in the likelihood and in the prior, i.e. no double dipping of the data if you want the posterior to correctly quantify uncertainty. It is however allowed to use **past data** for specifying the prior as long as that data are not used in the likelihood; for example, fitting the time series model to data on Swedish inflation data before 1985 and use those estimates as the prior mean. Since older data can be from a different economic regime, one would probably use a fairly large prior variance; this is similar to how we used an older survey for the Dirichlet prior in the mobile phone survey data.

We may base our prior on estimates of the model's parameters from **other data**, e.g. inflation data from other countries during the same time period 1985 – 2016. Other countries are certainly different from Sweden, but still relevant, especially data from similar countries.

Expert opinion

The ML estimate of the mean of the time series is $\hat{\mu}_{MLE} = 1.409$, which constrains the mean forecasts at longer horizon to end up at 1.409; see Figure 70. This is lower than the Central Bank of Sweden's inflation target at 2%. We can use this form of expert opinion as a $\mu \sim N(2, \tau_0^2)$ prior with a small prior variance τ_0^2 , if we trust the central bank experts. Prior information on the steady-state has been shown to improve forecasting performance for a number of economic variables; see [Villani \[2009\]](#).

Prior elicitation of the experts were made on a quantity that was well understood by central bank economists, the long run behavior of inflation. The challenge is to elicit prior beliefs from experts on quantities that the expert understands well. This will often involve observable quantities, like inflation, rather than abstract parameters in statistical models. The process is often iterative where model consequences from the initially given expert opinion are presented to the expert, who then adjusts the initial opinion. Eliciting expert opinions is a large area in itself, with help from cognitive science to account for the biases and shortcomings that are part of being a human.

Structured regularization priors

An important type of prior beliefs are priors that regularize, or shrink, parameter-rich models. **Regularization priors** are particularly popular in machine learning for probabilistically restricting

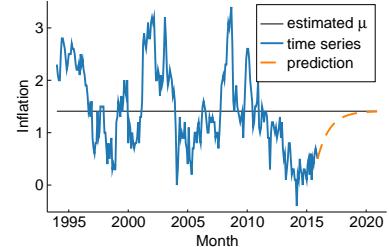


Figure 70: Swedish inflation 1995–2016 with 60 months ahead mean prediction in dashed orange.

past data

other data

Regularization priors

complex models that would otherwise easily overfit the data. There will be many examples of regularization priors later in the book, but we can get an first understanding of the concept from a commonly used prior for the autoregressive parameters ϕ_1, \dots, ϕ_p in the AR process. A regularization prior ϕ_1, \dots, ϕ_p makes it possible to use a large **lag length** p even on shorter time series. The prior embodies the idea that the magnitude of the ϕ_k are likely to be smaller for larger k , as in the following prior:

$$\phi_k \sim N\left(\mu_k, \frac{\tau^2}{k^2}\right), \quad (43)$$

where $\mu_k = 0$ for all k except for the first lag where $\mu_1 = 0.8$, for example. This centers the prior on the AR(1) process with coefficient $\phi_1 = 0.8$, which is a reasonable prior guess for Swedish inflation.

The hyperparameter τ is the prior standard deviation of ϕ_1 . The hyperparameter τ is called the **global shrinkage** since it has the effect of shrinking all ϕ_k toward their prior mean; this is the same effect as the prior standard deviation τ_0 had in the iid normal model in Chapter [Single-parameter models](#) where the posterior mean μ_n was shrunk toward the prior mean μ_0 via the weight w . Finally, the regularization part of the prior is that the factor $1/k^2$ reduces the prior variance of ϕ_k for longer lags; longer lags are more likely to be redundant a priori, and their ϕ_k will only be sizeable in the posterior if the data strongly suggest so.

Priors can more generally be used to incorporate **smoothness beliefs**. For example, we will later analyze nonlinear regression models where a response variable y is functionally related to an explanatory variable x via some function $f(x)$. Rather than assuming a restrictive functional form, most commonly linear, we often want $f(\cdot)$ to be flexible enough to adapt to almost any shape. However, our prior beliefs may still be that $f(\cdot)$ is smooth; Figure 71 shows examples of priors for function with wiggly and smooth beliefs. The parameter space here is the abstract space of functions, as will be explained in Chapter [Gaussian processes](#). We will in later chapters see many examples of quite elegant use of priors to impose smoothness without loosing desired flexibility. A well designed smoothness prior tames the flexibility in the right way and thereby helps to avoid overfitting the data. Note however that a regularization prior still represents subjective beliefs; my prior beliefs regarding the function $f(\cdot)$ puts higher prior probability on the smooth functions in the bottom part of Figure 71 than on the wiggly functions shown in the top part of the figure. This then *implies* a posterior that favors smoother functions, unless the data strongly suggest otherwise.

lag length

global shrinkage

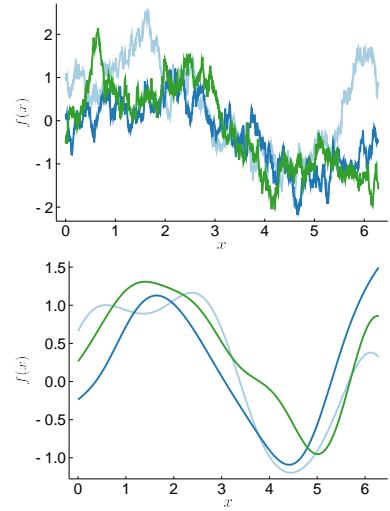


Figure 71: Three simulated draws from a prior over functions without smoothness beliefs (top) and with smooth beliefs (bottom).

smoothness beliefs

Hierarchical priors

The structure of the presented regularization prior for the AR(p) process is attractive, but it may be hard to specify an exact value for the global shrinkage τ . The solution is simple: if something is unknown to you, put a prior on it. This gives rise to the following **hierarchical prior** on the AR coefficients

hierarchical prior

$$p(\phi_1, \dots, \phi_p, \tau^2) = p(\phi_1|\tau^2) \cdots p(\phi_p|\tau^2)p(\tau^2),$$

where each $p(\phi_k|\tau^2)$ is the previous $N\left(\mu_k, \frac{\tau^2}{k^2}\right)$, with independence now only conditionally on τ^2 , and $p(\tau^2)$ is the marginal prior for the unknown prior hyperparameter τ^2 . The joint posterior $p(\mu, \phi_1, \dots, \phi_p, \sigma^2, \tau^2 | \mathbf{y})$ involves the now unknown τ^2 , so data will also inform us about τ^2 . Since τ^2 is a variance parameter, the prior $\tau^2 \sim \text{Inv-}\chi^2(\nu_0, \tau_0^2)$ is a natural choice. We still need to specify τ_0^2 our ‘best guess’ for τ^2 and the uncertainty via ν_0 , but the posterior is often considerably less sensitive to these prior hyperparameters further down the hierarchy, as will be demonstrated in a similar context in the chapter [Regularization](#).

Noninformative priors

It is often convenient to use a prior with relatively little information, at least for some model parameters. Eliciting priors takes effort and we sometimes prefer to specify priors for some parameters with a little less care than other key parameters. The data may also be known to be highly informative on some model parameters and the prior will therefore anyway be overruled by the likelihood. In short, it can be convenient to give some parameters a noninformative prior. A noninformative prior is a bit of a misnomer since any prior carries some information; see [Irony and Singpurwalla \[1997\]](#) for transcribed car dialogue among Bayesian statisticians about this topic. Consider for example the iid $\text{Bernoulli}(\theta)$ where $\theta \in [0, 1]$. The $\text{Uniform}(0, 1)$ distribution is a candidate for a noninformative prior since it assigns the same density to every possible value of θ . There are at least two arguments against this seemingly natural idea.

First, recall that the posterior from a $\theta \sim \text{Beta}(\alpha, \beta)$ prior is $\theta | \mathbf{x} \sim \text{Beta}(\alpha + s, \beta + f)$. This means that the prior carries the information equivalent to a prior sample of α successes and β failures. Since the $\text{Uniform}(0, 1)$ distribution is the $\text{Beta}(1, 1)$ distribution, the uniform prior is equivalent to a prior sample of $n = 2$ trials with one success and one failure; this is clearly *some* information. An alternative definition of a noninformative prior is the **zero sample prior** $\text{Beta}(\epsilon, \epsilon)$ where $\epsilon \downarrow 0$, i.e. ϵ is a tiny number; the posterior is then

zero sample prior

$\text{Beta}(s, f)$. The idea of the zero sample prior carries directly over the conjugate analysis for exponential family models presented in Figure 38 by letting v_0 and τ_0 go to zero.

A second argument against a uniform density as noninformative is that uniformity is typically not preserved when θ is transformed to an alternative parametrization $\phi = g(\theta)$, where $g(\cdot)$ is a one-to-one transformation; for example $g(\theta) = \log(\theta/(1-\theta))$, the log-odds transformation of the Bernoulli success probability θ . To see this we use the results on transformations of random variable in Figure 72 to obtain

$$p_\phi(\phi) = p_\theta(g^{-1}(\phi)) \left| \frac{\partial g^{-1}(\phi)}{\partial \phi} \right| = 1 \cdot \frac{e^\phi}{(1+e^\phi)^2},$$

since $p_\theta(\theta)$ is uniform and the inverse transformation is $g^{-1}(\phi) = e^\phi/(1+e^\phi)$. Hence, a uniform distribution for θ does not imply a uniform distribution on the log-odds. In the next section we will encounter rules for constructing priors that are guaranteed to be invariant to one-to-one transformations of the model parameter.

Invariant priors

As we saw in the previous section, a prior which is uniform in one parametrization is usually not uniform in another parametrization; the uniform distribution is not an **invariant prior** for θ in the Bernoulli model. Jeffreys' rule is a method for constructing priors that are guaranteed to be invariant to any one-to-one transformation of the parameter.

Definition (Jeffreys' rule). *Jeffreys' prior for a parameter vector θ in a model $p(\mathbf{x}|\theta)$ is of the form*

$$p(\theta) = |I(\theta)|^{1/2}. \quad (44)$$

where $I(\theta)$ is the Fisher information matrix and $|\cdot|$ denotes the matrix determinant.

We will for simplicity concentrate on the one-parameter version $p(\theta) = I(\theta)^{1/2}$ in this section. It can be proved that Jeffreys' prior is invariant to reparametrization [Migon et al., 2014], which was physicist Harold Jeffreys' original motivation for the rule [Jeffreys, 1998]. Invariance means that the following two ways to obtain a prior for θ give identical results:

- (A) apply Jeffreys' rule directly in the θ -parametrization to obtain

$$p_\theta(\theta) = I(\theta)^{1/2}.$$

Transforming variables

Let $X \sim p_X(x)$ and $Y = g(X)$, where $g(\cdot)$ is a one-to-one continuously differentiable transformation with inverse $X = g^{-1}(Y)$. The density of Y is then

$$p_Y(y) = p_X(g^{-1}(y)) \left| \frac{\partial}{\partial y} g^{-1}(y) \right|$$

Figure 72: Transformation of random variables.

invariant prior

Jeffreys' prior

(B) apply Jeffreys' rule in the ϕ -parametrization to first obtain

$$p_\phi(\phi) = I(\phi)^{1/2},$$

and then transform to $p_\theta(\theta)$ by the variable transformation formula in Fig 72

$$p_\theta(\theta) = p_\phi(\phi(\theta)) \left| \frac{d\phi(\theta)}{d\theta} \right| = I(\phi(\theta))^{1/2} \left| \frac{d\phi(\theta)}{d\theta} \right|.$$

EXAMPLE: JEFFREYS' PRIOR FOR BERNOULLI TRIALS. Consider once again the iid Bernoulli model

$$x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} \text{Bernoulli}(\theta),$$

with likelihood $\ln p(\mathbf{x}|\theta) = s \ln \theta + f \ln(1 - \theta)$. The first and second derivative of the log-likelihood are

$$\begin{aligned} \frac{d \log p(\mathbf{x}|\theta)}{d\theta} &= \frac{s}{\theta} - \frac{f}{(1-\theta)} \\ \frac{d^2 \log p(\mathbf{x}|\theta)}{d\theta^2} &= -\frac{s}{\theta^2} - \frac{f}{(1-\theta)^2} \end{aligned}$$

so that the Fisher information is (using lowercase letter for the random variable s and f)

$$I(\theta) = \frac{E_{\mathbf{x}|\theta}(s)}{\theta^2} + \frac{E_{\mathbf{x}|\theta}(f)}{(1-\theta)^2} = \frac{n\theta}{\theta^2} + \frac{n(1-\theta)}{(1-\theta)^2} = \frac{n}{\theta(1-\theta)}$$

Thus, the Jeffreys' prior is

$$p(\theta) = I(\theta)^{1/2} \propto \theta^{-1/2} (1-\theta)^{-1/2} \propto \text{Beta}(1/2, 1/2). \quad (45)$$

Hence Jeffreys' prior lies between the zero imaginary sample prior $\text{Beta}(\epsilon, \epsilon)$ and the uniform $\text{Beta}(1, 1)$. This derivation corresponds to Route A above. Exercise 1 shows that the same $\theta \sim \text{Beta}(1/2, 1/2)$ prior is obtained by taking Route B.

EXAMPLE: JEFFREYS' PRIOR FOR A GAUSSIAN VARIANCE. Consider the model $x_1, \dots, x_n | \theta \stackrel{\text{iid}}{\sim} N(\theta, \sigma^2)$. Let us also assume that θ is known and we use Jeffreys' rule to obtain the invariant prior for σ^2 . The log-likelihood is

$$\log p(\mathbf{x}|\sigma^2) = -\frac{1}{2} \log(2\pi) - \frac{1}{2} \log(\sigma^2) - \frac{\sum_{i=1}^n (x_i - \theta)^2}{2\sigma^2}$$

with first and second derivative

$$\begin{aligned} \frac{\partial}{\partial \sigma^2} \log p(\mathbf{x}|\sigma^2) &= -\frac{1}{2\sigma^2} + \frac{\sum_{i=1}^n (x_i - \theta)^2}{2(\sigma^2)^2} \\ \frac{\partial^2}{\partial (\sigma^2)^2} \log p(\mathbf{x}|\sigma^2) &= \frac{1}{2(\sigma^2)^2} - \frac{\sum_{i=1}^n (x_i - \theta)^2}{(\sigma^2)^3}. \end{aligned}$$

Since $\mathbb{E}_x \sum_{i=1}^n (x_i - \theta)^2 = \sum_{i=1}^n \mathbb{E}_{x_i} (x_i - \theta)^2 = n\sigma^2$ we have

$$I(\sigma^2) = -\frac{1}{2(\sigma^2)^2} + \frac{n\sigma^2}{(\sigma^2)^3} = -\frac{1}{2(\sigma^2)^2} + \frac{n}{(\sigma^2)^2} = \frac{n-1/2}{(\sigma^2)^2},$$

so Jeffreys' prior for the variance is

$$p(\sigma^2) = I(\sigma^2)^{1/2} \propto \frac{1}{\sigma^2},$$

which also implies that Jeffreys' prior for standard deviation is $p(\sigma) \propto \frac{1}{\sigma}$ by the variable transformation formula in Figure 72 and the invariance of the Jeffreys' prior. Since

$$\int_0^\infty \frac{1}{\sigma} d\sigma = \infty$$

Jeffreys' rule gives an **improper prior** in this case, i.e. a not a proper density since its integral diverges. Improper priors are somewhat strange, but can be successfully used in practice if the posterior density is known to be proper, i.e. has a finite integral over the whole parameter space. The $1/\sigma$ form of Jeffreys' prior may seem peculiar as it seemingly favors small values for σ . One way of understanding this prior is that it corresponds to a uniform distribution on $\log \sigma \in \mathbb{R}$. In the case where θ and σ^2 are unknown, the multiparameter version of Jeffreys' rule shows that Jeffreys prior for σ is still $1/\sigma$ and the prior for θ is uniform.

improper prior

Jeffreys' rule has a serious drawback: it violates the likelihood principle; see Section Bayesian learning and the likelihood principle. The reason is that Jeffreys' rule is based on the Fisher information, which is an expectation with respect to the sampling distribution $p(x|\theta)$. Exercise 2 asks you to derive Jeffreys' prior for binary data obtained by negative binomial sampling, instead of Bernoulli trials. This exercise shows that Jeffreys' prior for the success probability θ is not the Beta($1/2, 1/2$) that we obtained for Bernoulli trials.

Probably the most promising so called Objective Bayes approach is the **reference prior** proposed by José Bernardo based on information arguments. It is motivated as a non-informative prior useful for scientific reporting where one wants to present posterior results to a wide audience using a single well understood prior. The reference prior is invariant to one-to-one transformations and is in fact equal to Jeffreys' prior when the usual regularity conditions for likelihood inference apply. The reference prior is more general however, and avoids some of problems that have been found with Jeffreys' rule; see Bernardo and Smith [2009] for a comprehensive introduction to reference priors.

reference prior

EXERCISES

1. Show that using Jeffreys rule to obtain a prior for the log odds $\phi \equiv \log \theta / (1 - \theta)$ in Bernoulli trials implies the same Beta(1/2, 1/2) prior for θ (i.e. that Route A and B in the text give the same prior).
2. Derive Jeffreys' prior for the success probability θ in the negative binomial model for a dataset where n trials were needed to obtain a predetermined s number of successes. Compare with the Jeffreys' prior derived for the Bernoulli model in the text. Discuss the implication for the likelihood principle.

NOTEBOOKS

1. See the notebook [priors](#).

Regression

Regression models are the most important of all statistical models as they appear as a component in nearly any situation where an output variable y is modeled as function of a set of input variables $\mathbf{x} = (x_1, \dots, x_p)^\top$, where \top denotes vector transpose. The input variables are often called **covariates**, predictors or **features**, and the output variable is most commonly termed the **response variable** or target variable. In the chapter [Classification](#) we will see regression models for a binary response variable and also for response variables of other data types, for example counts. Regression is also the basis for deep neural networks where a linear combination of covariates are passed through several nonlinear activation functions before finally being linked to the response.

The basic **Gaussian linear regression model** is

$$y_i = \mathbf{x}_i^\top \boldsymbol{\beta} + \varepsilon_i, \quad \varepsilon_i \stackrel{iid}{\sim} N(0, \sigma^2) \quad \text{for } i = 1, \dots, n, \quad (46)$$

where \mathbf{x}_i is a vector with observations on the p covariates and $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)^\top$ is the vector of **regression coefficients**. The β_j are called **weights** in the machine learning literature and are therefore frequently denoted by w_j . The model is said to be **homoscedastic** since the error variance σ^2 is the same for all observations.

It is convenient to stack all n response observations in a vector $\mathbf{y} = (y_1, \dots, y_n)^\top$ and the covariate observations vectors as rows in the $n \times p$ covariate matrix $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^\top$. The Gaussian linear regression model can then be expressed as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \stackrel{iid}{\sim} N(0, \sigma^2 I_n), \quad (47)$$

where $\boldsymbol{\varepsilon}$ is vector with all the ε_i and $N(0, \sigma^2 I_n)$ is the multivariate normal distribution with diagonal covariance matrix $\sigma^2 I_n$ and I_n is the identity matrix; the simple diagonal structure of $\text{Cov}(\boldsymbol{\varepsilon})$ reflects the assumption that the ε_i are independent with the same variance.

Likelihood and MLE

The likelihood for the linear regression model with homoscedastic Gaussian errors is given by the following multivariate normal distri-

covariates

features

response variable

Gaussian linear regression model

regression coefficients

weights

homoscedastic

bution

$$\mathbf{y}|\boldsymbol{\beta}, \sigma^2, \mathbf{X} \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2 I_n), \quad (48)$$

where we note that the covariates \mathbf{X} are assumed fixed so the likelihood is the distribution of only the response \mathbf{y} .

The **least squares estimator** $\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ is well known to minimize the sum of squared **residuals**

$$Q(\boldsymbol{\beta}) \equiv (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}).$$

When the errors are homoscedastic Gaussian, $\hat{\boldsymbol{\beta}}$ is also the MLE since the log-likelihood from (48) is a constant plus $-(1/2\sigma^2)Q(\boldsymbol{\beta})$.

The sampling distribution of the MLE is easily obtained since $\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ is a linear function of \mathbf{y} and $(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$ is a constant matrix. Since $\mathbf{y}|\boldsymbol{\beta}, \sigma^2, \mathbf{X} \sim N(\mathbf{X}\boldsymbol{\beta}, \sigma^2 I_n)$, the frequentist sampling distribution of $\hat{\boldsymbol{\beta}}$ is obtained by applying the result in Figure 73 with $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$, $\Sigma = \sigma^2 I_n$ and $\mathbf{A} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}$ to obtain

$$\hat{\boldsymbol{\beta}}|\boldsymbol{\beta}, \sigma^2, \mathbf{X} \sim N(\boldsymbol{\beta}, \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}),$$

from which we also see that the MLE is unbiased for $\boldsymbol{\beta}$.

The MLE for σ^2 can be shown to be $\hat{\sigma}^2 \equiv (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})/n$. The estimator $\hat{\sigma}^2$ is biased for σ^2 , and the following unbiased estimator is typically used instead

$$s^2 \equiv \frac{(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})}{n-p}.$$

Non-informative prior

We will start with the invariant Jeffreys' prior (see Section [Invariant priors](#)) which can be shown to be

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

i.e. an improper uniform distribution for $\boldsymbol{\beta}$ independently of σ^2 ; note that σ^2 has the same $1/\sigma^2$ prior as in the iid normal model derived in [Invariant priors](#).

The joint posterior for $\boldsymbol{\beta}$ and σ^2 is given by Bayes' theorem as

$$\begin{aligned} p(\boldsymbol{\beta}, \sigma^2 | \mathbf{y}) &\propto p(\mathbf{y}|\boldsymbol{\beta}, \sigma^2) p(\boldsymbol{\beta}, \sigma^2) \propto N(\mathbf{y}|\mathbf{X}\boldsymbol{\beta}, \sigma^2 I_n) \cdot \frac{1}{\sigma^2} \\ &= |2\pi\sigma^2 I_n|^{-1/2} \exp \left\{ -\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) \right\} \cdot \frac{1}{\sigma^2}, \end{aligned} \quad (49)$$

where the conditioning on the fixed covariates \mathbf{X} is suppressed to simplify the notation. Now, $(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$ can be rewritten using the MLE $\hat{\boldsymbol{\beta}}$ as

$$(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) = (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) + (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^\top \mathbf{X}^\top \mathbf{X} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}), \quad (50)$$

least squares estimator
residuals

Linear transformation of Gaussians

Let $\mathbf{x} \sim N(\boldsymbol{\mu}, \Sigma)$ be multivariate Gaussian in p dimensions and \mathbf{A} a constant full rank $m \times p$ matrix. Then

$$\mathbf{Ax} \sim N(\mathbf{A}\boldsymbol{\mu}, \mathbf{A}\Sigma\mathbf{A}^\top).$$

Particularly, for $m = 1$ and $\mathbf{A} = (a_1, \dots, a_p)^\top$, a row vector, we get that linear combinations $\sum_{j=1}^p a_j x_j$ of Gaussian variables are Gaussian.

Figure 73: Linear transformation of Gaussians.

which can be directly verified by substituting the definition of $\hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$. Recall from linear algebra that the determinant of a diagonal matrix is the product of its diagonal elements, so $|2\pi\sigma^2 I_n| = (2\pi\sigma^2)^n \propto (\sigma^2)^n$. Using this result and (50) in (49) we obtain the posterior

$$p(\boldsymbol{\beta}, \sigma^2 | \mathbf{y}) \propto (\sigma^2)^{-(n+2)/2} \exp \left\{ -\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\hat{\beta})^\top (\mathbf{y} - \mathbf{X}\hat{\beta}) \right\} \quad (51)$$

$$\cdot \exp \left\{ -\frac{1}{2\sigma^2} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^\top \mathbf{X}^\top \mathbf{X} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) \right\} \quad (52)$$

The posterior is most transparent if we use the decomposition of the joint posterior

$$p(\boldsymbol{\beta}, \sigma^2 | \mathbf{y}) = p(\boldsymbol{\beta} | \sigma^2, \mathbf{y}) p(\sigma^2 | \mathbf{y}).$$

Focusing first on $p(\boldsymbol{\beta} | \sigma^2, \mathbf{y}, \mathbf{X})$ we only need to be concerned with the last factor in (51) as it is the only part that depends on $\boldsymbol{\beta}$; note that $\hat{\boldsymbol{\beta}}$ only depends on the data. We immediately recognize this last factor as proportional to the multivariate normal density, so

$$\boldsymbol{\beta} | \sigma^2, \mathbf{y} \sim N(\hat{\boldsymbol{\beta}}, \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}).$$

The marginal posterior of σ^2 is obtained by integrating out $\boldsymbol{\beta}$ in (51)

$$\begin{aligned} p(\sigma^2 | \mathbf{y}) &= \int p(\boldsymbol{\beta}, \sigma^2 | \mathbf{y}) d\boldsymbol{\beta} \\ &\propto (\sigma^2)^{-(n+2)/2} \exp \left\{ -\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \right\} \\ &\quad \cdot \int \exp \left\{ -\frac{1}{2\sigma^2} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^\top \mathbf{X}^\top \mathbf{X} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}) \right\} d\boldsymbol{\beta} \\ &\propto (\sigma^2)^{-(n+2)/2} \exp \left\{ -\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \right\} (\sigma^2)^{p/2}, \end{aligned}$$

where the last proportionality comes from the fact that

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

for any p -vectors \mathbf{x} and $\boldsymbol{\mu}$, and positive definite matrix Σ since we know that the $N(\mathbf{x} | \boldsymbol{\mu}, \Sigma)$ density integrates to one over \mathbb{R}^p . The marginal posterior for σ^2 is therefore

$$p(\sigma^2 | \mathbf{y}) \propto (\sigma^2)^{-[1+(n-p)/2]} \exp \left\{ -\frac{1}{2\sigma^2} (n-p)s^2 \right\}, \quad (53)$$

which can be recognized as proportional to the $\text{Inv-}\chi^2(n-p, s^2)$ density.

We summarize the prior-to-posterior updating in Gaussian linear regression with a noninformative prior in Figure 74.

Gaussian linear regression with non-informative prior

Model: $\mathbf{y} = \mathbf{X}\beta + \varepsilon, \quad \varepsilon \stackrel{iid}{\sim} N(0, \sigma^2 I_n)$

Prior: $p(\beta, \sigma^2) \propto 1/\sigma^2$

Posterior: $\beta|\sigma^2, \mathbf{y}, \mathbf{X} \sim N(\hat{\beta}, \sigma^2(\mathbf{X}^\top \mathbf{X})^{-1})$
 $\sigma^2|\mathbf{y}, \mathbf{X} \sim \text{Inv}-\chi^2(n - p, s^2)$

where $\hat{\beta} \equiv (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ and $s^2 \equiv (\mathbf{y} - \mathbf{X}\hat{\beta})^\top (\mathbf{y} - \mathbf{X}\hat{\beta}) / (n - p)$.

Figure 74: Prior-to-Posterior updating for the Gaussian linear regression with non-informative prior.

Conjugate prior

Let us now turn to the more interesting case with a conjugate prior for the Gaussian linear regression. Recall that the conjugate prior for the iid Normal model $x_1, \dots, x_n | \theta, \sigma^2 \sim N(\theta, \sigma^2)$ was of the form $p(\theta, \sigma^2) = p(\theta|\sigma^2)p(\sigma^2)$ where

$$\theta|\sigma^2 \sim N(\mu_0, \sigma^2/\kappa_0)$$

$$\sigma^2 \sim \text{Inv}-\chi^2(\nu_0, \sigma_0^2).$$

The conjugate prior in linear regression is very similar

$$\beta|\sigma^2 \sim N(\mu_0, \sigma^2 \Omega_0^{-1}) \tag{54}$$

$$\sigma^2 \sim \text{Inv}-\chi^2(\nu_0, \sigma_0^2), \tag{55}$$

with the prior sample size κ_0 replaced by the $p \times p$ precision matrix Ω_0 .

A detailed elicitation of the matrix Ω_0 can be demanding. One simple choice is $\Omega_0 = \kappa_0 I_p$ which corresponds to using the same prior variance of σ^2/κ_0 for each regression coefficient and assuming that the regression coefficients are a priori independent, since $\sigma^2 \Omega_0^{-1}$ is diagonal. Another convenient choice is Zellner's prior where $\Omega_0 = \kappa_0 (\mathbf{X}^\top \mathbf{X})$; the covariates are assumed to be known and so can be used when formulating a prior. One way to understand Zellner's prior is that the prior covariance of β , $\kappa_0 \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}$, is a scaled version of the sampling covariance matrix of the MLE $\mathbb{V}(\hat{\beta}) = \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}$. Zellner's prior there automatically adjusts to the potentially different scales of the covariates. The covariance matrix in Zellner's prior can more generally be defined as a scaled version of the Fisher information, i.e. the prior information is proportional to the expected information from a sample of size n . By setting $\kappa_0 = 1/n$, Zellner's prior therefore becomes a noninformative **unit information prior** with information content equal to the expected information from just a single observation. We will have more to say about Ω_0 in the chapter [Regularization](#).

unit information prior

Gaussian linear regression with conjugate prior

Model: $\mathbf{y} = \mathbf{X}\beta + \varepsilon, \quad \varepsilon \stackrel{iid}{\sim} N(0, \sigma^2 I_n)$

Prior: $\beta | \sigma^2 \sim N(\mu_0, \sigma^2 \Omega_0^{-1})$
 $\sigma^2 | \mathbf{y}, \mathbf{X} \sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2)$

Posterior: $\beta | \sigma^2, \mathbf{y}, \mathbf{X} \sim N(\mu_n, \sigma^2 \Omega_n^{-1})$
 $\sigma^2 | \mathbf{y}, \mathbf{X} \sim \text{Inv-}\chi^2(\nu_n, \sigma_n^2)$
 $\beta | \mathbf{y} \sim t_{\nu_n}(\mu_n, \sigma_n^2 \Omega_n^{-1})$

where

$$\begin{aligned} \mu_n &= \Omega_n^{-1} (\mathbf{X}^\top \mathbf{X} \hat{\beta} + \Omega_0 \mu_0), \quad \hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}, \quad \Omega_n = \mathbf{X}^\top \mathbf{X} + \Omega_0, \\ \nu_n \sigma_n^2 &= \nu_0 \sigma_0^2 + (n - p) s^2 + (\mu_n - \hat{\beta})^\top \mathbf{X}^\top \mathbf{X} (\mu_n - \hat{\beta}) \\ &+ (\mu_n - \mu_0)^\top \Omega_0 (\mu_n - \mu_0) \text{ and } s^2 \equiv (\mathbf{y} - \mathbf{X} \hat{\beta})^\top (\mathbf{y} - \mathbf{X} \hat{\beta}) / (n - p). \end{aligned}$$

Figure 75: Prior-to-Posterior updating for the Gaussian linear regression with conjugate prior.

Figure 75 shows that the prior in (54) is indeed a conjugate prior. Figure 75 also gives the marginal posterior of β as multivariate- t distribution. The proof of these results are given at the end of this chapter. Figure 76 gives some Julia code for computing the posterior hyperparameters and for simulating posterior draws.

BIKE SHARE DATA

PROOFS

This section derives the posterior distribution for linear regression with a conjugate prior in Figure 75.

The joint posterior is

$$\begin{aligned} p(\beta, \sigma^2 | \mathbf{y}) &\propto p(\mathbf{y} | \beta, \sigma^2) p(\beta, \sigma^2) \\ &\propto |2\pi\sigma^2 I_n|^{-1/2} \exp\left(-\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\beta)^\top (\mathbf{y} - \mathbf{X}\beta)\right) \\ &\times |2\pi\sigma^2 \Omega_0^{-1}|^{-1/2} \exp\left(-\frac{1}{2\sigma^2} (\beta - \mu_0)^\top \Omega_0 (\beta - \mu_0)\right) \\ &\times (\sigma^2)^{-(\nu_0/2+1)} \exp\left(-\frac{1}{2\sigma^2} \nu_0 \sigma_0^2\right) \\ &\propto (\sigma^2)^{-((\nu_0+n+p)/2+1)} \exp\left(-\frac{1}{2\sigma^2} (\nu_0 \sigma_0^2 + (n-p)s^2)\right) \\ &\times \exp\left(-\frac{1}{2\sigma^2} ((\beta - \hat{\beta})^\top \mathbf{X}^\top \mathbf{X} (\beta - \hat{\beta}) + (\beta - \mu_0)^\top \Omega_0 (\beta - \mu_0))\right), \end{aligned}$$

where $s^2 = (\mathbf{y} - \mathbf{X} \hat{\beta})^\top (\mathbf{y} - \mathbf{X} \hat{\beta}) / (n - p)$ as before. Completing the

Figure 76: Julia code for linear regression with a conjugate prior

```

using Distributions, LinearAlgebra
ScaledInverseChiSq(ν, τ²) = InverseGamma(ν/2, ν*τ²/2)

function BayesLinReg(y::Vector, X, μ₀, Ω₀, ν₀, σ²₀, nSim)

    # Compute posterior hyperparameters
    n = length(y)
    p = size(X,2)
    XX = X'*X
    βhat = X \ y
    Ωₙ = Symmetric(XX + Ω₀)
    μₙ = Ωₙ \ (XX*βhat + Ω₀*μ₀)
    νₙ = ν₀ + n
    σ²ₙ = (y-X*βhat)'*(y-X*βhat)/(n-p)
    σ²ₙ = (ν₀*σ²₀+(n-p)*σ²ₙ+(μₙ-βhat)'*X'*X*(μₙ-βhat)+(μₙ-μ₀)'*Ω₀*(μₙ-μ₀))/νₙ
    println(σ²ₙ)

    # Sampling from posterior
    invΩₙ = inv(Ωₙ)
    σ²sim = zeros(nSim)
    βsim = zeros(nSim,p)
    for i ∈ 1:nSim
        # Simulate from p(σ²|y,X)
        σ² = rand(ScaledInverseChiSq(νₙ,σ²ₙ))
        σ²sim[i] = σ²

        # Simulate from p(β|σ²,y,X)
        β = rand(MvNormal(μₙ,σ²*invΩₙ))
        βsim[i,:] = β'
    end
    return μₙ, Ωₙ, νₙ, σ²ₙ, βsim, σ²sim
end

```

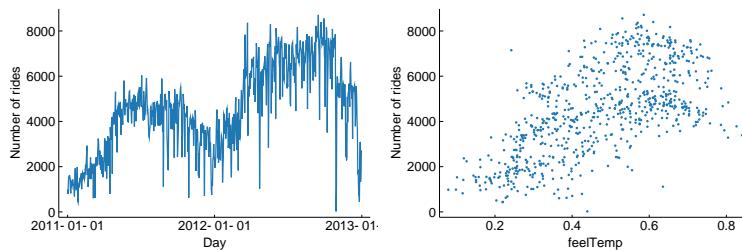


Figure 77: Daily bike share data

squares in the exponents using the result in Figure 65 gives

$$\begin{aligned} & (\beta - \hat{\beta})^\top \mathbf{X}^\top \mathbf{X}(\beta - \hat{\beta}) + (\beta - \mu_0)^\top \Omega_0(\beta - \mu_0) = \\ & (\beta - \mu_n)^\top \Omega_n(\beta - \mu_n) + (\mu_n - \hat{\beta})^\top \mathbf{X}^\top \mathbf{X}(\mu_n - \hat{\beta}) + (\mu_n - \mu_0)^\top \Omega_0(\mu_n - \mu_0), \end{aligned}$$

where $\mu_n = \Omega_n^{-1}(\mathbf{X}^\top \mathbf{X}\hat{\beta} + \Omega_0\mu_0)$. Hence,

$$\begin{aligned} p(\beta, \sigma^2 | \mathbf{y}) & \propto (\sigma^2)^{-((\nu_n+p)/2+1)} \exp\left(-\frac{\nu_n \sigma_n^2}{2\sigma^2}\right) \\ & \times \exp\left(-\frac{1}{2\sigma^2}(\beta - \mu_n)^\top \Omega_n(\beta - \mu_n)\right) \end{aligned} \quad (56)$$

where $\nu_n = \nu_0 + n$ and $\nu_n \sigma_n^2 = \nu_0 \sigma_0^2 + (n-p)s^2 + (\mu_n - \hat{\beta})^\top \mathbf{X}^\top \mathbf{X}(\mu_n - \hat{\beta}) + (\mu_n - \mu_0)^\top \Omega_0(\mu_n - \mu_0)$. Now,

$$\begin{aligned} p(\beta, \sigma^2 | \mathbf{y}) & \propto (\sigma^2)^{-((\nu_n+p)/2+1)} \exp\left(-\frac{\nu_n \sigma_n^2}{2\sigma^2}\right) |2\pi\sigma^2\Omega_n^{-1}|^{1/2} \\ & \times |2\pi\sigma^2\Omega_n^{-1}|^{-1/2} \exp\left(-\frac{1}{2\sigma^2}(\beta - \mu_n)^\top \Omega_n(\beta - \mu_n)\right) \\ & \propto (\sigma^2)^{-(\nu_n/2+1)} \exp\left(-\frac{\nu_n \sigma_n^2}{2\sigma^2}\right) \\ & \times |2\pi\sigma^2\Omega_n^{-1}|^{-1/2} \exp\left(-\frac{1}{2\sigma^2}(\beta - \mu_n)^\top \Omega_n(\beta - \mu_n)\right). \end{aligned}$$

From the second factor we see that $\beta | \sigma^2, \mathbf{y} \sim N(\mu_n, \sigma^2\Omega_n^{-1})$ and from the first factor that $\sigma^2 | \mathbf{y} \sim \text{Inv-}\chi^2(\nu_n, \sigma_n^2)$.

The marginal posterior of β is obtained by integrating $p(\beta, \sigma^2 | \mathbf{y})$ in (56) with respect to σ^2 using properties of the Inv- χ^2 distribution

$$\begin{aligned} p(\beta | \mathbf{y}) & \propto \int (\sigma^2)^{-((\nu_n+p)/2+1)} \times \exp\left(-\frac{1}{2\sigma^2}(\nu_n \sigma_n^2 + (\beta - \mu_n)^\top \Omega_n(\beta - \mu_n))\right) d\sigma^2 \\ & \propto \left((\nu_n \sigma_n^2 + (\beta - \mu_n)^\top \Omega_n(\beta - \mu_n))/2\right)^{-(\nu_n+p)/2} \\ & \propto \left(1 + \frac{1}{\nu_n}(\beta - \mu_n)^\top \sigma^{-2}\Omega_n(\beta - \mu_n)\right)^{-(\nu_n+p)/2} \end{aligned}$$

which is proportional to the multivariate student- t density

$$\beta | \mathbf{y} \sim t_{\nu_n}(\mu_n, \sigma_n^2\Omega_n^{-1}).$$

EXERCISES

1. This is the first problem.
2. This is the second problem.

NOTEBOOKS

1. See the notebook regression.

Prediction and Decision making

TODO! write intro text.

Bayesian prediction

We will occasionally use subscript on expectations, e.g. $\mathbb{E}_{\theta|y}(\theta)$ to denote which distribution the expectation is taken with respect to. Hence,

$$\mathbb{E}_{\theta|y}(\theta) \equiv \int \theta p(\theta|y)d\theta.$$

$$p(\tilde{y}|y) = \int_{\theta} p(\tilde{y}|\theta, y)p(\theta|y)d\theta$$

Prediction in normal model with known variance

My streaming service becomes unreliable and buffers at speeds below 5Mbit/sec. I am therefore particularly interested in this 'catastrophic' event happening tonight while watching my favourite movie. Finding the probability of a *single* measurement lower than 5MBit/sec is an exercise in prediction.

The Gaussian model $\tilde{y} \sim N(\theta, \sigma^2)$ for my internet speed can be trivially expressed as $\tilde{y} = \theta + \tilde{\varepsilon}$, where $\tilde{\varepsilon} \sim N(0, \sigma^2)$. Since we already know that the posterior for θ is $N(\mu_n, \tau_n^2)$ we see that \tilde{y} is the sum of two Gaussian variables, and the predictive distribution for \tilde{y} is therefore also Gaussian (Figure 73). To obtain the mean and variance of this predictive distribution it is helpful to first condition on θ and then 'undo' the conditioning by integrating with respect to the posterior for θ . This two-step approach of computing the mean and variance of random variables by first conditioning on another random variable are called the iteration laws; specifically the **law of iterated expectation** and the **law of total variance**. Figure 78 gives these laws in the case of two generic random variables X and Y as typically presented in introductory probability textbooks. Figure 79

Iteration laws

Law of iterated expectation:

$$\mathbb{E}_X(X) = \mathbb{E}_Y(\mathbb{E}_{X|Y}(X))$$

Law of total variance:

$$\begin{aligned} \mathbb{V}_X(X) &= \mathbb{E}_Y(\mathbb{V}_{X|Y}(X)) \\ &\quad + \mathbb{V}_Y(\mathbb{E}_{X|Y}(X)) \end{aligned}$$

Figure 78: Law of iterated expectations and law of total variance.

Iteration laws for Bayes

Marginal posterior mean:

$$\mathbb{E}_{\theta_1|y}(\theta_1) = \mathbb{E}_{\theta_2|y}(\mathbb{E}_{\theta_1|\theta_2,y}(\theta_1))$$

Marginal posterior variance:

$$\begin{aligned} \mathbb{V}_{\theta_1|y}(\theta_1) &= \mathbb{E}_{\theta_2|y}(\mathbb{V}_{\theta_1|\theta_2,y}(\theta_1)) \\ &\quad + \mathbb{V}_{\theta_2|y}(\mathbb{E}_{\theta_1|\theta_2,y}(\theta_1)) \end{aligned}$$

Figure 79: Iteration laws applied to compute marginal posterior moments given some data y .

law of iterated expectation

law of total variance

are the exact same laws but written in the context of computing the marginal posterior mean and variance for a parameter.

The predictive mean of \tilde{y} can now be computed by first computing the mean given θ

$$\mathbb{E}_{\tilde{y}|\mathbf{y},\theta}(\tilde{y}) = \theta$$

and then undo the conditioning in the second step by taking the posterior expectation

$$\mathbb{E}(\tilde{y}|\mathbf{y}) = \mathbb{E}_{\theta|\mathbf{y}}(\theta) = \mu_n,$$

since μ_n is by definition the posterior mean of θ . The predictive variance is similarly given by the law of total variance as

$$\begin{aligned}\mathbb{V}(\tilde{y}|\mathbf{y}) &= \mathbb{E}_{\theta|\mathbf{y}}[\mathbb{V}_{\tilde{y}|\mathbf{y},\theta}(\tilde{y})] + \mathbb{V}_{\theta|\mathbf{y}}[\mathbb{E}_{\tilde{y}|\mathbf{y},\theta}(\tilde{y})] \\ &= \mathbb{E}_{\theta|\mathbf{y}}(\sigma^2) + \mathbb{V}_{\theta|\mathbf{y}}(\theta) \\ &= \sigma^2 + \tau_n^2.\end{aligned}$$

Hence, the posterior predictive distribution is

$$\tilde{y}|\mathbf{y} \sim N(\mu_n, \sigma^2 + \tau_n^2).$$

The predictive variance is the sum of the model variance σ^2 and the posterior variance of θ , τ_n^2 , which represents the parameter uncertainty from not knowing θ when we make the prediction. The model variance σ^2 comes from each observation not being completely predictable even if the $N(\theta, \sigma^2)$ model was entirely known. The parameter uncertainty will disappear with more training data since $\tau_n^2 \rightarrow 0$ as $n \rightarrow \infty$. These two sources of predictive uncertainty appear at least implicitly in all models, and their relative importance depends on size of the training sample, the fit and complexity of the model.

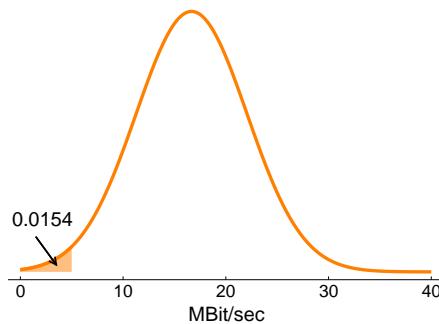


Figure 8o: Predictive density for the internet download speed example with $n = 5$ training observations, and marks out the probability of interest, $\Pr(\tilde{y}|y_1, \dots, y_5) \approx 0.0154$.

Figure 8o plots the predictive distribution for the internet download speed example with $n = 5$ training observations, and marks out the probability of interest, $\Pr(\tilde{y}|y_1, \dots, y_5) \approx 0.0154$.

Prediction in linear regression

Consider now prediction in the linear regression model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \stackrel{iid}{\sim} N(0, \sigma^2 I_n). \quad (57)$$

Using a training dataset (\mathbf{y}, \mathbf{X}) with n observations we have obtained the posterior $\sigma^2|\mathbf{y} \sim \text{Inv}-\chi^2(\nu_n, \sigma_n^2)$ and $\boldsymbol{\beta}|\sigma^2, \mathbf{y} \sim N(\boldsymbol{\mu}_n, \sigma^2 \Omega_n^{-1})$ using the conjugate prior as described in the Chapter [Regression](#); the conditioning on the fixed covariates \mathbf{X} in the training data is not explicitly written out.

Interest now centers on predicting the response $\tilde{\mathbf{y}}$ for \tilde{n} new observations using the $\tilde{n} \times p$ covariate matrix $\tilde{\mathbf{X}}$. The joint posterior predictive distribution for all \tilde{n} elements of $\tilde{\mathbf{y}}$ is then

$$p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \mathbf{y}) = \iint p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \boldsymbol{\beta}, \sigma^2) p(\boldsymbol{\beta}, \sigma^2|\mathbf{y}) d\boldsymbol{\beta} d\sigma^2. \quad (58)$$

Note how I have implicitly used some conditional independencies to reduce the clutter in the conditioning; for example $p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \mathbf{y}, \boldsymbol{\beta}, \sigma^2) = p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \boldsymbol{\beta}, \sigma^2)$ and $p(\boldsymbol{\beta}, \sigma^2|\mathbf{y}, \tilde{\mathbf{X}}) = p(\boldsymbol{\beta}, \sigma^2|\mathbf{y})$.

We will compute the posterior predictive distribution in (58) using two steps:

i) integrate out $\boldsymbol{\beta}$ to get $p(\tilde{\mathbf{y}}|\sigma^2, \tilde{\mathbf{X}}, \mathbf{y}) = \int p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \boldsymbol{\beta}, \sigma^2) p(\boldsymbol{\beta}|\sigma^2, \mathbf{y}) d\boldsymbol{\beta}$, and then

ii) integrate out σ^2 to obtain $p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \mathbf{y}) = \int p(\tilde{\mathbf{y}}|\sigma^2, \tilde{\mathbf{X}}, \mathbf{y}) p(\sigma^2|\mathbf{y}) d\sigma^2$.

Since $\tilde{\mathbf{y}} = \tilde{\mathbf{X}}\boldsymbol{\beta} + \tilde{\boldsymbol{\varepsilon}}$, and $\boldsymbol{\beta}$ and $\tilde{\boldsymbol{\varepsilon}}$ are both normal, we immediately see that $p(\tilde{\mathbf{y}}|\sigma^2, \mathbf{y})$ is multivariate normal with

$$\begin{aligned} \mathbb{E}(\tilde{\mathbf{y}}|\sigma^2) &= \mathbb{E}(\tilde{\mathbf{X}}\boldsymbol{\beta}) = \tilde{\mathbf{X}}\boldsymbol{\mu}_n \\ \mathbb{V}(\tilde{\mathbf{y}}|\sigma^2) &= \mathbb{V}(\tilde{\mathbf{X}}\boldsymbol{\beta}) + \mathbb{V}(\tilde{\boldsymbol{\varepsilon}}) = \tilde{\mathbf{X}}\sigma^2 \Omega_n^{-1} \tilde{\mathbf{X}}^\top + \sigma^2 I_{\tilde{n}} = \sigma^2 \tilde{\Sigma}, \end{aligned}$$

where $\tilde{\Sigma} = I_{\tilde{n}} + \tilde{\mathbf{X}}\Omega_n^{-1}\tilde{\mathbf{X}}^\top$; note that the expectation and variances are with respect to the posterior $p(\boldsymbol{\beta}|\sigma^2, \mathbf{y})$. Hence,

$$\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \mathbf{y}, \sigma^2 \sim N(\tilde{\mathbf{X}}\boldsymbol{\mu}_n, \sigma^2 \tilde{\Sigma}).$$

Now, since $\sigma^2|\mathbf{y} \sim \text{Inv}-\chi^2(\nu_n, \sigma_n^2)$, we have

$$\begin{aligned}
p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \mathbf{y}) &= \int p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \sigma^2, \mathbf{y})p(\sigma^2|\mathbf{y})d\sigma^2 \\
&= \int |2\pi\sigma^2\tilde{\Sigma}|^{-1/2} \exp\left(-\frac{1}{2\sigma^2}(\tilde{\mathbf{y}} - \tilde{\mathbf{X}}\boldsymbol{\mu}_n)^\top\tilde{\Sigma}^{-1}(\tilde{\mathbf{y}} - \tilde{\mathbf{X}}\boldsymbol{\mu}_n)\right) \\
&\quad \times \frac{(\nu_n\sigma_n^2/2)^{\nu_n/2}}{\Gamma(\nu_n/2)} (\sigma^2)^{-(\nu_n/2+1)} \exp\left(-\frac{\nu_n\sigma_n^2}{2\sigma^2}\right) d\sigma^2 \\
&= |2\pi\tilde{\Sigma}|^{-1/2} \frac{(\nu_n\sigma_n^2/2)^{\nu_n/2}}{\Gamma(\nu_n/2)} \\
&\quad \times \int (\sigma^2)^{-((\nu_n+\tilde{n})/2+1)} \exp\left(-\frac{\nu_n\sigma_n^2 + a(\mathbf{y})}{2\sigma^2}\right) d\sigma^2 \\
&= (2\pi)^{-\tilde{n}/2} |\tilde{\Sigma}|^{-1/2} \frac{(\nu_n\sigma_n^2/2)^{(\nu_n+\tilde{n})/2} \Gamma((\nu_n+\tilde{n})/2)}{((\nu_n\sigma_n^2 + a(\mathbf{y}))/2)^{(\nu_n+\tilde{n})/2} \Gamma(\nu_n/2)}
\end{aligned}$$

where $a(\tilde{\mathbf{y}}) = (\tilde{\mathbf{y}} - \tilde{\mathbf{X}}\boldsymbol{\mu}_n)^\top\tilde{\Sigma}^{-1}(\tilde{\mathbf{y}} - \tilde{\mathbf{X}}\boldsymbol{\mu}_n)$, and the last equality follows from the integrand begin proportional to a $\text{Inv}-\chi^2$ distribution. The density above can with a little bit of simple algebra be written as

$$\begin{aligned}
p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \mathbf{y}) &= \frac{\Gamma((\nu_n+\tilde{n})/2)}{\Gamma(\nu_n/2)(\pi\nu_n)^{\tilde{n}/2}|\sigma_n^2\tilde{\Sigma}|^{1/2}} \\
&\quad \times \left(1 + \frac{1}{\nu_n}(\tilde{\mathbf{y}} - \tilde{\mathbf{X}}\boldsymbol{\mu}_n)^\top(\sigma_n^2\tilde{\Sigma})^{-1}(\tilde{\mathbf{y}} - \tilde{\mathbf{X}}\boldsymbol{\mu}_n)\right)^{-(\nu_n+\tilde{n})/2},
\end{aligned}$$

which can be recognized as the density of a **multivariate student-t distribution**; Bayesian prediction in linear regression with a conjugate prior is summarized in Figure 81.

multivariate student-t distribution

Predictive density conjugate Gaussian linear regression

Model: $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon} \stackrel{iid}{\sim} \mathcal{N}(0, \sigma^2 I_n)$

Posterior: $\boldsymbol{\beta}|\sigma^2, \mathbf{y}, \mathbf{X} \sim \mathcal{N}(\boldsymbol{\mu}_n, \sigma^2\Omega_n^{-1})$
 $\sigma^2|\mathbf{y}, \mathbf{X} \sim \text{Inv}-\chi^2(\nu_n, \sigma_n^2)$

Predictive density for \tilde{n} observations with covariate matrix $\tilde{\mathbf{X}}$:

$$\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \mathbf{y} \sim t_{\nu_n}(\tilde{\mathbf{X}}\boldsymbol{\mu}_n, \sigma_n^2(\mathbf{I}_{\tilde{n}} + \tilde{\mathbf{X}}\Omega_n^{-1}\tilde{\mathbf{X}}^\top))$$

using the posterior hyperparameters in Figure 75.

It took us some work to get here, but the effort was worthwhile. The predictive distribution $p(\tilde{\mathbf{y}}|\tilde{\mathbf{X}}, \mathbf{y})$ is a practically important joint probability density of $\tilde{\mathbf{y}}$ that includes uncertainty from two sources:

- i) errors $\boldsymbol{\varepsilon}$, represented by the $\sigma_n^2\mathbf{I}_{\tilde{n}}$ term, and
- ii) parameter uncertainty, from the term $\sigma_n^2(\tilde{\mathbf{X}}\Omega_n^{-1}\tilde{\mathbf{X}}^\top)$.

Figure 81: Predictive density in Gaussian linear regression with a conjugate prior.

The parameter uncertainty will vanish with large training samples since it can be shown that $\Omega_n^{-1} \xrightarrow{p} \mathbf{0}$ and $\sigma_n^2 \xrightarrow{p} \sigma^2$ as $n \rightarrow \infty$, under the common assumption that $n^{-1}\mathbf{X}^\top\mathbf{X}$ converges to a constant non-singular matrix. In the chapter [Model comparison](#) we will see how the posterior predictive distribution can also incorporate model uncertainty, and in chapter [Variable selection](#) how to handle the uncertainty in the choice of covariates in regression and classification.

Some additional real-world prediction problems

I will now illustrate Bayesian prediction in two more complex problems. The problems are presented here as motivational examples to show how simulation can be used for Bayesian prediction in real applications; all details will not be given and the examples are not meant to be fully understood at this point.

PREDICTING INFLATION WITH AN AUTOREGRESSIVE PROCESS.

Imagine that you have the task of predicting the future development of a time series, for example forecasting the Swedish inflation in the coming 12 quarters. Not only would you like to have a mean prediction, but also some notation of predictive uncertainty.

A popular model for macroeconomic time series forecasting is the autoregressive process with p lags, AR(p), introduced in the chapter [Priors](#):

$$y_t = \mu + \phi_1(y_{t-1} - \mu) + \dots + \phi_p(y_{t-p} - \mu) + \varepsilon_t, \quad \varepsilon_t \stackrel{\text{iid}}{\sim} N(0, \sigma^2), \quad (59)$$

where y_t is the time series observed at time t , y_{t-k} is the k th lagged value of the time series and ε_t are future shocks to the time series.

Having observed training data $\mathbf{y}_{1:T} \equiv (y_1, \dots, y_T)$ up to time T , we now want the joint predictive density of the time series in the h coming time periods $\tilde{\mathbf{y}}_{T+1:T+h} \equiv (\tilde{y}_{T+1}, \dots, \tilde{y}_{T+h})$. This predictive density can as usual be written as an integral with respect to the posterior distribution,

$$p(\tilde{\mathbf{y}}_{T+1:T+h} | \mathbf{y}_{1:T}) = \int p(\tilde{\mathbf{y}}_{T+1:T+h} | \mathbf{y}_{1:T}, \boldsymbol{\theta}) p(\boldsymbol{\theta} | \mathbf{y}_{1:T}) d\boldsymbol{\theta},$$

where $\boldsymbol{\theta} = (\mu, \phi_1, \dots, \phi_p, \sigma^2)$ is the vector of parameters in the AR(p) process and $p(\boldsymbol{\theta} | \mathbf{y}_{1:T})$ is the posterior distribution of the parameters based on the training data.

We can simulate from the predictive distribution $p(\tilde{\mathbf{y}}_{T+1:T+h} | \mathbf{y}_{1:T})$ by repeating the following two steps for $i = 1, \dots, m$:

- simulate a posterior parameter draw $\boldsymbol{\theta}^{(i)} \sim p(\boldsymbol{\theta} | \mathbf{y}_{1:T})$
- simulate a h -steps-ahead realization path $\tilde{\mathbf{y}}_{T+1:T+h}^{(i)}$ from the model $p(\tilde{\mathbf{y}}_{T+1:T+h} | \mathbf{y}_{1:T}, \boldsymbol{\theta}^{(i)})$ conditional on $\boldsymbol{\theta}^{(i)}$.

The first step above will be described in Chapter [Posterior simulation](#). The second step is implemented using the usual sequential decomposition of a joint distribution

$$\begin{aligned} p(\tilde{\mathbf{y}}_{T+1:T+h} | \mathbf{y}_{1:T}, \theta) = & p(\tilde{\mathbf{y}}_{T+1} | \mathbf{y}_{1:T}, \theta) p(\tilde{\mathbf{y}}_{T+2} | \mathbf{y}_{1:T+1}, \theta) \\ & \cdots p(\tilde{\mathbf{y}}_{T+h} | \mathbf{y}_{1:T+h-1}, \theta). \end{aligned} \quad (60)$$

We can simulate from each term in (60) forward in time, i.e. from left to right, by iterating on (59) with a new simulated future shock, ε_{T+j} injected at each time step. Since the AR(p) process is a **Markov process** of order p (see Figure 82) it is sufficient to condition on the p most recent time observations in each term instead of the full training sample $\mathbf{y}_{1:T}$. Note also that with exception of $p(\tilde{\mathbf{y}}_{T+1} | \mathbf{y}_{1:T}, \theta)$, all terms in (60) conditions on future, yet unobserved values, which have been simulated in earlier time steps. The algorithm is detailed in Figure 83 where this is made explicit by highlighting such data points in orange. Using this algorithm with $m = 10,000$ draws produces the $h = 12$ -steps-ahead predictive distribution for Swedish inflation in Figure 84.

Predictive distribution - AR process.

```

Input: time series  $\mathbf{y}_{1:T} = (y_1, \dots, y_T)$   

        number of predictive draws  $m$ .  

        forecast horizon  $h$ .  

for  $i$  in  $1:m$  do  

     $\mu, \phi_1, \dots, \phi_p, \sigma \leftarrow \text{rPOSTERIORAR}(\mathbf{y}_{1:T}, \text{Prior})$   

     $\varepsilon_{T+1} \leftarrow \text{rNORM}(0, \sigma)$   

     $\tilde{y}_{T+1} \leftarrow \mu + \phi_1(y_T - \mu) + \dots + \phi_p(y_{T+1-p} - \mu) + \varepsilon_{T+1}$   

     $\varepsilon_{T+2} \leftarrow \text{rNORM}(0, \sigma)$   

     $\tilde{y}_{T+2} \leftarrow \mu + \phi_1(\tilde{y}_{T+1} - \mu) + \dots + \phi_p(y_{T+2-p} - \mu) + \varepsilon_{T+2}$   

     $\vdots$   

     $\varepsilon_{T+h} \leftarrow \text{rNORM}(0, \sigma)$   

     $\tilde{y}_{T+h} \leftarrow \mu + \phi_1(\tilde{y}_{T+h-1} - \mu) + \dots + \phi_p(\tilde{y}_{T+h-p} - \mu) + \varepsilon_{T+h}$   

end  

Output:  $m$  draws from the joint predictive density:  

 $p(\tilde{\mathbf{y}}_{T+1}, \dots, \tilde{\mathbf{y}}_{T+h} | \mathbf{y}_{1:T}).$ 
```

cess X_1, X_2, \dots is said to be **first-order Markov** if

$$\Pr(X_{n+1} | \mathbf{X}_{1:n}) = \Pr(X_{n+1} | X_n),$$

i.e. if the distribution of future values are independent of the past, conditional on the most recent value.

A process is p th order **Markov** if the distribution of future values are independent of the past, conditional on the p most recent values.

A Markov process in discrete time is also called a **Markov Chain**.

Figure 82: Markov processes.

Markov process

Figure 83: Algorithm for simulating from the joint h -step-ahead predictive distribution of an AR process. The function `rPOSTERIORAR()` uses Gibbs sampling and will be presented in Chapter [Posterior simulation](#). The terms in orange font are future values used in the prediction which have been simulated in earlier time steps.

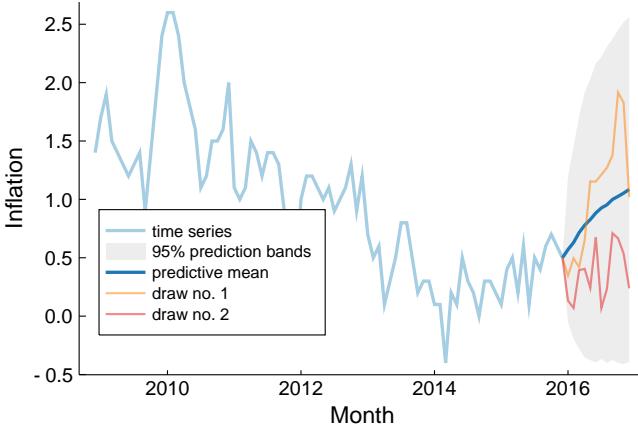


Figure 84: Predictive distribution $h = 12$ steps ahead for Swedish inflation represented by a mean prediction in dark blue and 95% predictive intervals as the gray region. Two of the $m = 10,000$ simulated paths from the algorithm in Figure 83 are marked out.

PREDICTING AUCTION PRICES. In Chapter [Single-parameter models](#) we inferred the mean number of bidders in a internet auction using the iid Poisson model. The Poisson model can be extended to a regression model with a mean depending on auction-specific covariates, such as the seller's reservation price, which we saw already in Chapter [Single-parameter models](#) was an important determinant of the number of bidders. A Poisson regression for the number of bidders r in an auction with covariates \mathbf{w} is $r|\mathbf{w} \sim \text{Pois}(\lambda)$, where $\lambda = \exp(\mathbf{w}^\top \gamma)$. Note that the covariates \mathbf{w} are auction-specific so each auction has its own Poisson mean λ reflecting the specifics (reservation price, seller's rating etc) of that specific auction. The reason for using the exponential function to link the covariates to the Poisson mean λ is that this guarantees that λ is positive.

We will return to a Bayesian analysis of the Poisson regression for the number of bidders in Chapter [Classification](#); this model will here be a component in a bigger model for the final price of the auctioned item. The training dataset includes also all bids in each of the $n = 1,000$ auctions. There are two complications that needs to be considered when modeling the price. First, since bidders compete, they are strategic and their disclosed bids b need not be the same as their true valuation v of auctioned object. Game theory can be used to find the optimal bid function $b(v, r, \mu, \sigma)$, mapping the valuations to the observed bids; the optimal bid function depends on the number of bidders r , as well as the mean μ and standard deviation in the bidders evaluations, σ , for the given auction. The second complication is that the bidding system at eBay is such that the winner of the auction pays a price equal to the *second* largest bid. The following simulation scheme describes a simplified version of the model used in [Wegmann and Villani \[2011\]](#):

1. Simulate the number of bidders $\tilde{r}|\tilde{\mathbf{w}} \sim \text{Pois}(\tilde{\lambda})$, where $\tilde{\lambda} =$

$\exp(\tilde{\mathbf{w}}^\top \gamma)$ and $\tilde{\mathbf{w}}$ are the covariates for λ .

2. Simulate the valuations of all \tilde{r} bidders from the linear regression $N(\tilde{\mu}, \sigma^2)$ where $\tilde{\mu} = \tilde{\mathbf{x}}^\top \beta$ is the regression function depending on covariates $\tilde{\mathbf{x}}$ that determine the mean valuation.
3. Compute bids for all \tilde{r} bidders using the optimal bid function $b(v, \tilde{r}, \tilde{\mu}, \sigma)$.
4. Return the second largest bid as the final price.

The algorithm in Figure 85 summarizes this process of simulating from the predictive distribution, including the sampling of the posterior for the model parameters.

Predictive distribution - internet auction price.

```

Input: training auction bids  $\mathbf{Y}$ 
      training auction covariates  $\mathbf{W}$  for  $\lambda$ .
      training auction covariates  $\mathbf{X}$  for  $\mu$ .
      test auction covariates  $\tilde{\mathbf{w}}$  for  $\lambda$ .
      test auction covariates  $\tilde{\mathbf{x}}$  for  $\mu$ .
      number of predictive draws  $m$ .

for  $i$  in  $1:m$  do
     $\beta, \gamma, \sigma \leftarrow \text{rPostAuction}(\mathbf{Y}, \mathbf{X}, \mathbf{W}, \text{Prior})$  # parameters
     $\tilde{r} \leftarrow \text{rPois}(\tilde{\lambda}),$  where  $\tilde{\lambda} = \exp(\tilde{\mathbf{w}}^\top \gamma)$  # bidders
     $\tilde{\mathbf{v}}_{1:\tilde{r}} \leftarrow \text{rNorm}(\tilde{\mu}, \sigma),$  where  $\tilde{\mu} = \tilde{\mathbf{x}}^\top \beta$  # all valuations  $v$ 
     $\mathbf{b}_{1:\tilde{r}} \leftarrow \text{BidFunction}(\tilde{\mathbf{v}}_{1:\tilde{r}}, \tilde{r}, \tilde{\mu}, \sigma)$  # all bids
     $\tilde{p} \leftarrow \text{SECONDLARGEST}(\mathbf{b}_{1:\tilde{r}})$  # final price is 2nd largest bid
end

Output:  $m$  draws from the predictive distribution of the
      final price  $\tilde{p}$  in an auction.

```

Figure 85: Algorithm for simulating from the predictive distribution of selling price in internet coin auction with covariates $\tilde{\mathbf{x}}$ for the mean valuation and covariates $\tilde{\mathbf{w}}$ for modeling the mean number of bidders in the auction. The function rPostAuction simulates from the joint posterior of all model parameters using the Metropolis-Hastings algorithm described in Chapter Posterior simulation.

Figure 86 shows the predictive distribution of two test auctions from the full model in Wegmann and Villani [2011]. The predictive distribution contains three parts: i) the probability of no bids ($\tilde{r} = 0$), ii) the probability of exactly one bid ($\tilde{r} = 1$), in which the price is the seller's reservation price, and iii) the predictive density of the price given at least two bids. For the auction to the left in Figure 86 the actual outcome was more than two bids and a final price of \$41.00, which was fairly well predicted by the model: the probability of $\tilde{r} \leq 1$ was close to zero and \$41.5 has a relatively high density. The auction to the right in Figure 86 ended without any bids and this was

predicted with a probability of 0.150; the probability of a price equal to the reservation price \$11.45 (the green dot) was 0.269.

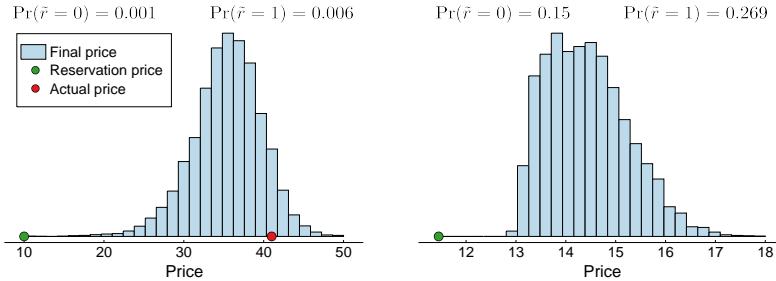


Figure 86: Predictive distributions of the final price in two auctions. The green dot marks out the sellers reservation price and the red dot marks out the realized price. The auction in the right hand graph has no red dot since the auction ended without any bids. The predicted probability of no bids and one bid (buyer pays the reservation price) are written in the graph titles. The histograms represent the predictive densities given at least two bids.

Bayesian decisions

Predictions play a major role in modern statistical analysis and machine learning, but the final aim is often **decision making under uncertainty**, with the predictive distribution as an essential component. This is obvious in AI applications, where self-driving cars or automatic stock trading apps need to constantly make decisions to reach pre-determined goals.

One can argue that decisions are nearly always the final aim, even when this is not as apparent as for automatic AI systems. Consider for example data from a clinical trial where the interest is to quantify the reduction in blood pressure from a given dose of beta-blocker medicine. A first idea would be to **infer** the regression coefficient β in linear regression of blood pressure (y) on the covariates dosage (x) and to check if the value $\beta = 0$ (no effect) is included in a 95% HPD credible interval.

A more interesting goal is **predicting** the blood pressure reduction for a given dosage, particularly if additional subject covariates, such as age, sex, exercise habits etc, are used in the regression model to obtain personalized predictions.

The ultimate goal however is to **make a decision** if a particular patient should be given the medicine. To answer this question we clearly need personalized predictions of the blood pressure reduction and its subsequent effect of reducing the probability of stroke, but also a valuation of the cost and the risk of potential side effects of taking the medicine. This section will introduce the Bayesian framework for making such decisions under uncertainty.

Actions and Utility

Let $a \in \mathcal{A}$ be an **action** in a set \mathcal{A} of possible actions. Let $\theta \in \Theta$ rep-

decision making under uncertainty

resent an unknown quantity. The consequences of choosing action a when θ turns out to be θ is quantified by a **utility function** $u(a, \theta)$. The utility function is subjective since the consequences of the actions typically varies from person to person. Table 3 present the utility of different action-unknown pairs in an example with a discrete set of actions and a discrete set of possible values for θ .

	θ_1	θ_2	\dots	θ_K
a_1	$u(a_1, \theta_1)$	$u(a_1, \theta_2)$	\dots	$u(a_1, \theta_K)$
a_2	$u(a_2, \theta_1)$	$u(a_2, \theta_2)$	\dots	$u(a_2, \theta_K)$
\vdots	\vdots	\vdots		\vdots
a_J	$u(a_J, \theta_1)$	$u(a_J, \theta_2)$	\dots	$u(a_J, \theta_K)$

utility function

Table 3: Utility table.

Table 4 present a toy decision problem where the choice is between bringing or not bringing an umbrella with you today. The consequences of this decision depends on the weather during the day. The best outcome is when you have chosen not to bring the umbrella and it turns out to be a sunny day. The worst outcome is when it rains and you left the umbrella home.

	Rain	Sun
No umbrella	-50	50
Umbrella	10	30

Table 4: Utility table.

Here are some more interesting decision problems.

SURGERY A surgeon needs to decide if a delicate surgery should be performed ($a = 1$) or not ($a = 0$). The surgery can be successful ($\theta = 1$) or lead to severe complications ($\theta = 0$). The probability of a successful operation can be computed based on the patient's characteristics. The utility function may be difficult to assess, but should involve the consequences of the patient as well as the cost of the operation. This is an example with discrete \mathcal{A} and Θ .

CENTRAL BANK'S INTEREST RATE DECISIONS. An central bank with an explicit inflation target needs to continually decide the level of their lending rate (a) to simultaneously reach an pre-determined target level for future inflation (θ_1) and to reduce future unemployment (θ_2). A simplified utility function could be

$$u(a, \theta) = \omega (\theta_1(a) - \bar{\theta}_1)^2 - (1 - \omega)\theta_2(a),$$

where $\theta = (\theta_1, \theta_2)$, $\bar{\theta}_1$ is the inflation target, ω is the weight of the inflation target relative to the unemployment, and both unknowns θ_1 and θ_2 are functions of the interest rate, a . Here the set of actions \mathcal{A} can be considered discrete (repo rate changes are in quarter percentage units) and Θ is two-dimensional and continuous.

PRICE REDUCTION ON ELECTRIC CARS. A government wants to give a price deduction on purchases of environmentally friendly electric cars (a) in an attempt to minimize future global warming. This is a complex decision problems with many unknowns. The government may settle for the intermediate goal of maximizing the expected utility from the CO₂ reduction from the price deduction (θ), net of the monetary cost of the deduction. Both \mathcal{A} and Θ are continuous spaces here.

FIRMS' STOCKING DECISIONS. Deciding how much of a product to keep in stock is a balance act where too much stock is costly in storage, and too little stock runs the risk of not being able to deliver on time. Let a be the number of items in stock, θ the unknown number of items demanded by the customers in the coming period and p the set price for the product. A utility function for the firm may have the form

$$u(a, \theta) = \begin{cases} p \cdot \theta - c_1(a - \theta) & \text{if } a \geq \theta \\ p \cdot a - c_2(\theta - a)^2 & \text{if } a < \theta, \end{cases}$$

where c_1 and c_2 are positive constants. In the first case, too much stock was kept ($a \geq \theta$) and the utility is the profit, i.e. revenue $p \cdot \theta$ minus stocking costs for unsold items (c_1 each). In the second case, the firm kept too small stock, can only sell a units and suffers a reputation cost of not being a trustworthy firm that delivers on time. The reputation cost is considered to be quadratic in the number of undelivered items (many people complaining on social media etc).

Maximizing expected utility

There have been a large number of heuristic decision rules proposed in the literature. As an example, one such rule is the **maximin rule**: choose the action that gives the highest utility if the worst possible outcome of θ happens. In the umbrella example in Table 4 we see that the maximin decision is to always carry an umbrella since the worst utility for this choice is 10 (it rains) whereas if you choose not to carry an umbrella, the utility could be as low as -50 if it rains. The problem with the minimax rule, and many other heuristics, is that it completely ignores the probability of rain. Always bringing an umbrella may be a decent rule for rainy Bergen in Norway, but not for sunny California.

The Bayesian solution to a decision problem is instead based on the **posterior expected utility** of an action

$$\bar{u}(a) \equiv \mathbb{E}_{\theta|x} [u(a, \theta)] = \int u(a, \theta) p(\theta|x) d\theta, \quad (61)$$

from which the **optimal Bayesian decision** is to choose the action

maximin rule

posterior expected utility

optimal Bayesian decision

$a \in \mathcal{A}$ that maximizes posterior expected utility:

$$a^* = \arg \max_{a \in \mathcal{A}} \bar{u}(a). \quad (62)$$

The Bayesian decision rule is naturally based on averaging over the unknown θ with respect to your best quantification of uncertainty, the posterior distribution; brake the Bayesian eggs and you can enjoy a Bayesian omelette.

Figure 87 illustrates the optimal Bayesian decision in the umbrella toy decision problem in Table 4. Note how the probability for rain must be at least 0.25 for the Bayesian to make the same decision as the constantly umbrella carrying pessimist following the maximin rule.

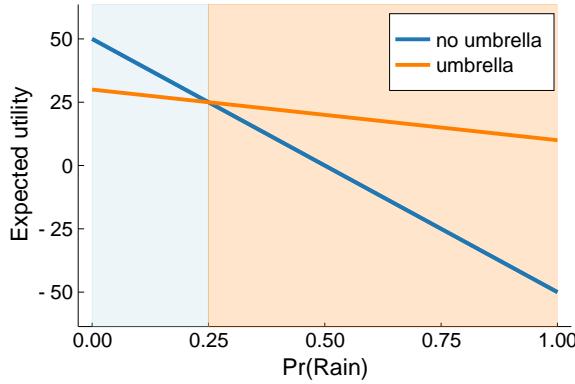


Figure 87: Expected utility of bringing an umbrella as function of the probability of rain. The shaded regions mark out the action that maximizes expected utility.

An interesting feature of the Bayesian theory is that it implies the **separation principle**, i.e. that inference and decision problems can and should be kept separate:

separation principle

1. first learn a posterior distribution for the unknown state of the world θ and then
2. set up a utility function $u(a, \theta)$ that values the consequence of actions $a \in \mathcal{A}$, to finally
3. choose the optimal action that maximizes posterior expected utility $\bar{u}(a)$.

Finding the optimal Bayesian decision involves computing the integral in (61), which is often analytically intractable. A simple approach is to compute the integral by Monte Carlo integration

$$\bar{u}(a) \equiv \mathbb{E}_{\theta|x} [u(a, \theta)] \approx m^{-1} \sum_{i=1}^m u(a, \theta^{(i)}), \quad (63)$$

where $\theta^{(1)}, \dots, \theta^{(m)} \sim p(\theta|x)$ are posterior draws. Expression (63) can be optimized numerically, see Chapter [Classification](#), to find the approximate Bayes decision a^* .

Point estimate as a decision problem

The chapter [Single-parameter models](#) presented ways of summarizing a posterior distribution by a measure of posterior location, e.g. the posterior mean, median or mode. Choosing between these location measures is a decision problem where the action a is the **point estimate** of the unknown parameter θ . Reporting the estimate a when the unknown is really θ gives utility $u(a, \theta)$. For example, with a **quadratic utility** $u(a, \theta) = -(a - \theta)^2$, the optimal decision is to summarize the posterior distribution $p(\theta|x)$ with the posterior mean, $E(\theta|x)$. To see this, note that the negative posterior expected utility is

$$\mathbb{E}_{\theta|x}(a - \theta)^2 = \mathbb{E}_{\theta|x}(a - E(\theta|x) - (\theta - E(\theta|x)))^2 = (a - E(\theta|x))^2 + V(\theta|x),$$

since the cross-term is zero by the fact that $\mathbb{E}_{\theta|x}(\theta - E(\theta|x)) = 0$.

Maximizing the posterior expected utility is the same as minimizing $\mathbb{E}(a - \theta)^2$. Hence, since $V(\theta|x)$ does not depend on a , the posterior mean $a = E(\theta|x)$ is the optimal estimate for the quadratic utility function.

Similarly, one can show that the posterior median is optimal under the **linear utility** $u(a, \theta) = -|a - \theta|$. The posterior mode, the θ value with highest posterior density, seems like a sensible summary, but actually corresponds to the rather peculiar **zero-one utility**

$$u(a, \theta) = \begin{cases} 0 & \text{if } a = \theta \\ -1 & \text{if } a \neq \theta. \end{cases}$$

The zero-one utility hence gives a constant loss (negative utility) regardless of the size of the estimation error $a - \theta$, except when the estimate is spot on.

The linear, quadratic and zero-one utility are all symmetric in the error $a - \theta$. The following so called **lin-lin utility** function values over- and underestimation differently.

$$u(a, \theta) = \begin{cases} -c_1|a - \theta| & \text{if } a \leq \theta \\ -c_2|a - \theta| & \text{if } a > \theta. \end{cases}$$

where c_1 and c_2 are positive constants. A lin-lin loss is for example appropriate for budget spending prediction, where underestimation is worse than overestimation. The optimal estimate under lin-lin loss can be shown to be the $c_1/(c_1 + c_2) \cdot 100\%$ **percentile** of the posterior distribution $p(\theta|x)$, i.e. the value that has exactly $c_1/(c_1 + c_2)$ of the probability mass to the left. For example, with $c_1 = 9$ and $c_2 = 1$, i.e. the loss from underestimation is 9 larger than for overestimation, the optimal estimate is the 90% percentile of $p(\theta|x)$.

The four presented utility function are plotted in Figure 88 as function of the estimation error $a - \theta$.

point estimate

quadratic utility

linear utility

zero-one utility

lin-lin utility

percentile

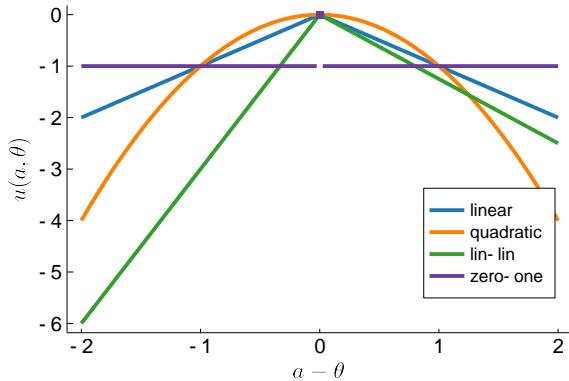


Figure 88: Utility functions for point estimation as a function of estimation error $a - \theta$. The lin-lin utility has $c_1 = 3$ and $c_2 = 1.25$.

EXERCISES

1. (a) Let $x_1, \dots, x_n \stackrel{iid}{\sim} \text{Bern}(\theta)$, with a $\text{Beta}(\alpha, \beta)$ prior for θ . Derive the predictive distribution for x_{n+1} .
 - (b) You need to decide if you bring your umbrella during your daily walk. It has rained on two days during the last ten days, and you assess those ten days to be representative also for the weather today, the 11th day. Your utility for the action-state combinations are given in the table below. Assume a $\text{Beta}(1, 1)$ prior for θ . Compute the Bayesian decision.
 - (c) How sensitive is your decision in (b) to the changes in the prior hyperparameters, α and β ?
2. (a) Let x_i be the number of sales of a product on month i . Let $x_1, \dots, x_n \stackrel{iid}{\sim} N(\theta, \sigma^2)$ be the (approximate) distribution for the sales, and let $\theta \sim N(200, 50^2)$ a priori. Assume that $\sigma^2 = 25^2$ and that we have observed $n = 5$ and $\bar{x} = 320.4$. Compute the predictive distribution for x_6 .
 - (b) The company has the choice of performing a marketing campaign for their product. The marketing campaign costs 300 and is believed to increase sales by 20% compared to when no campaign is performed. The company sells the product for $p = 10$ dollar and the cost of producing the product is $q = 5$ dollar. There are no fixed production costs. Assume that the company's utility is described by $U(y) = 1 - \exp(-y/1000)$, where y is the total profit from sales in the next month. Should the company perform the marketing campaign? Hint: the expected value of the exponential function of a normal random variable $S \sim N(\mu, \sigma^2)$ is $\mathbb{E}(\exp(S)) = \exp(\mu + \sigma^2/2)$.

NOTEBOOKS

1. See the notebook [Prediction and Decision](#).

Classification

EXERCISES

1. This is the first problem.
2. This is the second problem.

NOTEBOOKS

1. See the notebook **Classification**.

Posterior simulation

Gibbs sampling

Markov Chain Monte Carlo

Hamiltonian Monte Carlo

Probabilistic programming frameworks

Variational inference

Regularization

POLYNOMIAL REGRESSION As a first step toward flexible nonlinear regression modeling, let us consider the Gaussian polynomial regression model

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_p x^p + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2)$$

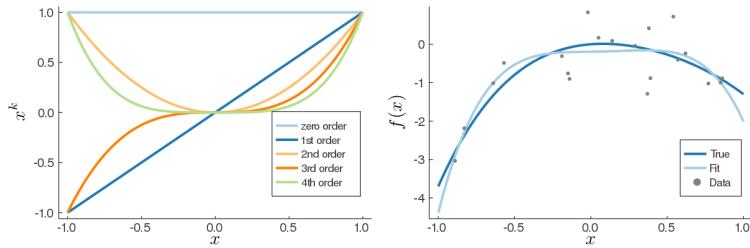


Figure 89: Polynomial regression.

L₂-regularization and Ridge

L₁-regularization and Lasso

Global-local regularization and Horseshoe

Laplace distribution

$X \sim \text{Laplace}(\mu, \beta)$ for $X \in \mathbb{R}$.

$$\begin{aligned} p(x) &= \frac{1}{2\beta} \exp\left(-\frac{|x - \mu|}{\beta}\right) \\ \mathbb{E}(X) &= \mu \\ \mathbb{V}(X) &= 2\beta^2 \end{aligned}$$

Figure 90: Laplace distribution.

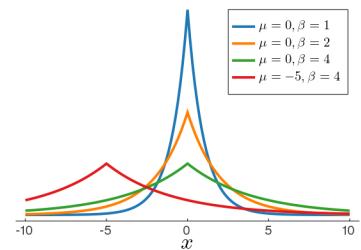


Figure 91: Some Laplace distributions.

Model comparison

Posterior model probabilities

Linear regression

The marginal likelihood for the linear regression model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \stackrel{iid}{\sim} \mathcal{N}(0, \sigma^2 I_n), \quad (64)$$

is given by

$$p(\mathbf{y}|\mathbf{X}) = \iint p(\mathbf{y}|\boldsymbol{\beta}, \sigma^2, \mathbf{X}) p(\boldsymbol{\beta}, \sigma^2) d\boldsymbol{\beta} d\sigma^2. \quad (65)$$

The marginal likelihood is a special case of the posterior predictive distribution in (??) when the posterior is based on $n = 0$ data points, i.e. when the parameters are integrated with respect to the prior, and the object of prediction is the training data \mathbf{y} ; for this reason, the marginal likelihood is sometimes called the **prior predictive distribution**. Note that the marginal likelihood is not measuring in-sample training error since the prediction for the training data \mathbf{y} is only using prior information for the model parameters $\boldsymbol{\beta}$ and σ^2 . Hence setting $n = 0$ and $\tilde{\mathbf{y}} = \mathbf{y}$ we immediately have the marginal likelihood for the linear regression model

$$\mathbf{y}|\mathbf{X} \sim t_{\nu_0} \left(\mathbf{x}\boldsymbol{\mu}_0, \sigma_0^2 (\mathbf{I}_n + \mathbf{X}\Omega_0^{-1}\mathbf{X}^\top) \right). \quad (66)$$

prior predictive distribution

Bayesian cross-validation

- M-completed? - Generalization performance.
- WAIC - Cross-validation

Variable selection

Gaussian processes

Gaussian processes

Mixture models

Finite mixtures

Mixtures of regressions

Latent Dirichlet allocation

Infinite mixtures

Dynamic models and sequential inference

Dynamic models

- Time-varying regression models
- State-space models (with control)

Bayesian filtering and smoothing

- The Kalman filter (Bayesian approach)
- Forward filtering backward smoothing

Sequential Monte Carlo

Basic particle filter

Sequential decision making

- Bayesian updating is key
- Markov Decision process
- Reinforcement learning
- Bellman's equation?

Bibliography

José M Bernardo and Adrian FM Smith. *Bayesian theory*, volume 405.

John Wiley & Sons, 2009.

George Casella and Roger L Berger. *Statistical inference*, volume 2.

Duxbury Pacific Grove, CA, 2002.

Dheeru Dua and Casey Graff. UCI machine learning repository, 2017.

URL <http://archive.ics.uci.edu/ml/datasets/Spambase/>.

Andrew Gelman, John B Carlin, Hal S Stern, David B Dunson, Aki Vehtari, and Donald B Rubin. *Bayesian data analysis*, volume 3rd edition. CRC press, 2013.

Telba Z Irony and Nozer D Singpurwalla. Non-informative priors do not exist - a dialogue with José M. Bernardo. *Journal of Statistical Planning and Inference*, 65(1):159–177, 1997.

Harold Jeffreys. *The theory of probability*. OUP Oxford, 1998.

Helio S Migon, Dani Gamerman, and Francisco Louzada. *Statistical inference: an integrated approach*. CRC press, 2014.

Rolf Sundberg. *Statistical modelling by exponential families*, volume 12. Cambridge University Press, 2019.

Mattias Villani. Steady-state priors for vector autoregressions. *Journal of Applied Econometrics*, 24(4):630–650, 2009.

Bertil Wegmann and Mattias Villani. Bayesian inference in structural second-price common value auctions. *Journal of Business & Economic Statistics*, 29(3):382–396, 2011.

Index

- action, 83
- autoregressive model, 58
- batch learning, 28
- Bayes estimator, 21
- Bayes' theorem, 15
- Bernoulli distribution, 10
- Bernoulli trials, 10
- Beta distribution, 19
- Binomial distribution, 12
- Birnbaum's theorem, 24
- Categorical data, 47
- central limit theorem, 47
- coefficient of variation, 46
- conjugate prior, 20, 31
- convergence in distribution, 46
- convergence in probability, 45
- covariates, 67
- credibility interval, 32
- decision making under uncertainty, 83
- dependent observations, 57
- dutch book argument, 14
- eBayCoin dataset, 29
- equal tail credibility interval, 32
- estimate, 11
- exponential family, 35
- Factorization criterion, 34
- features, 67
- Fisher information, 54
- Fisher information matrix, 54
- frequentist probability, 14
- Gamma distribution, 29
- Gaussian linear regression model, 67
- global shrinkage, 60
- hierarchical prior, 61
- Highest Posterior Density (HPD) region, 32
- homoscedastic, 67
- hyperparameters, 25
- iid, 10
- imaginary prior sample, 20
- improper prior, 64
- Internet speed dataset, 26, 42, 44
- invariant prior, 62
- inverse Gamma distribution, 41
- Jeffreys' prior, 62
- joint posterior distribution, 39
- lag length, 60
- lagged value, 58
- law of iterated expectation, 75
- law of large numbers, 45
- law of total probability, 15
- law of total variance, 75
- least squares estimator, 68
- license, 2
- likelihood function, 10
- Likelihood principle, 23
- likelihood surface, 39
- lin-lin utility, 87
- linear utility, 87
- long run properties, 12
- Markov Chain, 80
- Markov process, 80
- maximin rule, 85
- maximum likelihood estimator, 11
- mobile phone survey data, 48
- multi-class, 47
- multinomial distribution, 48
- multivariate student-*t* distribution, 78
- natural parameter, 35
- negative binomial distribution, 23
- nuisance parameters, 40
- observed information, 54
- observed information matrix, 54
- one-hot encoding, 47
- online learning, 27
- optimal Bayesian decision, 85
- ordinal data, 47
- other data, 59
- parameter space, 9
- past data, 59
- percentile, 87
- personal degree of belief, 14
- point estimate, 87
- Poisson distribution, 28
- posterior, 16
- posterior density, 17
- posterior draws, 44
- posterior expected utility, 85
- posterior median, 87
- posterior mode, 87
- prior, 16
- prior density, 17
- prior elicitation, 19
- prior predictive distribution, 97
- quadratic utility, 87
- reference prior, 64
- regression, 67
- regression coefficients, 67
- Regularization priors, 59
- residuals, 68

- response variable, 67
- sampling distribution, 12
- sampling variance, 12
- scaled inverse chi-squared distribution, 41
- separation principle, 86
- simulation consistent, 45
- smoothness beliefs, 60
- SpamBase dataset, 21
- stationary, 58
- steady-state form, 58
- stochastic process, 57
- student-*t* distribution, 35
- subjective consensus, 18
- subjective probability, 13
- Sufficiency principle, 34
- Sufficient statistic, 34
- time series, 57
- unbiased, 12
- uniform distribution, 19
- uniform distribution on the unit simplex, 49
- unit information prior, 70
- unit simplex, 49
- utility function, 84
- weights, 67
- zero sample prior, 61
- zero-one utility, 87