PSYC 573 Bayesian Data Analysis (2024 Fall): Course Notes

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Preface

There will be some math in this notes. Don't worry if you feel the math is challenging; for applied focused students, it is much more important to understand the concepts of Bayesian methods than to understand the mathematical symbols, as they usually can be handled by the software.

Part I

Week 1

1 Introduction

1.1 History of Bayesian Statistics

Here is a nice brief video that covers some of the 250+ years of history of Bayesian statistics:

https://www.youtube.com/watch?v=BcvLAw-JRss

If you are interested in learning more about the story, check out the popular science book, "The theory that would not die," by McGrayne (2011)

1.1.1 Thomas Bayes (1701–1762)

You may find a biography of Bayes from https://www.britannica.com/biography/Thomas-Bayes. There is also a nice story in the book by Lambert (2018). He was an English Presbyterian minister. The important work he wrote that founded Bayesian statistics was "An Essay Towards Solving a Problem in the Doctrine of Chances," which he did not publish and was later discovered and edited by his friend, Richard Price, after Bayes's death [1]

1.1.2 Pierre-Simon Laplace (1749–1827)

Laplace, a French Mathematician, was an important figure in not just Bayesian statistics but other areas of mathematics, astronomy, and physics. We know much more about the work by Laplace than by Bayes, and Laplace has worked independently on the inverse probability problem (i.e., P[Parameter|Data]). Indeed, he was credited for largely formalizing the Bayesian interpretation of probability and most of the machinery for Bayesian statistics, and making it a useful technique for different problems, despite the discipline being called "Bayesian." His other contributions include the methods of least squares and the central limit theorem. See a short biography of him at https://www.britannica.com/biography/Pierre-Simon-marquis-de-Laplace.

[1] Price is another important figure in mathematics and philosophy, and had taken Bayes' theorem and applied it to insurance and moral philosophy.

1.1.3 20th Century

Until the early 1920s, the *inverse probability* method, which is based on what is now called Bayes's Theorem, was pretty much the predominant point of view of statistics. Then a point of view later known as *frequentist* statistics arrived, and quickly became the mainstream school of thinking for statistical inferences, and is still the primary framework for quantitative research. In the early 1920s, frequentist scholars, most notably R. A. Fisher and Jerzy Neyman, criticized Bayesian inference for using subjective elements in an objective discipline. In Fisher's words,

> The theory of inverse probability is founded upon an error, and must be wholly rejected—Fisher, 1925

Ironically, the term *Bayesian* was first used in one of Fisher's works. And interestingly, Fisher actually thought he "[had] been doing almost exactly what Bayes had done in the 18th century."[2]

Despite criticisms from frequentist scholars, Bayesian methods have been used by scholars in the Allies in World War II, such as Alan Turing, in an algorithm to break coded messages in the Enigma machine that the German Navy used to communicate. However, because of the more complex mathematics involved in Bayesian statistics, Bayesian statistics is limited to straight-forward problems and theoretical discussions until the early 1980s, when computing speed increased tremendously and made *Markov Chain Monte Carlo*—the primary algorithm for Bayesian estimation in modern Bayesian statistics—feasible. With the help of increased computing speed, Bayesian statistics has come back and been used as an alternative way of thinking, especially given the growing dissatisfaction towards the misuse of frequentist statistics by some scholars across disciplines. Bayesian estimation methods have also been applied to many new research questions where frequentist approaches work less well, as well as in big data analytics and machine learning.

1.2 Motivations for Using Bayesian Methods

Based on my personal experience, Bayesian methods are used quite often in statistics and related departments, as it is consistent and coherent, in contrast to frequentist where a new and probably ad hoc procedure needed to be developed to handle a new problem. For Bayesian, as long as you can formulate a model, you just run the analysis the same way as you would for simpler problems, or in Bayesian people's words "turning the Bayesian crank," and likely the difficulties would be more technical than theoretical, which is usually solved with better computational speed.

Social and behavioral scientists are relatively slow to adopt the Bayesian method, but things have been changing. In a recently accepted paper by Van De Schoot et al. (2017), the authors

[2] See the paper by John Aldrich on this.

reviewed papers in psychology between 1990 and 2015 and found that whereas less than 10% of the papers from 1990 to 1996 mentioned "Bayesian", the proportion increased steadily and was found in close to 45% of the psychology papers in 2015. Among studies using Bayesian methods, more than 1/4 cited computational problems (e.g., nonconvergence) in frequentist methods as a reason, and about 13% cited the need to incorporate prior knowledge into the estimation process. The other reasons included the flexibility of Bayesian methods for complex and nonstandard problems, and the use of techniques traditionally attached to Bayesian such as missing data and model comparisons.

1.2.1 Problem with classical (frequentist) statistics

The rise of Bayesian methods is also related to the statistical reform movement in the past two decades. The problem is that applied researchers are obsessed with $p < .05$ and often misinterpreted a small p-value as something that it isn't (read Gigerenzer, 2004). Some scholars coined the term p-hacking to refer to the practice of obtaining statistical significance by choosing to test the data in a certain way, either consciously or subconsciously (e.g., dichotomizing using mean or median, trying the same hypothesis using different measures of the same variable, etc). This is closely related to the recent "replication crisis" in scientific research, with psychology being in the center under close scrutiny.

Bayesian is no panacea to the problem. Indeed, if misused, it can give rise to the same problems as statistical significance. My goal in this class is to help you appreciate the Bayesian tradition of embracing the uncertainty in your results, and adopt rigorous model checking and comprehensive reporting rather than relying merely on a p-value. I see this as the most important mission for someone teaching statistics.

1.3 Comparing Bayesian and Frequentist Statistics

Attributes	Frequentist	Bayesian
Interpretation of probability	Frequentist	Subjectivist
Uncertainty	How estimates vary in repeated sampling from the same population	How much prior beliefs about parameters change in light of data
What's relevant?	Current data set + all that might have been observed	Only the data set that is actually observed
How to proceed with analyses	MLE; ad hoc and depends on problems	"Turning the Bayesian crank"

1.4 Software for Bayesian Statistics

The following summarizes some of the most popular Bayesian software. Currently, JAGS and Stan are the most popular. General statistical programs like SPSS, SAS, and Stata also have some support for Bayesian analyses as well.

- WinBUGS
  - Bayesian inference Using Gibbs Sampling
  - Free, and most popular until late 2000s. Many Bayesian scholars still use WinBUGS
  - No further development
  - One can communicate from R to WinBUGS using the package `R2WinBUGS`
- JAGS
  - Just Another Gibbs Sampler
  - Very similar to WinBUGS, but written in C++, and supports user-defined functionality
  - Cross-platform compatibility
  - One can communicate from R to JAGS using the package `rjags` or `runjags`
- Stan
  - Named in honour of Stanislaw Ulam, who invented the Markov Chain Monte Carlo method
  - Uses new algorithms that are different from Gibbs sampling
  - Under very active development
  - Can interface with R through the package `rstan`, and the R packages `rstanarm` and `brms` automates the procedure for fitting models in Stan for many commonly used models

Part II

Week 2

2 Probability

2.1 History of Probability

2.1.1 Games of chance

Correspondence between French Mathematicians (Pierre de Fermat and Blaise Pascal) on gambling problem by Antoine Gombaud, Chevalier de Méré. The problem is roughly of the form[1]:

> Imagine two people playing a multi-round game. In each round, each person has an equal chance of winning. The first person who wins six rounds will get a huge cash prize. Now, consider a scenario in which A and B have played six rounds, where A has won five and B has won one. At that time, the game had to be stopped due to a thunderstorm. Since neither A nor B have reached six wins, instead of giving the prize to either one of them, they agree to divide up the prize. What would be a fair way to do so?

The discussion led to the formalization of using mathematics to solve the problem. Basically, one way is to say if A has a 97% chance of winning the prize eventually and B has a 3% chance, then A should get 97% of the prize.

2.2 Different Ways to Interpret Probability

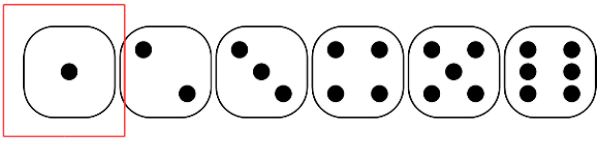
There are multiple perspectives for understanding probability.[2] What you've learned in your statistics training is likely based on the *frequentist* interpretation of probability (and thus frequentist statistics), whereas the foundation of what you will learn in this class is the *subjectivist* interpretation of probability. Understanding the different perspectives on probability is helpful for understanding the Bayesian framework.

You don't need to commit to one interpretation of probability in order to conduct Bayesian data analysis.

[1] see the exact form at https://en.wikipedia.org/wiki/Problem_of_points
[2] See http://plato.stanford.edu/entries/probability-interpret/ for more information

2.2.1 Classical Interpretation

This is an earlier perspective and is based on counting rules. The idea is that probability is equally distributed among all "indifferent" outcomes. "Indifferent" outcomes are those where a person has no evidence to say that one outcome is more likely than another. For example, when one throws a die, one does not think that a certain number is more likely than another unless one knows that the die is biased. In this case, there are six equally likely outcomes, so the probability of each outcome is 1 / 6.



2.2.2 Frequentist Interpretation

The frequentist interpretation states that probability is essentially the long-run relative frequency of an outcome. For example, to find the probability of getting a "1" when throwing a die, one can repeat the experiment many times, as illustrated below:

Trial	Outcome
1	2
2	3
3	1
4	3
5	1
6	1
7	5
8	6
9	3
10	3

And we can plot the relative frequency of "1"s in the trials:

As you can see, with more trials, the relative frequency approaches 1 / 6. It's the reason why in introductory statistics, many of the concepts require you to think in terms of repeated sampling (e.g., sampling distribution, p-values, standard errors, confidence intervals), because

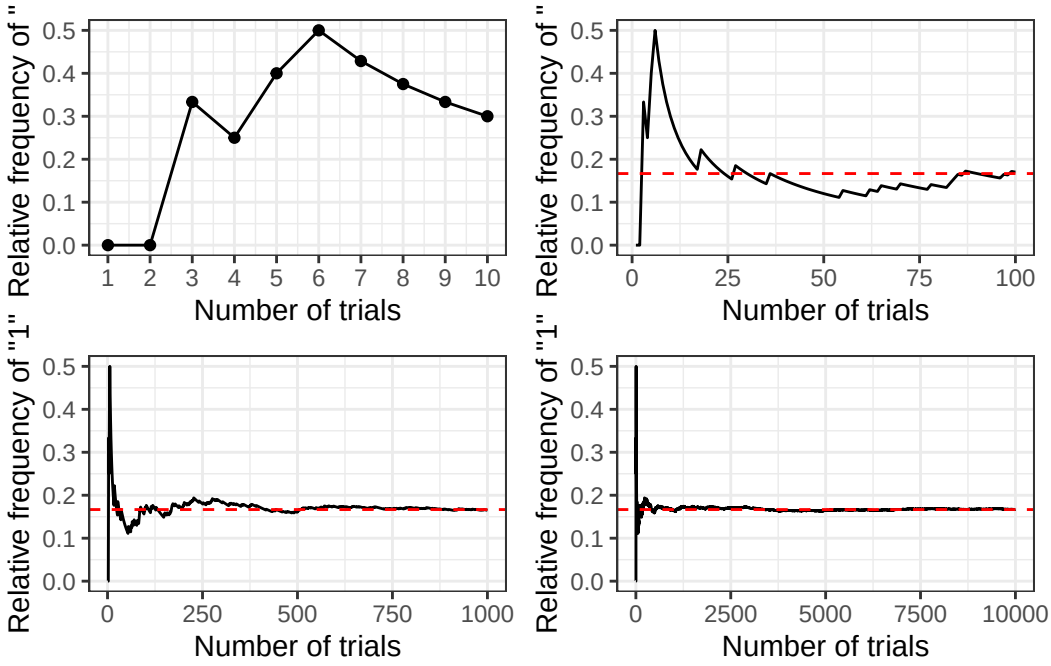


Figure 2.1: Relative frequency when repeatedly rolling a die.

probability in this framework is only possible when the outcome can be repeated. It's also the reason why we don't talk about something like:

- the probability of the null hypothesis being true, or
- the probability that the population mean is in the interval [75.5, 80.5],

because the population is fixed and cannot be repeated. Only the samples can be repeated, so probability in frequentist statistics is only about samples.

2.2.2.1 Problem of the single case

Because of the frequentist's reference to long-run relative frequency, it does not make sense to talk about the probability of an event that cannot be repeated under this framework. For example, it does not make sense to talk about

- the probability that the Democrats/Republicans will win the 2028 US Presidential Election, or
- the probability that the LA Chargers winning the 2024 Super Bowl, or
- the probability that it will rain on Christmas Day in LA in 2024,

because all these are specific events that cannot be repeated. However, it is common for laypeople to talk about probabilities or chances for these events.

2.2.3 Subjectivist Interpretation

The frequentist interpretation is sometimes called the "objectivist view," as the reference of probability is based on empirical evidence of long-run relative frequency (albeit hypothetical in many cases). In contrast, the *subjectivist* view of probability is based on one's belief. For example, when I say that the probability of getting a "1" from rolling a die is 1 / 6, it reflects the state of my mind about the die. My belief can arise from different sources: Maybe I make the die and know it is a fair one; maybe I saw someone throwing the die 1,000 times, and the number of "1"s was close to 1,000 / 6, or maybe someone I trust and with authority says that the die has a 1-in-6 chance of showing a "1".

The "subjective" component has been criticized a lot by frequentist scholars, sometimes unfairly. To be clear, what "subjective" here means is that probability reflects the state of one's mind instead of the state of the world, and so it is totally fine that two people can have different beliefs about the same event. However, it does not mean that probability is arbitrary, as the beliefs are subjected to the constraints of the axioms of probability as well as the condition that the person possessing such beliefs is *rational*.[3] Therefore, if two persons are exposed to the same information, they should form similar, though likely not identical, beliefs about the event.

The subjective interpretation works perfectly fine with single events, as one can have a belief about whether it rains on a particular day or a belief about a particular election result.

2.2.3.1 Calibrating a subjective belief

In order to represent one's belief by probability, one needs to assign a nonzero value to every plausible outcome of an event. This has been the job of odds-makers for a long time. Indeed, a lot of the development in the field of probability has to do with coming up with a fair bet. The process of assigning probabilities to outcomes of an event according to one's belief is called *calibration*. For example, consider three possible outcomes for tomorrow's weather. For simplicity, consider three mutually exclusive possible outcomes: sunny, cloudy, and rainy.

To calibrate my belief, consider first if you bet \$10, and the return is (a) \$30 for sunny, (b) \$30 for cloudy, and (c) \$30 for rainy. Which one will you bet? If you're like me in LA, I'm pretty sure I'll bet on (a), as I think that it is more likely to have a sunny day. This means that setting $P(\text{sunny}) = P(\text{cloudy}) = P(\text{rainy}) = 1 / 3$ is not a good reflection of my belief.

[3] In a purely subjectivist view of probability, assigning a probability P to an event does not require any justifications, as long as it follows the axioms of probability. For example, I can say that the probability of me winning the lottery and thus becoming the wealthiest person on earth tomorrow is 95%, which by definition would make the probability of me not winning the lottery 5%. Most Bayesian scholars, however, do not endorse this version of subjectivist probability and require justifications of one's beliefs (that have some correspondence to the world).

Now consider the bet with the returns (a) \$20 for sunny, (b) \$30 for cloudy, and (c) \$60 for rainy. This would reflect the belief that there is a 50% chance of a sunny day, 33.33% chance of a cloudy day, and 16.67% chance of a rainy day. Will you take the bet? This is an improvement from the last one, but I would still say a sunny day is a good bet, which suggests that the probability of 50% is too low for a sunny day. The idea is to continue iterating until it is hard to consider (a), (b), or (c) as a clear betting favorite. For me, this would end up being something like (a) \$16.7 for sunny, (b) \$33.3 for cloudy, and (c) \$100 for rainy, which would correspond to 60% sunny, 30% cloudy, and 10% rainy.

If it's hard for you to consider the gambling analogy, an alternative way is to consider how many times is a sunny day more likely than a non-sunny day, and how many times is a cloudy day more likely than a rainy day. For example, I may consider a sunny day to be twice as likely as a non-sunny day, which would give the probability of a sunny day to be 66.67%. Then, if I also think that a cloudy day is three times as likely as a rainy day, I would assign a probability of $33.33\% \times 3 \,/\, 4 = 25\%$ for a cloudy day, and a probability of $33.33\% \times 1 \,/\, 4 = 8.33\%$ for a rainy day.

The process of calibrating one's belief plays a key role in Bayesian data analysis, namely in the form of formulating a *prior* probability distribution.

2.3 Basics of Probability

Kolmogorov axioms

For an event A_i (e.g., getting a "1" from throwing a die)

- $P(A_i) \geq 0$ [All probabilities are non-negative]
- $P(A_1 \cup A_2 \cup \cdots) = 1$ [Union of all possibilities is 1]
- $P(A_1) + P(A_2) = P(A_1 \text{ or } A_2)$ [Addition rule]

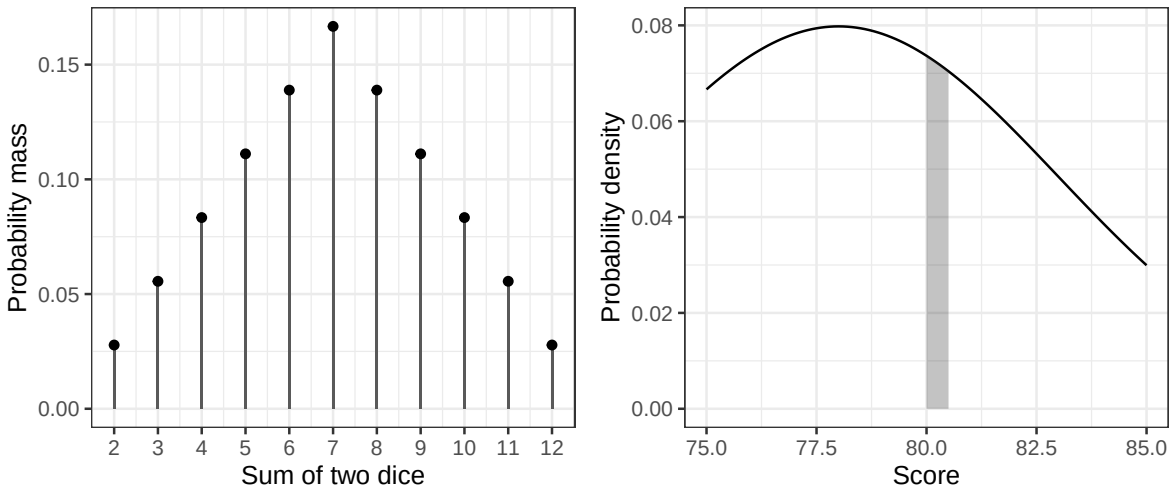
Consider two events, for example, on throwing a die,

- A: The number is odd
- B: The number is larger than or equal to 4

Assuming that die is (believed to be) fair, you can verify that the probability of A is $P(A) = 3 \,/\, 6 = 1 \,/\, 2$, and the probability of B is also $P(B) = 3 \,/\, 6 = 1 \,/\, 2$.

2.3.1 Probability Distributions

- Discrete event (e.g., the outcome of throwing a die or an election): probability *mass*. The probability is nonzero, at least for some outcomes. The graph below on the left shows the probability mass of the sum of the numbers from two dice.
- Continuous event (e.g., temperature): probability *density*.[4] The probability is basically zero for any outcome. Instead, the probability density is approximated by $P(A \leq a \leq A + h)/h$ for a very small h.
  - For example, to find the probability density that a person's well-being score is 80, we first find the probability that a person scores between 80 and 80.5 (or 80 and 80.0005), and divide that probability by 0.5 (or 0.0005). See the shaded area of the graph below on the right.



(a) Probability mass

(b) Probability density

Figure 2.2: Examples of probability distributions

> **i** For this course, as in the textbook, we use $P(x)$ to mean both the probability mass for an outcome x when the event is discrete, and the probability density at an outcome x when the event is continuous.

[4] For many problems in the social and behavioral sciences, the measured variables are not truly continuous, but we still use continuous distributions to approximate them.

2.3.1.1 Example: Normal Distribution

$$P(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2}\left[\frac{x-\mu}{\sigma}\right]^2\right)$$

```
# Write a function to compute the density of an outcome x
# for a normal distribution
my_normal_density <- function(x, mu, sigma) {
    exp(- ((x - mu) / sigma) ^2 / 2) / (sigma * sqrt(2 * pi))
}
# For example, density at x = 36 in a normal distribution
# with mu = 50 and sigma = 10
my_normal_density(36, mu = 50, sigma = 10)
```

```
#> [1] 0.01497275
```

2.3.2 Summarizing a Probability Distribution

While it is useful to know the probability mass/density of every possible outcome, in many situations, it is helpful to summarize a distribution by some numbers.

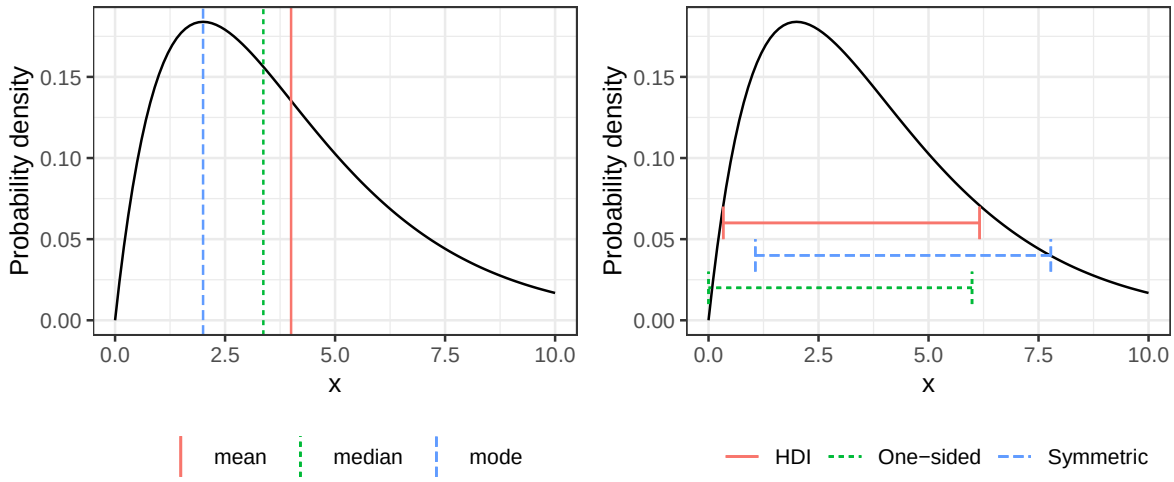
2.3.2.1 Central Tendency

- Mean: $E(X) = \int x \cdot P(x)dx$
- Median: 50th percentile; the median of X is Mdn_X such that $P(X \leq Mdn_X) = 1 \ / \ 2$
- Mode: A value with maximum probability mass/density

See Figure 2.3a for examples.

2.3.2.2 Dispersion

- Variance: $V(X) = E[X - E(X)]^2$
  - Standard deviation: $\sigma(X) = \sqrt{V(X)}$
- Median absolute deviation (MAD): $1.4826 \times Mdn(|X - Mdn_X|)$



(a) Central Tendency

(b) Interval

Figure 2.3: Measures of central tendency and interval

2.3.2.3 Interval

Use $C(X)$ to denote an interval. A $W\%$ interval means $P(X \in C[X]) \approx W\%$

- One-sided interval: $C(X)$ is half-bounded
- Symmetric $W\%$ interval: $C(X) = [L(X), U(X)]$ is bounded, with $P(X < L[X]) = P(X > U[X]) \approx W\%/2$
  - Also called *equal-tailed* interval
- Highest density $W\%$ interval (HDI): $P(x_c) \geq P(x_o)$ for every x_c in $C(X)$ and every x_o outside $C(X)$. In general, the HDI is the shortest $W\%$ interval.

The plot in Figure 2.3b shows several 80% intervals.

2.3.2.4 Computing Summaries of Sample Distributions Using R

```
# Simulate data from a half-Student's t distribution with
# df = 4, and call it sim_s
sim_s <- rt(10000, df = 4) # can be both positive and negative
sim_s <- abs(sim_s) # take the absolute values
ggplot(data.frame(x = sim_s), aes(x = x)) +
    geom_histogram(binwidth = 0.1)
```

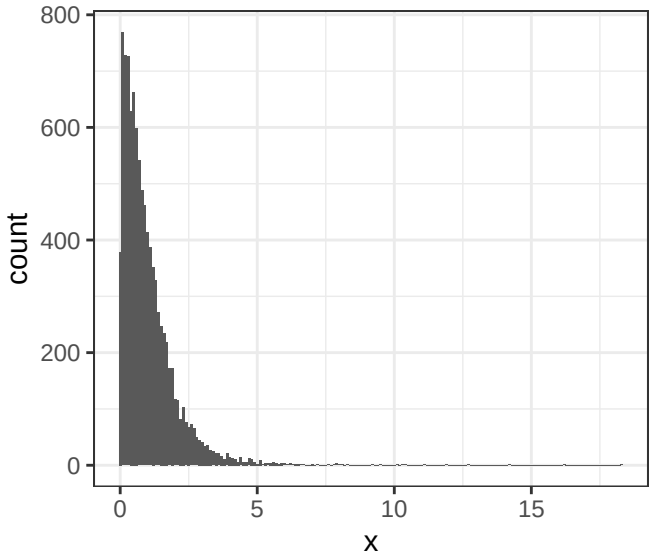


Figure 2.4: Simulated density of a half-Student's t distribution

```
# Central tendency
# (note: the mode is difficult to compute for continuous
# variables, and rarely used in this course.)
c(mean = mean(sim_s),
  median = median(sim_s),
  mode = density(sim_s, bw = "SJ")$x[
      which.max(density(sim_s, bw = "SJ")$y)
  ])
```

```
#>      mean    median      mode
#> 1.0082926 0.7426326 0.1021776
```

```
# Dispersion
c(
    variance = var(sim_s),
    sd = sd(sim_s),
    mad = mad(sim_s)
)
```

```
#>  variance        sd       mad
#> 1.0231058 1.0114869 0.6996741
```

```r
# 80% Interval
c(`0%` = 0, quantile(sim_s, probs = .8)) # right-sided
```

```
#>     0%    80%
#> 0.0000 1.5598
```

```r
c(quantile(sim_s, probs = .2), `100%` = Inf) # left-sided
```

```
#>       20%      100%
#> 0.2680906       Inf
```

```r
quantile(sim_s, probs = c(.1, .9)) # equal-tailed/symmetric
```

```
#>       10%       90%
#> 0.1299027 2.1371636
```

```r
HDInterval::hdi(sim_s)
```

```
#>        lower        upper
#> 0.0003616342 2.7992620765
#> attr(,"credMass")
#> [1] 0.95
```

2.3.3 Multiple Variables

- Joint probability: $P(X, Y)$
- Marginal probability:

$$P(X) = \int P(X, y)dy$$

$$P(Y) = \int P(x, Y)dx$$

  - The probability that outcome X happens, regardless of what values Y take.

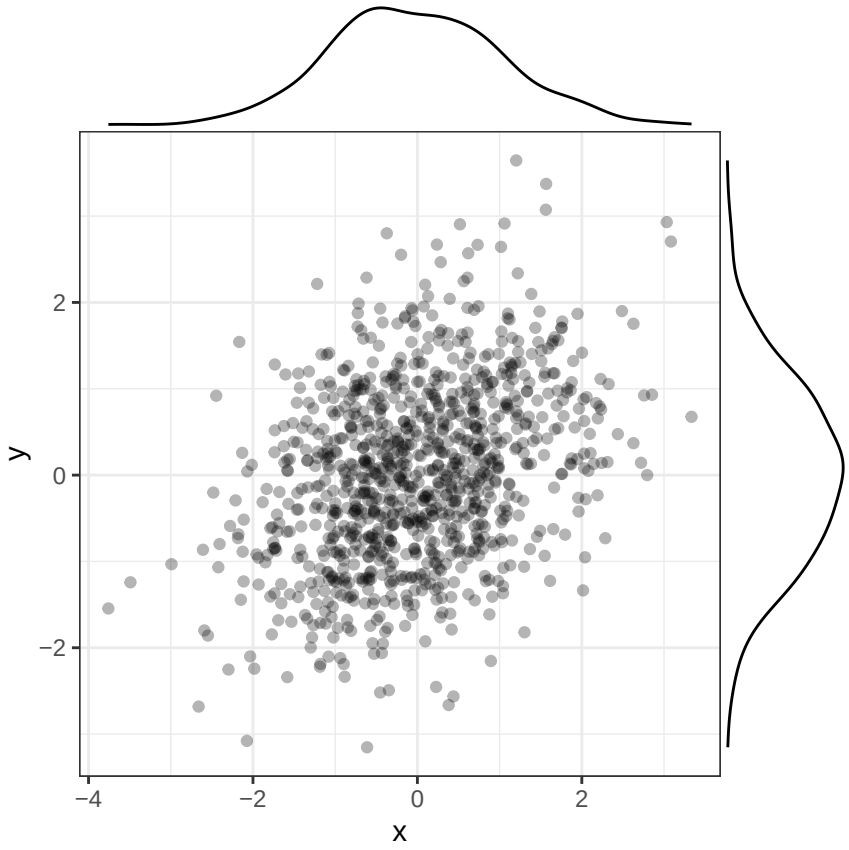


Figure 2.5: Joint and Marginal Distributions

2.3.3.1 Conditional Probability

Conditional probability is the probability of an event given some other information. In the real world, you can say that everything is conditional. For example, the probability of getting an odd number on throwing a die is 1/2 is conditional on the die being fair. We use $P(A \mid B)$ to represent the the conditional probability of event A given event B..

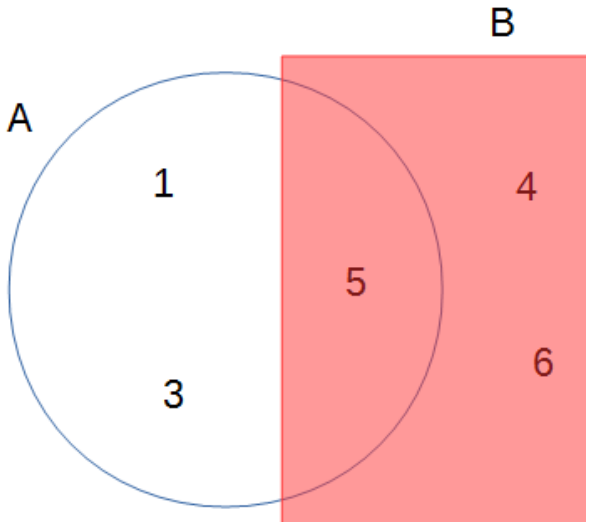
Continuing from the previous example, $P(A \mid B)$ is the conditional probability of getting an odd number, *knowing that the number is at least 4*. By definition, conditional probability is the probability that both A and B happen, divided by the probability that B happens.

> **!** **Conditional Probability**
>
> $$P(A \mid B) = \frac{P(A, B)}{P(B)}$$

In the example, $P(A, B) = 1 \ / \ 6$, because 5 is the only even number ≥ 4 when throwing a die. Thus,

$$\begin{aligned} P(A \mid B) &= 1/3 \\ &= \frac{P(A, B)}{P(B)} \\ &= \frac{1/6}{1/2} \end{aligned}$$

This picture should make it clear:



> ! Please recognize that $P(A \mid B) \neq P(B \mid A)$. For example, when throwing a die, $P(\text{number is six} \mid \text{even number}) = 1/3$, but $P(\text{even number} \mid \text{number is six})$ is 1.

2.3.3.2 Independence

> ! Two events, A and B, are independent if $P(A \mid B) = P(A)$

This means that any knowledge of B does not (or should not) affect one's belief about A. Consider the example:

- A: A die shows five or more
- B: A die shows an odd number

Here is the joint probability

	>= 5	<= 4
odd	1/6	2/6
even	1/6	2/6

So the conditional probability of $P(>= 5 \mid \text{odd}) = (1/6) / (1/2) = 1/3$, which is the same as $P(>= 5 \mid \text{even}) = (1/6) / (1/2) = 1/3$. Similarly it can be verified that $P(<= 4 \mid \text{odd}) = P(<= 4 \mid \text{even}) = 2/3$. Therefore, A and B are independent.

On the other hand, for the example

- A: A die shows four or more
- B: A die shows an odd number

the joint probabilities are

	>= 4	<= 3
odd	1/6	2/6
even	2/6	1/6

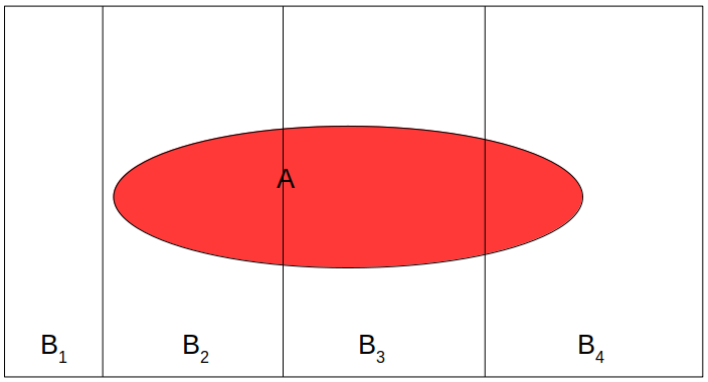
Obviously, A and B are not independent because once we know that the number is four or above, the probability of whether it is an odd number or not changes.

! Independence can also be expressed as

If A and B are independent, $P(A, B) = P(A)P(B)$

2.3.4 Law of Total Probability

When we talk about conditional probability, like $B_1 = 4$ or above and $B_2 = 3$ or below, we can get $P(A \mid B_1)$ and $P(A \mid B_2)$ (see the figure below), we refer $P(A)$ as the *marginal probability*, meaning that the probability of A without knowledge of B.



If $B_1, B_2, \cdots, B_n$ are all mutually exclusive possibilities for an event (so they add up to a probability of 1), then

! **Law of Total Probability**

$$\begin{aligned} P(A) &= P(A, B_1) + P(A, B_2) + \cdots + P(A, B_n) \\ &= P(A \mid B_1)P(B_1) + P(A \mid B_2)P(B_2) + \cdots + P(A \mid B_n)P(B_n) \\ &= \sum_{k=1}^{n} P(A \mid B_k)P(B_k) \end{aligned}$$

3 Bayes's Theorem

The Bayes's theorem is, surprisingly (or unsurprisingly), very simple:

$$P(B \mid A) = \frac{P(A \mid B)P(B)}{P(A)}$$

More generally, we can expand it to incorporate the law of total probability to make it more applicable to data analysis. Consider B_i as one of the n many possible mutually exclusive events, then

$$\begin{aligned} P(B_i \mid A) &= \frac{P(A \mid B_i)P(B_i)}{P(A)} \\ &= \frac{P(A \mid B_i)P(B_i)}{P(A \mid B_1)P(B_1) + P(A \mid B_2)P(B_2) + \cdots + P(A \mid B_n)P(B_n)} \\ &= \frac{P(A \mid B_i)P(B_i)}{\sum_{k=1}^{n} P(A \mid B_k)P(B_k)} \end{aligned}$$

If B_i is a continuous variable, we will replace the sum by an integral,

$$P(B_i \mid A) = \frac{P(A \mid B_i)P(B_i)}{\int_k P(A \mid B_k)P(B_k)}$$

The denominator is not important for practical Bayesian analysis, therefore, it is sufficient to write the above equality as

$$P(B_i \mid A) \propto P(A \mid B_i)P(B_i)$$

3.1 Example 1: Base rate fallacy (From Wikipedia)

3.1.1 Question

A police officer stops a driver *at random* and does a breathalyzer test for the driver. The breathalyzer is known to detect true drunkenness 100% of the time, but in 1% of the cases, it

gives a false positive when the driver is sober. We also know that, in general, for every 1,000 drivers passing through that spot, one is driving drunk. Suppose that the breathalyzer shows positive for the driver. What is the probability that the driver is truly drunk?

3.1.2 Solution

$P(\text{positive}|\text{drunk}) = 1$
$P(\text{positive}|\text{sober}) = 0.01$
$P(\text{drunk}) = 1/1000$
$P(\text{sober}) = 999/1000$

Using Bayes' Theorem,

$$\begin{aligned} P(\text{drunk}|\text{positive}) &= \frac{P(\text{positive}|\text{drunk})P(\text{drunk})}{P(\text{positive}|\text{drunk})P(\text{drunk}) + P(\text{positive}|\text{sober})P(\text{sober})} \\ &= \frac{1 \times 0.001}{1 \times 0.001 + 0.01 \times 0.999} \\ &= 100/1099 \approx 0.091 \end{aligned}$$

So there is less than a 10% chance that the driver is drunk even when the breathalyzer shows positive.

You can verify that with a simulation using R:

```
set.seed(4)
truly_drunk <- c(rep("drunk", 100), rep("sober", 100 * 999))
table(truly_drunk)
```

```
#> truly_drunk
#> drunk sober
#>   100 99900
```

```
breathalyzer_test <- ifelse(truly_drunk == "drunk",
    # If drunk, 100% chance of showing positive
    "positive",
    # If not drunk, 1% chance of showing positive
    sample(c("positive", "negative"), 999000,
        replace = TRUE, prob = c(.01, .99)
    )
)
# Check the probability p(positive | sober)
table(breathalyzer_test[truly_drunk == "sober"])
```

```
#>
#> negative positive
#>    98903      997
```

```
# 997 / 99900 = 0.00997998, so the error rate is less than 1%
# Now, Check the probability p(drunk | positive)
table(truly_drunk[breathalyzer_test == "positive"])
```

```
#>
#> drunk sober
#>   100   997
```

```
# 100 / (100 + 997) = 0.0911577, which is only 9.1%!
```

3.2 Bayesian Statistics

`Bayesian statistics` is a way to estimate some parameter θ (i.e., some quantities of interest, such as the population mean, regression coefficient, etc) by applying Bayes' Theorem.

$$P(\theta|D) \propto P(D|\theta)P(\theta)$$

There are three components in the above equality:

- $P(D|\theta)$, the probability that you observe data D, given the parameter θ; this is called the `likelihood` (Note: It is the likelihood of θ, but probability about y)
- $P(\theta)$, the probability distribution θ, without referring to the data D. This usually requires appeals to one's degree of belief, and so is called the *prior*
- $P(\theta|y)$, the updated probability distribution of θ, after observing the data D; this is called the *posterior*

On the other hand, classical/frequentist statistics focuses solely on the likelihood function.[1] In Bayesian statistics, the goal is to update one's belief about θ based on the observed data D.

[1]The likelihood function in classical/frequentist statistics is usually written as $P(y;\theta)$. You will notice that here, I write the likelihood for classical/frequentist statistics to be different from the one used in Bayesian statistics. This is intentional: In frequentist conceptualization, θ is fixed, and it does not make sense to talk about the probability of θ. This implies that we cannot condition on θ, because conditional probability is defined only when $P(\theta)$ is defined.

3.3 Example 2: Locating a Plane

Consider a highly simplified scenario of locating a missing plane in the sea. Assume that we know the plane, before missing, happened to be flying at the same latitude, heading west across the Pacific, so we only need to find its longitude. We want to go out to collect debris (data) so that we can narrow the location (θ) of the plane down.

3.3.1 Prior

We start with our prior. Assume that we have some rough idea where the plane should be, so we express our belief in a probability distribution like the following:

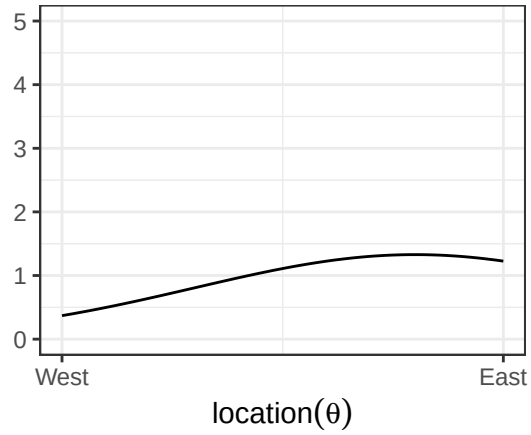


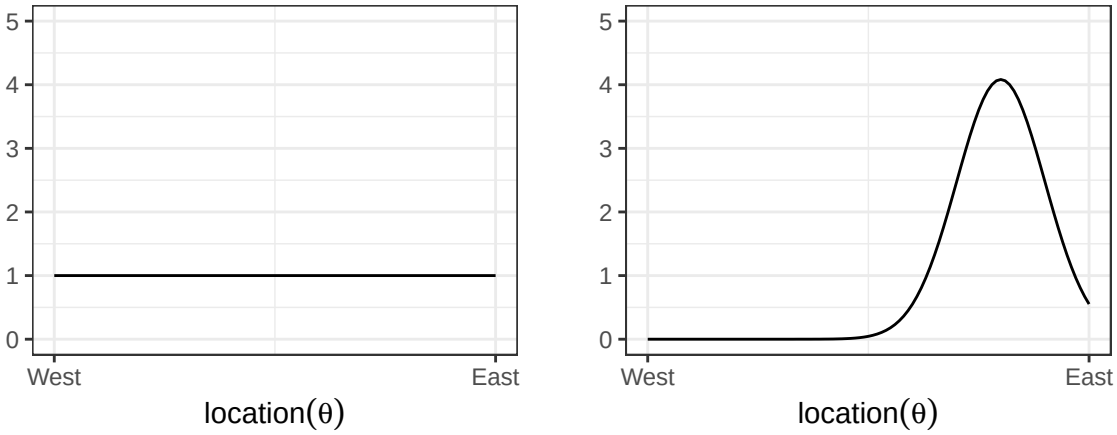
Figure 3.1: Prior distribution.

which says that our belief is that the plane is about twice more likely to be towards the east than towards the west. Below are two other options for priors (out of infinitely many), one providing virtually no information and the other encoding stronger information:

The prior is chosen to reflect the researcher's belief, so different researchers will likely formulate a different prior for the same problem, and that's okay as long as the prior is reasonable and justified. Later, we will learn that in regular Bayesian analyses, with a moderate sample size, different priors generally only make negligible differences.

3.3.2 Likelihood

Now, assume that we have collected debris in the locations shown in the graph,



(a) Noninformative prior.

(b) Informative prior.

Figure 3.2: More options for prior distribution.

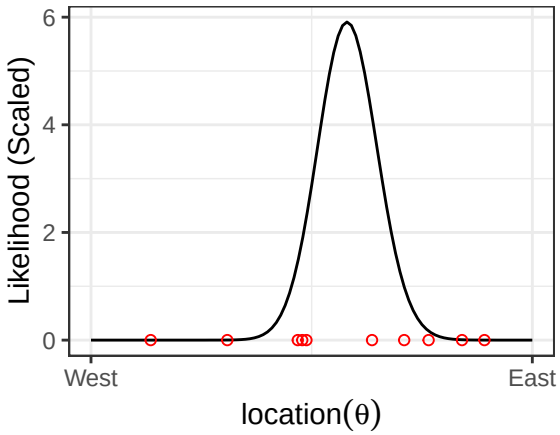


Figure 3.3

3.3.3 Posterior

Now, from Bayes's Theorem,

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

So we can simply multiply the prior probabilities and the likelihood to get the posterior probability for every location. A rescaling step is needed to ensure that the area under the curve will be 1, which is usually performed by the software.

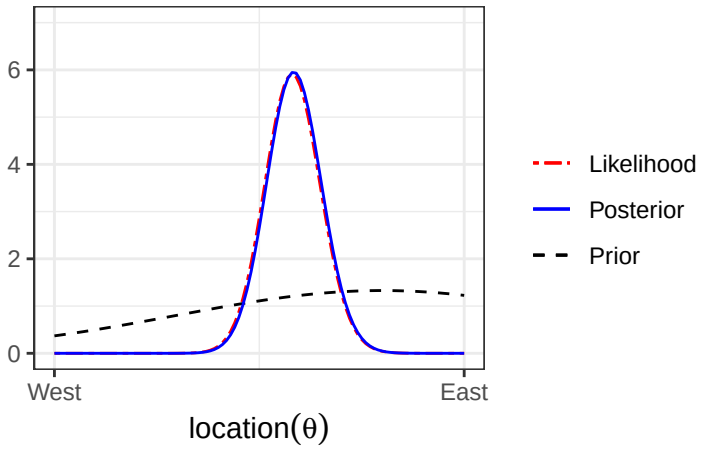


Figure 3.4

As illustrated below, the posterior distribution is a synthesis of (a) the prior and (b) the data (likelihood).

3.3.4 Influence of Prior

Figure 3.5 shows what happen with a stronger prior:

3.3.5 Influence of More Data

Figure 3.6 shows what happen with 20 more data points:

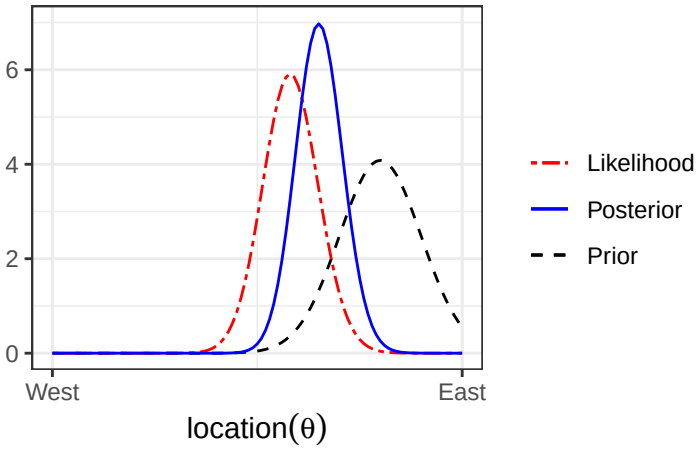


Figure 3.5

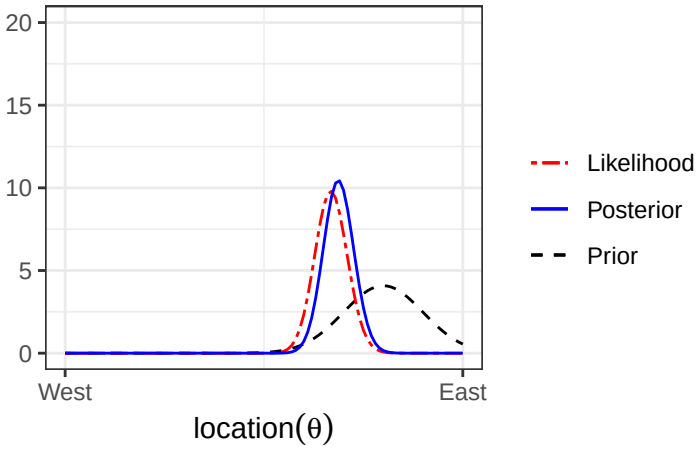


Figure 3.6

3.4 Data-Order Invariance

In many data analysis applications, researchers collect some data D_1, and then collect some more data D_2. An example would be researchers conducting two separate experiments to study the same research question. In Bayesian statistics, one can consider three ways to obtain the posterior:

1. Update the belief with D_1, and then with D_2
2. Update the belief with D_2, and then with D_1
3. Update the belief with both D_1 and D_2 simultaneously

Whether these three ways give the same posterior depends on whether **data-order invariance** holds. If the inference of D_1 does not depend on D_2, or vice versa, then all three ways lead to the same posterior. Specifically, if we have **conditional independence** such that

$$P(D_1, D_2 \mid \theta) = P(D_1 \mid \theta)P(D_2 \mid \theta),$$

then one can show all three ways give the same posterior (see section 4.4 and 4.5 of Johnson et al., 2022).

Exchangeability*

Exchangeability is an important concept in Bayesian statistics. Data are exchangeable when the joint distribution, $P(D_1, \ldots, D_N)$, does not depend on the ordering of the data. A simple way to think about it is if you scramble the order of your outcome variable in your data set and still can obtain the same statistical results, then the data are exchangeable. An example situation where data are not exchangeable is

- D_1 is from year 1990, D_2 is from year 2020, and the parameter θ changes from 1990 to 2020

When data are exchangeable, conditional independence would generally hold.[2]

3.5 Bernoulli Likelihood

For binary data y (e.g., coin flip, pass/fail, diagnosed/not), an intuitive way to analyze is to use a Bernoulli model:

$$P(y = 1 \mid \theta) = \theta$$
$$P(y = 0 \mid \theta) = 1 - \theta\text{'}$$

[2]The de Finetti's theorem shows that when the data are exchangeable and can be considered an infinite sequence (i.e., not from a tiny finite population), then the data are conditionally independent given some θ.

which is more compactly written as

$$P(y \mid \theta) = \theta^y (1-\theta)^{(1-y)},$$

where $\theta \in [0, 1]$ is the probability of a "1". You can verify that the compact form is the same as the longer form.

3.5.1 Multiple Observations

When there are more than one y, say $y_1, \ldots, y_N$, that are conditionally independent, we have

$$\begin{aligned} P(y_1, \ldots, y_N \mid \theta) &= \prod_{i=1}^{N} P(y_i \mid \theta) \\ &= \theta^{\sum_{i=1}^{N} y_i} (1-\theta)^{\sum_{i=1}^{N} (1-y_i)}, \\ &= \theta^z (1-\theta)^{N-z} \end{aligned}$$

where z is the number of "1"s (e.g., the number of heads in coin flips). Note that the likelihood only depends on z, not the individual ys. In other words, the likelihood is the same as long as there are z heads, regardless of when those heads occur.

Let's say $N = 4$ and $z = 1$. We can plot the likelihood in R:

```
# Write the likelihood as a function of theta
lik <- function(th, num_flips = 4, num_heads = 1) {
    th ^ num_heads * (1 - th) ^ (num_flips - num_heads)
}
# Likelihood of theta = 0.5
lik(0.5)
```

```
#> [1] 0.0625
```

```
# Plot the likelihood
ggplot(data.frame(th = c(0, 1)), aes(x = th)) +
    # `stat_function` for plotting a function
    stat_function(fun = lik) +
    # use `expression()` to get greek letters
    labs(x = expression(theta),
    y = "Likelihood with N = 4 and z = 1")
```

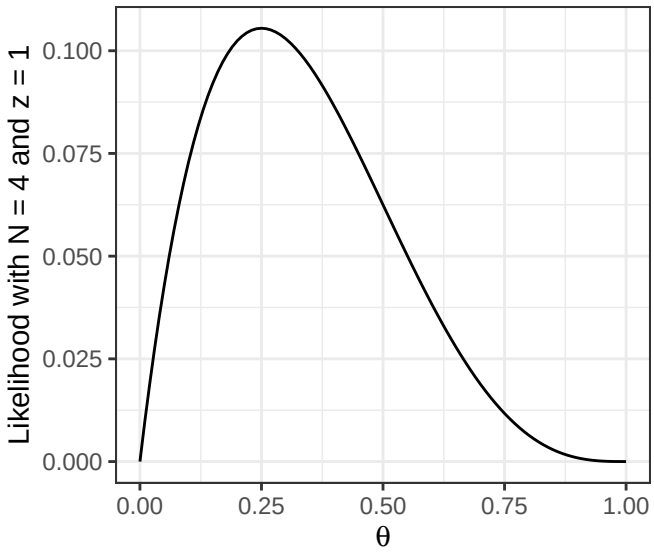


Figure 3.7: Binomial likelihood function with $N = 4$ and $z = 1$

3.5.2 Setting Priors

Remember again the relationship between the prior and the posterior:

$$P(\theta|y) \propto P(y|\theta)P(\theta)$$

The posterior distributions are mathematically determined once the priors and the likelihood are set. However, the mathematical form of the posterior is sometimes very difficult to deal with.

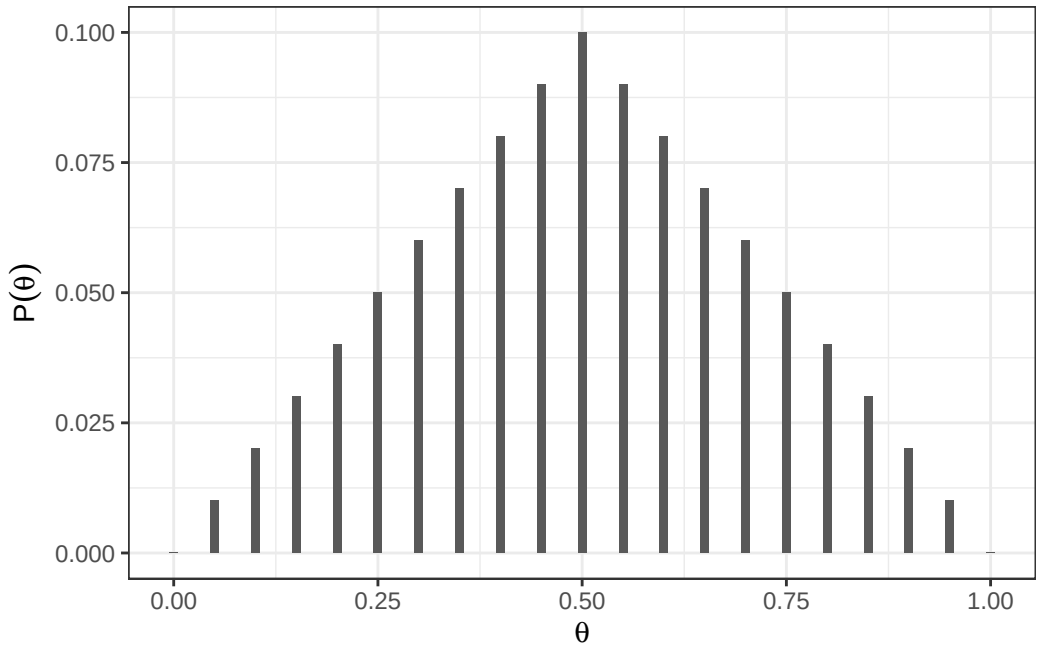
One straightforward, brute-force method is to discretize the parameter space into a number of points. For example, by taking $\theta = 0, 0.05, 0.10, \ldots, 0.90, 0.95, 1.00$, one can evaluate the posterior at these 21 **grid points**.

Let's use a prior that peaks at 0.5 and linearly decreases to both sides. I assume that $\theta = 0.5$ is twice as likely as $\theta = 0.25$ or $\theta = 0.75$ to reflect my belief that the coin is more likely to be fair.

```
# Define a grid for the parameter
grid_df <- data.frame(th = seq(0, 1, by = 0.05))
# Set the prior mass for each value on the grid
grid_df$pth <- c(0:10, 9:0)  # linearly increasing, then decreasing
# Convert pth to a proper distribution such that the value
# sum to one
```

```r
grid_df$pth <- grid_df$pth / sum(grid_df$pth)                                    ①
# Plot the prior
ggplot(grid_df, aes(x = th, y = pth)) +
    geom_col(aes(x = th, y = pth),
        width = 0.01,
    ) +
    labs(y = expression(P(theta)), x = expression(theta))
```

① This line ensures that the probability values sum to one. This is a trick we will use to obtain the posterior probability.



Prior Predictive Distribution

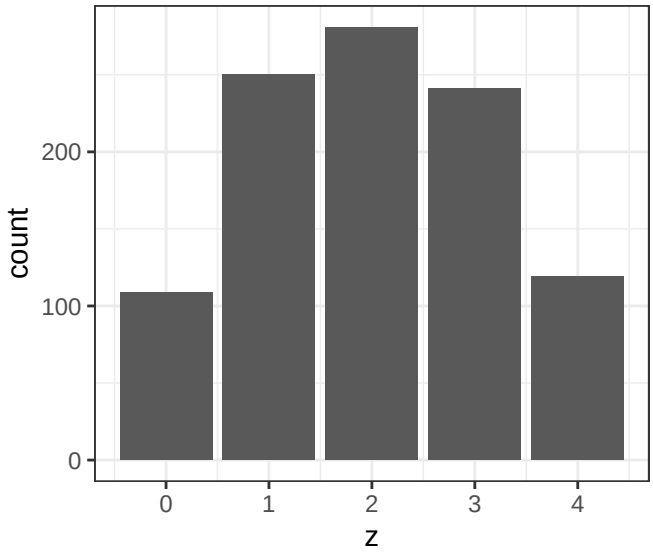
One way to check whether the prior is appropriate is to use the **prior predictive distribution**. Bayesian models are **generative** because they can be used to simulate data. The prior predictive distribution can be obtained by first simulating some θ values from the prior distribution and then simulating a data set for each θ.

```r
# Draw one theta
num_trials <- 4  # number of draws
sim_th1 <- sample(grid_df$th, size = 1,
                  # based on prior probability
                  prob = grid_df$pth)
# Simulate new data of four flips based on model
sim_y1 <- rbinom(num_trials, size = 1, prob = sim_th1)

# Repeat many times
# Set number of simulation draws
num_draws <- 1000
sim_th <- sample(grid_df$th, size = num_draws, replace = TRUE,
                 # based on prior probability
                 prob = grid_df$pth)
# Use a for loop
# Initialize output
sim_y <- matrix(NA, nrow = num_trials, ncol = num_draws)
for (s in seq_len(num_draws)) {
    # Store simulated data in the sth column
    sim_y[, s] <- rbinom(num_trials, size = 1, prob = sim_th[s])
}
# Show the first 10 simulated data sets based on prior:
sim_y[, 1:10]
```

```
#>      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
#> [1,]    1    0    0    1    0    1    0    0    0     1
#> [2,]    0    0    0    1    1    0    1    0    1     1
#> [3,]    1    0    0    1    0    0    0    1    1     1
#> [4,]    1    0    1    1    1    0    0    1    1     0
```

```r
# Show the distribution of number of heads
sim_heads <- colSums(sim_y)
ggplot(data.frame(z = sim_heads), aes(x = z)) +
    geom_bar()
```



The outcome seems to fit our intuition that it's more likely to be half heads and half tails, but there is a lot of uncertainty.

3.5.3 Summarizing the Posterior

```
grid_df <- grid_df |>
    mutate(
        # Use our previously defined lik() function
        py_th = lik(th, num_flips = 4, num_heads = 1),
        # Product of prior and likelihood
        `prior x lik` = pth * py_th,
        # Scaled the posterior
        pth_y = `prior x lik` / sum(`prior x lik`)
    )
# Print a table
knitr::kable(grid_df)
```

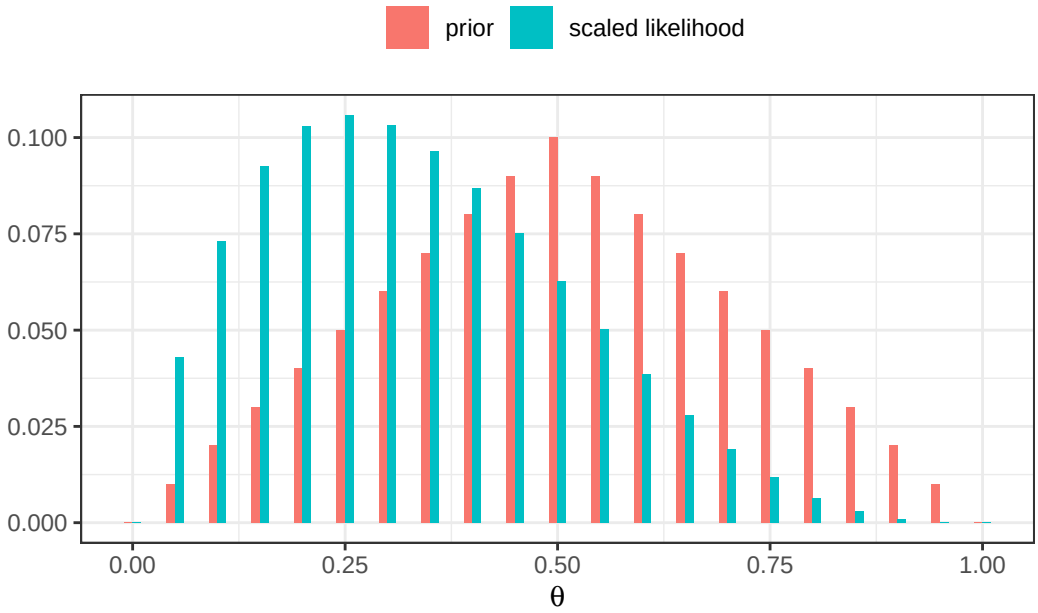
th	pth	py_th	prior x lik	pth_y
0.00	0.00	0.0000000	0.0000000	0.0000000
0.05	0.01	0.0428687	0.0004287	0.0073359
0.10	0.02	0.0729000	0.0014580	0.0249500
0.15	0.03	0.0921188	0.0027636	0.0472914

th	pth	py_th	prior x lik	pth_y
0.20	0.04	0.1024000	0.0040960	0.0700927
0.25	0.05	0.1054688	0.0052734	0.0902416
0.30	0.06	0.1029000	0.0061740	0.1056525
0.35	0.07	0.0961187	0.0067283	0.1151381
0.40	0.08	0.0864000	0.0069120	0.1182815
0.45	0.09	0.0748688	0.0067382	0.1153071
0.50	0.10	0.0625000	0.0062500	0.1069530
0.55	0.09	0.0501187	0.0045107	0.0771891
0.60	0.08	0.0384000	0.0030720	0.0525695
0.65	0.07	0.0278687	0.0019508	0.0333832
0.70	0.06	0.0189000	0.0011340	0.0194056
0.75	0.05	0.0117188	0.0005859	0.0100268
0.80	0.04	0.0064000	0.0002560	0.0043808
0.85	0.03	0.0028687	0.0000861	0.0014727
0.90	0.02	0.0009000	0.0000180	0.0003080
0.95	0.01	0.0001187	0.0000012	0.0000203
1.00	0.00	0.0000000	0.0000000	0.0000000

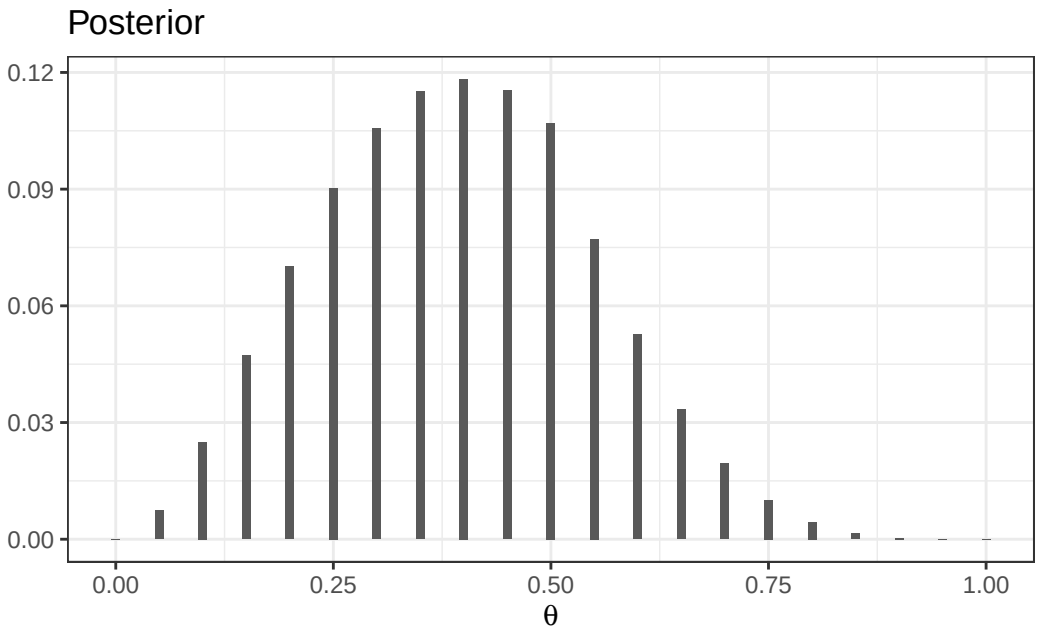
```
# Plot the prior/likelihood and the posterior
ggplot(data = grid_df, aes(x = th)) +
    geom_col(aes(x = th - 0.005, y = pth, fill = "prior"),
        width = 0.01,
    ) +
    geom_col(aes(x = th + 0.005, y = py_th / sum(py_th),
        fill = "scaled likelihood"), width = 0.01,
    ) +
    labs(fill = NULL, y = NULL, x = expression(theta)) +
    theme(legend.position = "top")
ggplot(data = grid_df, aes(x = th)) +
    geom_col(aes(x = th, y = pth_y), width = 0.01) +
    labs(
        fill = NULL, y = NULL, title = "Posterior",
        x = expression(theta)
    )
```

Figure 3.8b shows the posterior distribution, which represents our updated belief about θ. We can summarize it by simulating θ values from it and compute summary statistics:

```
# Define a function for computing posterior summary
summ_draw <- function(x) {
```



(a) Prior and likelihood



(b) Posterior

Figure 3.8: Bernoulli posterior distribution

```
    c(
        mean = mean(x),
        median = median(x),
        sd = sd(x),
        mad = mad(x),
        `ci.1` = quantile(x, prob = .1, names = FALSE),
        `ci.9` = quantile(x, prob = .9, names = FALSE)
    )
}
# Sample from the posterior
post_samples <- sample(
    grid_df$th,
    size = 1000, replace = TRUE,
    prob = grid_df$pth_y
)
summ_draw(post_samples)
```

```
#>      mean    median        sd       mad      ci.1      ci.9
#> 0.3848000 0.4000000 0.1538429 0.1482600 0.2000000 0.6000000
```

```
# Alternatively, use the `posterior` package
data.frame(theta = post_samples) |>
    posterior::summarize_draws()
```

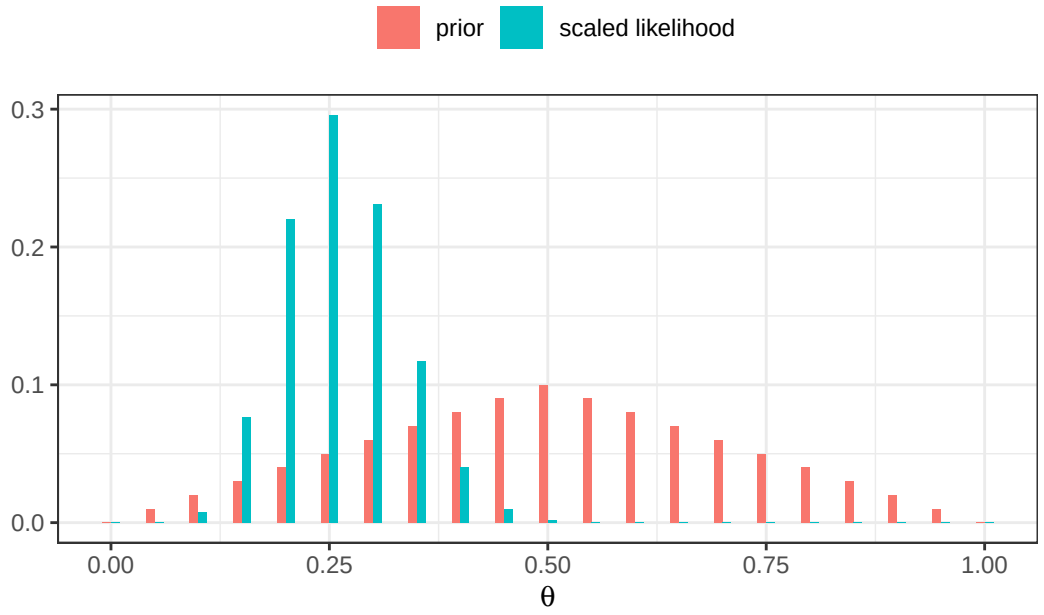
```
#> # A tibble: 1 x 10
#>   variable  mean median    sd   mad    q5   q95  rhat ess_bulk ess_tail
#>   <chr>    <dbl>  <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
#> 1 theta    0.385    0.4 0.154 0.148  0.15  0.65  1.00    1030.     721.
```

3.5.4 Influence of Sample Size

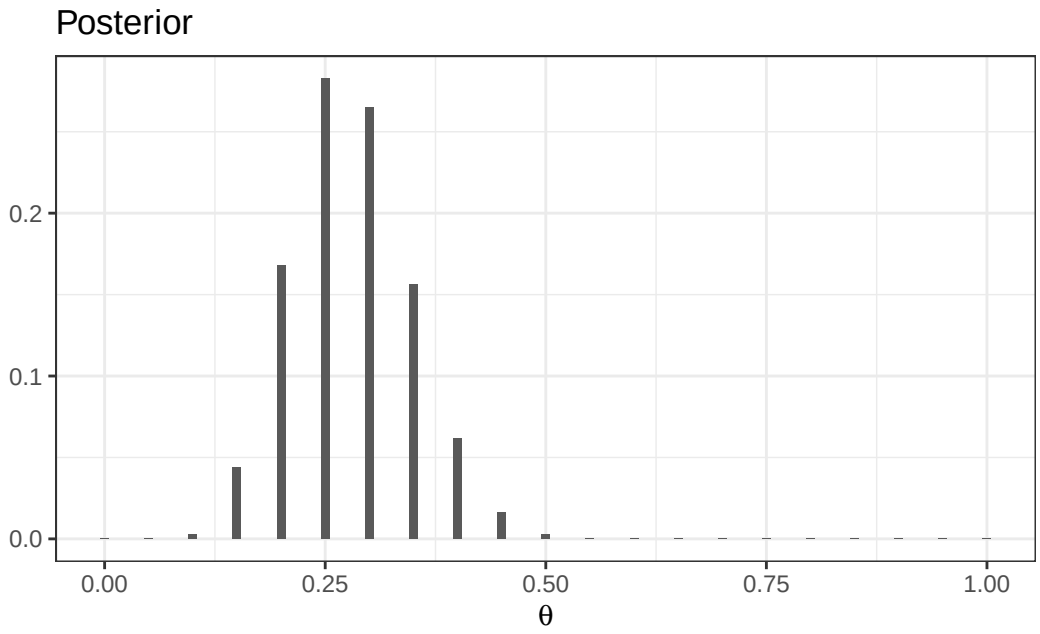
If, instead, we have $N = 40$ and $z = 10$, the posterior will be more similar to the likelihood.

```
grid_df2 <- grid_df |>
    mutate(
        # Use our previously defined lik() function
        py_th = lik(th, num_flips = 40, num_heads = 10),
        # Product of prior and likelihood
        `prior x lik` = pth * py_th,
        # Scaled the posterior
```

```
        pth_y = `prior x lik` / sum(`prior x lik`)
    )
# Plot the prior/likelihood and the posterior
ggplot(data = grid_df2, aes(x = th)) +
    geom_col(aes(x = th - 0.005, y = pth, fill = "prior"),
        width = 0.01,
    ) +
    geom_col(aes(x = th + 0.005, y = py_th / sum(py_th),
        fill = "scaled likelihood"), width = 0.01,
    ) +
    labs(fill = NULL, y = NULL, x = expression(theta)) +
    theme(legend.position = "top")
```




```
ggplot(data = grid_df2, aes(x = th)) +
    geom_col(aes(x = th, y = pth_y), width = 0.01) +
    labs(
        fill = NULL, y = NULL, title = "Posterior",
        x = expression(theta)
    )
```




```
# Sample from the posterior
post_samples <- sample(
    grid_df2$th,
    size = 1000, replace = TRUE,
    prob = grid_df2$pth_y
)
summ_draw(post_samples)
```

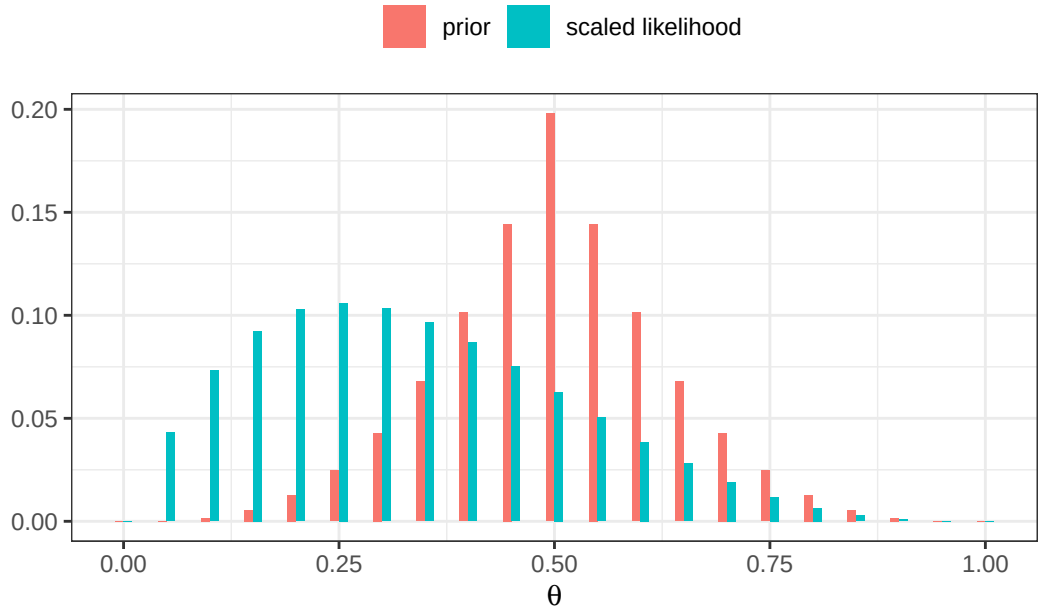
```
#>       mean     median         sd        mad       ci.1       ci.9
#> 0.28085000 0.30000000 0.06542215 0.07413000 0.20000000 0.35000000
```

3.5.5 Influence of Prior

If we have a very strong prior concentrated at $\theta = .5$, but still with $N = 40$ and $z = 10$, the posterior will be more similar to the prior.

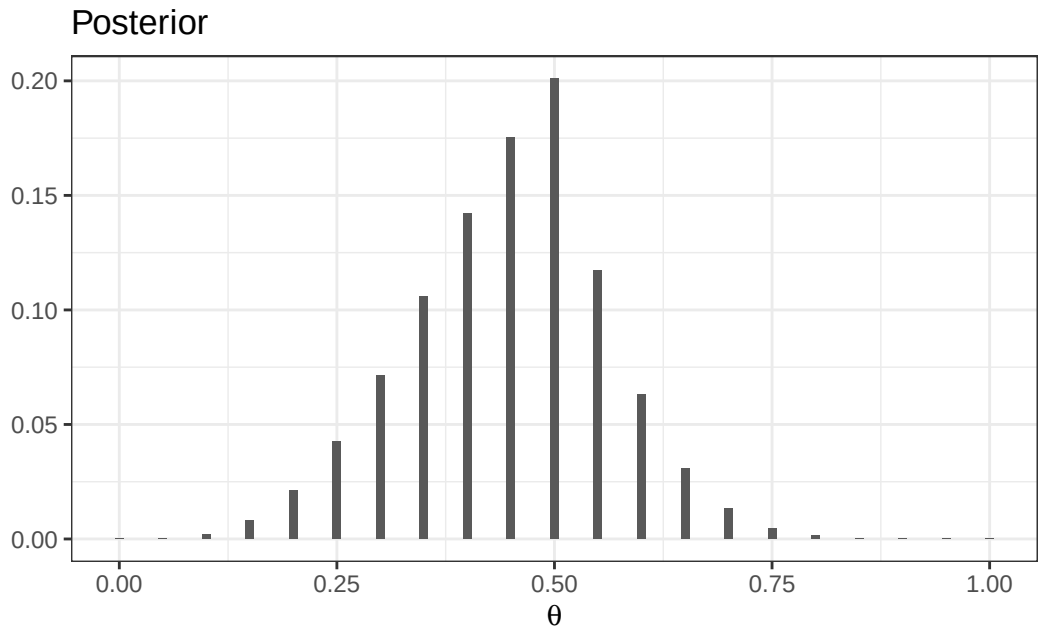
```
grid_df3 <- grid_df |>
    mutate(
        # stronger prior
        pth = pth ^ 3,
        # scale the prior to sume to 1
        pth = pth / sum(pth),
```

```
        # Use our previously defined lik() function
        py_th = lik(th, num_flips = 4, num_heads = 1),
        # Product of prior and likelihood
        `prior x lik` = pth * py_th,
        # Scaled the posterior
        pth_y = `prior x lik` / sum(`prior x lik`)
    )
# Plot the prior/likelihood and the posterior
ggplot(data = grid_df3, aes(x = th)) +
    geom_col(aes(x = th - 0.005, y = pth, fill = "prior"),
        width = 0.01,
    ) +
    geom_col(aes(x = th + 0.005, y = py_th / sum(py_th),
        fill = "scaled likelihood"), width = 0.01,
    ) +
    labs(fill = NULL, y = NULL, x = expression(theta)) +
    theme(legend.position = "top")
```




```
ggplot(data = grid_df3, aes(x = th)) +
    geom_col(aes(x = th, y = pth_y), width = 0.01) +
    labs(
        fill = NULL, y = NULL, title = "Posterior",
```

```
        x = expression(theta)
    )
```




```
# Sample from the posterior
post_samples <- sample(
    grid_df3$th,
    size = 1000, replace = TRUE,
    prob = grid_df3$pth_y
)
summ_draw(post_samples)
```

```
#>      mean    median        sd       mad      ci.1      ci.9
#> 0.4493000 0.4500000 0.1096656 0.0741300 0.3000000 0.6000000
```

```
# Alternatively, use the `posterior` package
data.frame(theta = post_samples) |>
    posterior::summarize_draws()
```

```
#> # A tibble: 1 x 10
#>   variable  mean median    sd    mad    q5   q95  rhat ess_bulk ess_tail
#>   <chr>    <dbl>  <dbl> <dbl>  <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
#> 1 theta    0.449   0.45 0.110 0.0741  0.25   0.6  1.00    1001.     899.
```

3.5.6 Remark on Grid Approximation

In this note, we discretized θ into a finite number of grid points to compute the posterior, mainly for pedagogical purposes. A big limitation is that our posterior will have no density for values other than the chosen grid points. While increasing the number of grid points (e.g., 1,000) can give more precision, the result is still not truly continuous. A bigger issue is that the computation breaks down when there is more than one parameter; if there are p parameters, with 1,000 grid points per parameter, one needs to evaluate the posterior probability for $1,000^p$ grid points, which is not feasible even with modern computers. So more efficient algorithms, namely Markov chain Monte Carlo (MCMC) methods, will be introduced as we progress in the course.

Part III

Week 3

4 Beta-Bernoulli Model

4.1 Steps of Bayesian Data Analysis

Some authors described the process as "turning the Bayesian Crank," as the same workflow applies to a variety of research scenarios.

Adapted from Gelman et al. (2020), I conceptualize Bayesian data analysis as the following steps:

1. **Identify/Collect the data** required to answer the research questions.
    - As a general recommendation, it is helpful to **visualize** the data to get a sense of how they look, as well as to inspect for potential anomalies in the data collection.
2. **Choose an initial statistical model** for the data in relation to the research questions. The model should have some theoretical justification and have parameters that are meaningful for the research questions. However, it is unlikely that any chosen model will capture everything important in the data, and this initial model will be modified and expanded in later steps.
3. **Specify prior distributions** for the model parameters. Although this is a subjective endeavor, the priors chosen should be sensible to a skeptical audience.
4. **Check the prior distributions**. It is recommended you conduct a **prior predictive check**, by simulating fake data based on the chosen model and prior distributions. This is especially important for complex models as the parameters are more difficult to interpret.
5. **Obtain the posterior distributions** for the model parameters. As described below and later in the course, this can be obtained by analytical or various mathematical approximations.
    - For mathematical approximations, one should check the algorithms for **convergence** to make sure the results closely mimic the target posterior distributions.
6. Conduct a **posterior predictive check** to examine the fit between the model and the data, i.e., whether the chosen model with the estimated parameters generates predictions that deviate from the data being analyzed on important features.
7. It is unlikely that your initial model fully describes the major aspects of the data as pertaining to your research questions. Therefore, one should repeat steps 2 to 6 to **specify and compare different models**.

8. If the fit between the model and the data is deemed satisfactory, one can proceed to **interpret the results** in the context of the research questions. It is also important to **visualize the results** in ways that are meaningful for the analysis.

4.2 Beta-Bernoulli Example

We will be using a built-in data set in R about patients diagnosed with AIDS in Australia before July 1, 1991. Here is a description of the variables (from the R documentation):

Figure 4.1: Figure from https://commons.wikimedia.org/wiki/File:Australia_states_1931-present.png

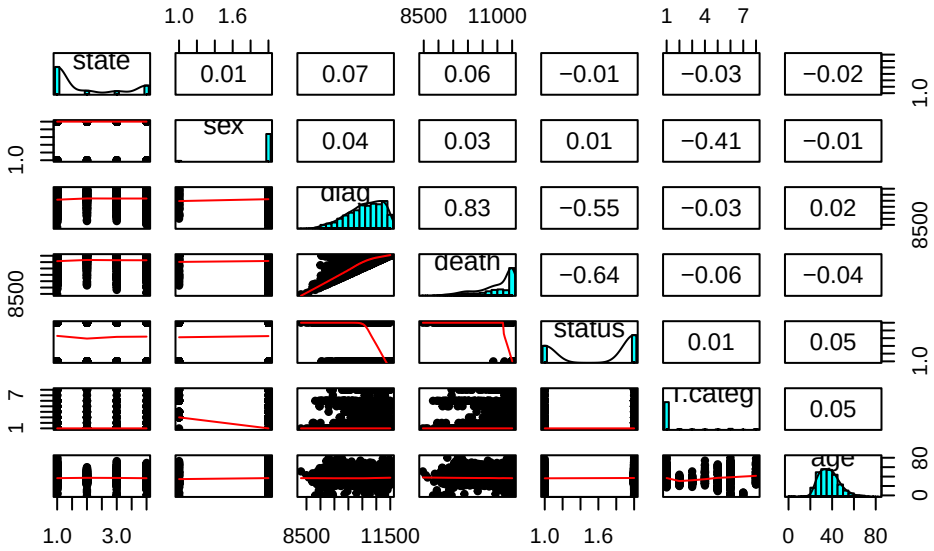
- `state`: Grouped state of origin: "NSW"includes ACT and "other" is WA, SA, NT, and TAS.
- `sex`: Sex of patient.
- `diag`:(Julian) date of diagnosis.
- `death`: (Julian) date of death or end of observation.
- `status`: "A" (alive) or "D" (dead) at end of observation.
- `T.categ`: Reported transmission category.
- `age`: Age (years) at diagnosis.

You should always first plot your data and get some summary statistics:

```
data("Aids2", package = "MASS")
head(Aids2)
```

```
  state sex  diag death status T.categ age
1   NSW   M 10905 11081      D      hs  35
2   NSW   M 11029 11096      D      hs  53
3   NSW   M  9551  9983      D      hs  42
4   NSW   M  9577  9654      D    haem  44
5   NSW   M 10015 10290      D      hs  39
6   NSW   M  9971 10344      D      hs  36
```

```
pairs.panels(Aids2, ellipses = FALSE)
```



We will be using the `status` variable. Our simple research question is:

> What was the death rate of AIDS in Australia when the data were collected?

4.2.1 Bernoulli Model

If we assume that the outcomes of the observations are exchangeable, meaning that the observations can be reordered in any way and still give the same inference, then one can choose a model:

$$y_i \sim \text{Bern}(\theta) \text{ for } i = 1, 2, \ldots, N$$

- y_i = status of observation i (0 = "A", 1 = "D")
- N = number of patients in the data set
- θ = probability of "D"[1]

The model states that: the sample data y follows a Bernoulli distribution with n with a parameter θ

When the data consist of binary observations, the variable is called a Bernoulli variable. It is conventional to denote one outcome as success and code it as 1, and the other as failure and code it as 0 (poor terminology, maybe, but that's by convention). Therefore, in the AIDS example, each observation is considered a "Bernoulli" outcome (Alive vs. Dead).

4.2.2 Exchangeability

To illustrate exchangeability in an example, say we take 6 rows in our data set:

```
     state sex  diag death status T.categ age
1      NSW   M 10905 11081      D      hs  35
31     NSW   F 10961 11504      A      id  30
1802   QLD   F  9495  9753      D   blood  66
1811   QLD   M 10770 11504      A    hsid  29
2129   VIC   M  8499  8568      D      hs  43
2137   VIC   M  9055  9394      D      hs  29
```

Now, when we reorder the column `status` to something like:

```
     state sex  diag death status T.categ age
1      NSW   M 10905 11081      D      hs  35
31     NSW   F 10961 11504      D      id  30
1802   QLD   F  9495  9753      D   blood  66
1811   QLD   M 10770 11504      A    hsid  29
2129   VIC   M  8499  8568      A      hs  43
2137   VIC   M  9055  9394      D      hs  29
```

[1] An additional thing to note for the Bernoulli/binomial model is that, instead of setting the prior on θ, sometimes we are more interested in setting the prior for a transformed parameter that has values between $-\infty$ and ∞, such as one on the *logit* scale (as related to logistic regression).

If the results are expected to be the same, then we say that the observations are assumed exchangeable. It happens when we assume that all observations have one common mean. However, if we think that there is a mean for females and a different mean for males, we cannot reorder the outcome randomly because they are no longer exchangeable (i.e., you cannot exchange a female score for a male score and expect to get the same results).

> **!** **Exchangeability**
>
> A set of observations is said to be exchangeable if their joint probability distribution stays the same under all permutations. Roughly speaking, it means that the observations can be reordered and still provide the same inferences.

4.2.3 Check the Support

It is important to identify the *support* of the parameter, θ. Because θ is a probability, its support is $[0, 1]$, meaning it is continuous and can take any value from 0 to 1. For a continuous parameter, there are infinitely many possible values, and it is impossible to specify our beliefs for each value. So, more commonly, we choose a probability density function with the same support as the parameter to express our prior belief.

4.2.4 Conjugate Prior: Beta Distribution

A commonly used family of prior distributions for a Bernoulli/binomial model is the *Beta distribution*, which has two parameters. We can write the prior as

$$P(\theta) \sim \text{Beta}(a, b)$$

a and b are the two hyperparameters. Here are a few examples:

You will notice that when $a > b$, there is more density closer to the right region (i.e., larger θ), and vice versa. Also, the variance decreases when a and b become larger.[2]

A nice interpretation of a and b in a Beta prior distribution is to consider

- $a - 1$ = number of prior 'successes' (e.g., "D")
- $b - 1$ = number of prior 'failures' (e.g., "A")

[2]The Beta$(1/2, 1/2)$ distribution is called a *Jeffreys prior* (https://en.wikipedia.org/wiki/Jeffreys_prior), which is derived according to some statistical principles for different models. One big advantage of a Jeffreys prior is that it is **invariant**, meaning that the prior will stay the same even under reparameterization. However, like conjugate priors, Jeffreys prior limits the choice of prior even when true prior information is available.

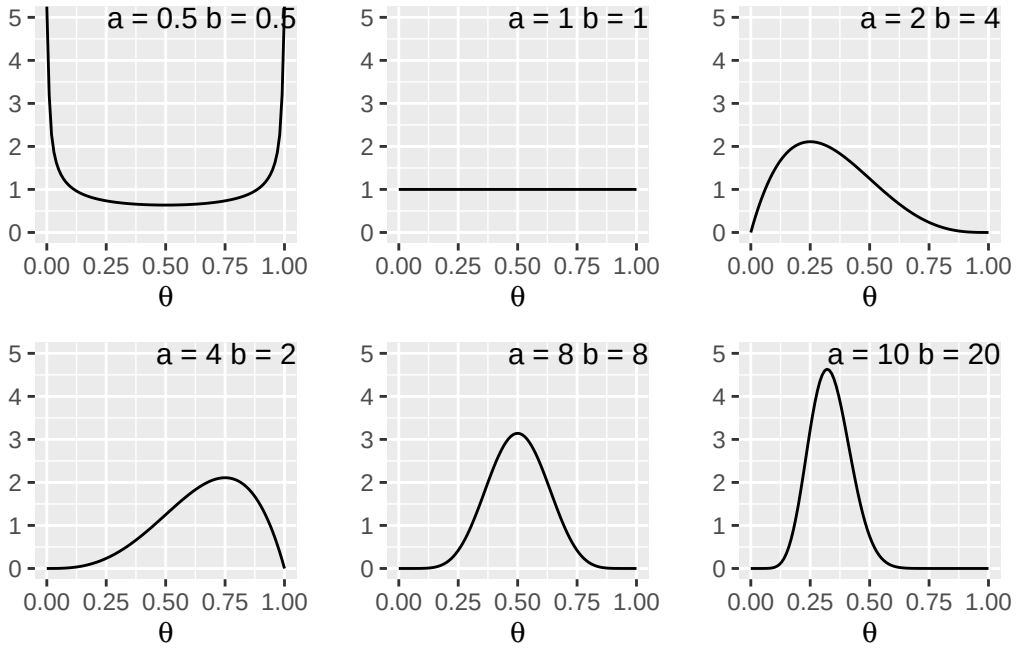


Figure 4.2: Beta distributions with different a and b values

Therefore, with Beta$(1, 1)$, one has seen 0 prior success and 0 failure, meaning that there is no prior information (i.e., *noninformative*). Therefore, it makes sense that all θ values are equally likely. On the other hand, if one chooses Beta$(10, 20)$, one has seen 9 prior successes and 19 prior failures, so one has quite a lot of prior information (indeed more than the data with only 10 observations), so this is a *strong* prior.

> The smaller the variance of the prior distribution, the stronger one's belief before looking at the data, the more prior information

So by manipulating the values of a and b, which are sometimes called *hyperparameters*, you can control the shape of the prior distribution as well as its strength, so it is quite flexible. Another advantage of using a beta prior is that it is a *conjugate prior* of the Bernoulli model, which means that the posterior distribution $P(\theta \mid y)$ is also a beta distribution, the same as the prior distribution, although with different parameter values.

> **!** **Conjugate Prior**
>
> For a specific model, conjugate priors yield posterior distributions in the same distribution family as the priors

Conjugacy greatly simplifies the computational burden for Bayesian analyses, so conjugate priors are almost the only ones used in earlier literature. However, this limited the applica-

tions of Bayesian methods, as for many problems, no conjugate priors can provide a realistic representation of one's belief. Modern Bayesian analysis instead relies on *simulation-based* methods to approximate the posterior distribution, which can accommodate almost any kind of prior distribution. Aside from a few examples in this note, mainly for pedagogical purposes, we will be using simulation-based methods in the coming weeks.

Proof of Conjugacy*

To derive the form of the posterior, first recognize that the Beta distribution has the form:

$$\begin{aligned} P(\theta) &= \mathrm{B}^{-1}(a, b)\theta^{a-1}(1-\theta)^{b-1} \\ &\propto \theta^{a-1}(1-\theta)^{b-1} \end{aligned}$$

Where $\mathrm{B}(\cdot)$ is the beta function which is not very important for the class. As the density function is a function of θ, it suffices to write only the terms that involve θ. Similarly,

$$P(\mathbf{y} \mid \theta) \propto \theta^{z}(1-\theta)^{N-z}.$$

Therefore,

$$\begin{aligned} P(\theta \mid \mathbf{y}) &\propto P(y \mid \theta)P(\theta) \\ &\propto \theta^{z}(1-\theta)^{N-z}\theta^{a-1}(1-\theta)^{b-1} \\ &= \theta^{a+z-1}(1-\theta)^{b+N-z-1}. \end{aligned}$$

If we let $a^* = a + z$, $b^* = b + N - z$, we can see that $P(\theta \mid \mathbf{y})$ is in the same form as the prior with a and b replaced by a^* and b^*. Therefore, the posterior is also a beta distribution. So the beta distribution is a conjugate prior for the Bernoulli model.

In this example, we will choose a *weakly informative* Beta(2, 2) prior, which represents a weak belief as below:

```
ggplot(data.frame(th = c(0, 1)), aes(x = th)) +
    stat_function(fun = dbeta, args = list(shape1 = 2, shape2 = 2)) +
    ylim(0, 3) +
    labs(y = "", x = expression(theta), title = "Beta(2, 2)")
```

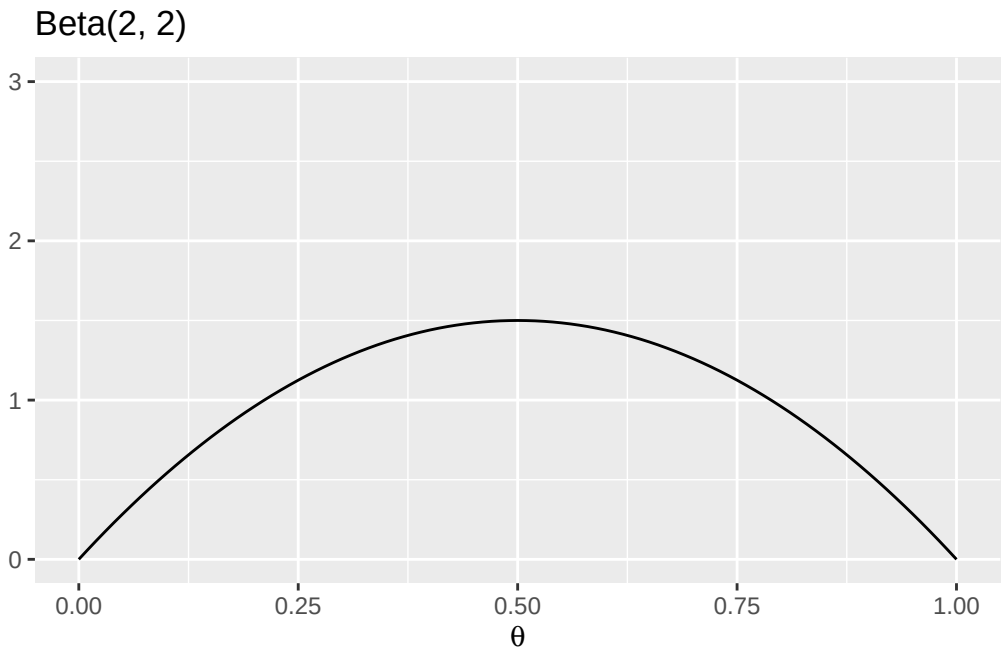


Figure 4.3: A weakly informative Beta(2, 2) prior

Don't Be Stubborn

> A good prior should give a non-zero probability/density for all possible values of a parameter

Otherwise, if the prior density for some parameter values is zero, the posterior density will be zero, regardless of how much the data support those parameter values

4.2.5 Data

```
count(Aids2, status)
```

```
  status    n
1      A 1082
2      D 1761
```

The likelihood function is highly concentrated. I ran into some numerical issues as the computation gave zero, so I plotted the log-likelihood instead.

```r
loglik <- function(th, N = 1082 + 1761, z = 1761) {
    z * log(th) + (N - z) * log(1 - th)
}
ggplot(data.frame(th = c(0.61, 0.63)), aes(x = th)) +
    stat_function(fun = loglik, n = 501) +
    labs(x = expression(theta), y = "Log-likelihood")
```

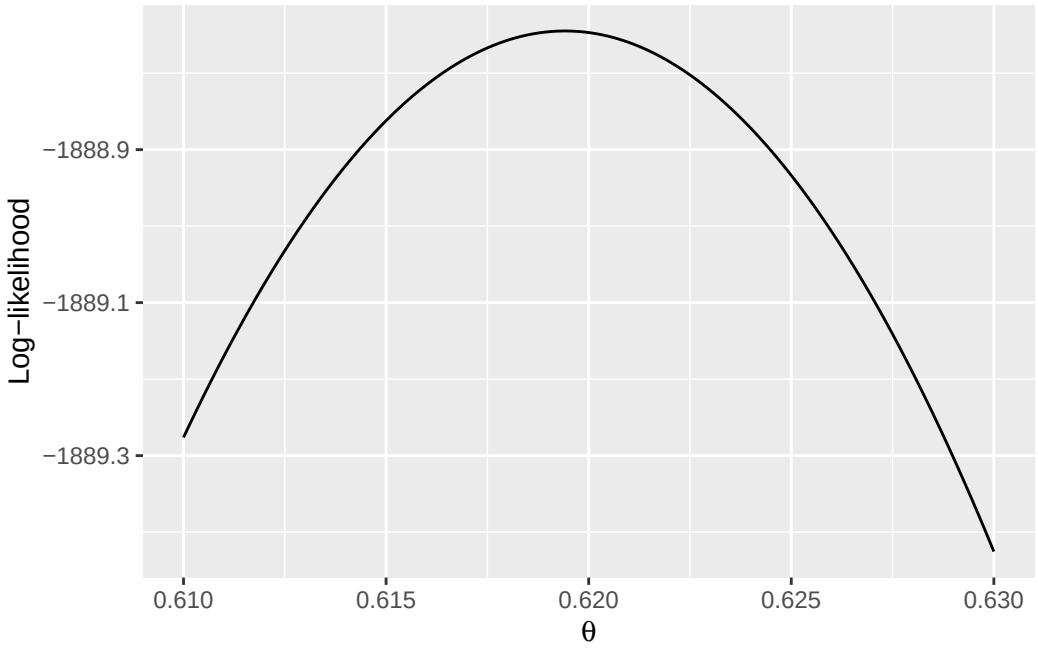


Figure 4.4: Log-likelihood function of the theta parameter

Note I only show a range of [0.610, 0.630] for the x-axis, which contains where the likelihood (thus also the log-likelihood) peaked.

4.2.6 Posterior

Based on the conjugacy, the posterior of θ is Beta(1,807, 1,116). As we are using a conjugate prior, the posterior is also a Beta distribution:

$$P(\theta \mid y) \sim \text{Beta}(a + z, b + N - z),$$

which is a distribution for $a + z - 1$ successes and $b + N - z$ failures. This makes perfect sense as our prior information has $a - 1$ successes and $b - 1$ failures, and from our data, we have y successes and $n - y$ failures, so our updated belief is based on adding up those successes and failures.

4.2.7 Summarize the posterior

```
set.seed(2119)
num_draws <- 1000
sim_theta <- rbeta(num_draws, shape1 = 1807, shape2 = 1116)
c(`Bayes estimate` = mean(sim_theta),
  `Posterior median` = median(sim_theta),
  `Posterior SD` = sd(sim_theta),
  `MAD` = mad(sim_theta),
  `90% Credible interval (equal-tailed)` = quantile(sim_theta, probs = c(.1, .9)),
  `90% HDI` = HDInterval::hdi(sim_theta, credMass = .9))
```

```
                            Bayes estimate
                                 0.618209694
                           Posterior median
                                 0.618382945
                              Posterior SD
                                 0.008829290
                                       MAD
                                 0.009254166
90% Credible interval (equal-tailed).10%
                                 0.606862338
90% Credible interval (equal-tailed).90%
                                 0.628990588
                               90% HDI.lower
                                 0.604051851
                               90% HDI.upper
                                 0.632766654
```

4.2.8 Posterior Predictive Check

Now, we need to know whether the model fits the data well. We do not have much to check for a Bernoulli model if we only have the `status` variable. However, as there is information for other variables, we can use them to check the exchangeability assumption. For example, we can ask whether the data from different state categories are exchangeable. The death rate across the 4 state categories are

```
       status
state      A    D
  NSW    664 1116
```

```
  Other  107  142
  QLD     78  148
  VIC    233  355
```

```
       status
state           A         D
  NSW   0.3730337 0.6269663
  Other 0.4297189 0.5702811
  QLD   0.3451327 0.6548673
  VIC   0.3962585 0.6037415
```

We can now generate predictions from our posterior distribution and model.

```
plist <- vector("list", 12L)
plist[[1]] <- ggplot(
    Aids2,
    aes(x = state, y = mean(status == "D"), fill = state)
) +
    geom_bar(stat = "identity") +
    guides(fill = "none") +
    labs(x = "Observed data", y = "Number of Deaths") +
    theme(axis.title.x = element_text(color = "red")) +
    ylim(0, 1200)
for (i in 1:11) {
    # Get the a value from posterior samples
    theta_post <- rbeta(1, 1763, 1084)
    # For each plausible theta value, generate a status variable
    status_new <- sample(c("D", "A"), nrow(Aids2),
        replace = TRUE,
        prob = c(theta_post, 1 - theta_post)
    )
    df_new <- Aids2 |>
        mutate(status = factor(status_new))
    plist[[i + 1]] <- plist[[1]] %+% df_new +
        labs(x = paste("Simulated data", i)) +
        theme(axis.title.x = element_text(color = "black"))
}
gridExtra::grid.arrange(grobs = plist, nrow = 3)
```

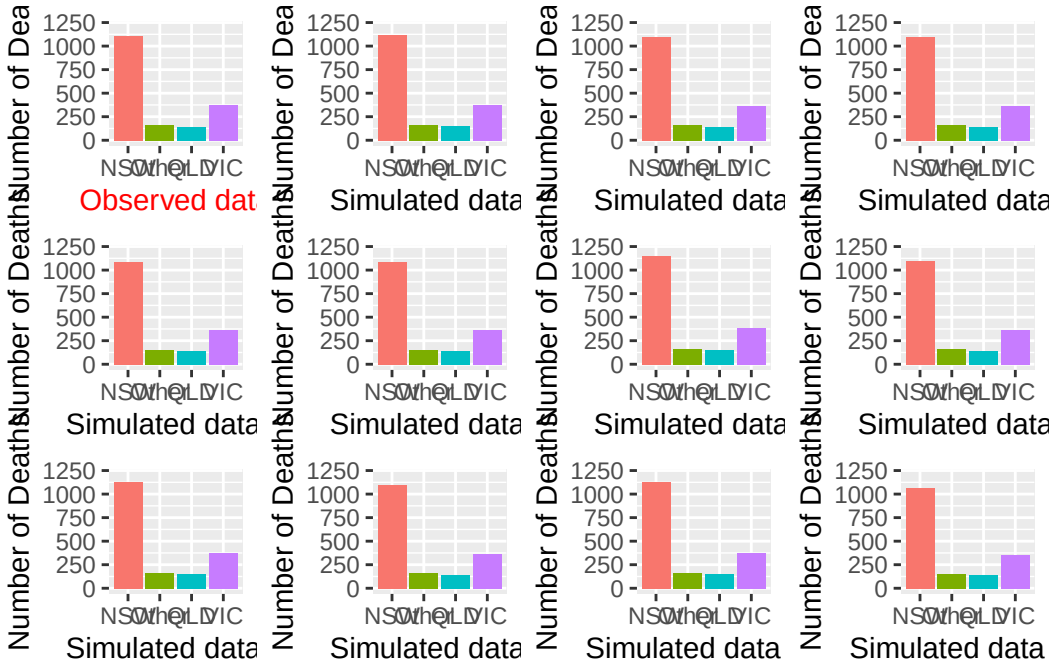


Figure 4.5: Posterior predictive check by comparing the observed data with 11 simulated data sets based on the model

So the observed data (the first subplot) look similar to the simulated data. We can also conduct a posterior predictive check by a test statistic for subgroups. Here, we will use the `bayesplot` package and look at fit across groups:

```
# Draw posterior samples of theta
post_sample <- rbeta(1e4, 1807, 1116)
# Initialize a S by N matrix to store the simulated data
y_tilde <- matrix(NA,
                  nrow = length(post_sample),
                  ncol = length(Aids2$status))
for (s in seq_along(post_sample)) {
    theta_s <- post_sample[s]
    status_new <- sample(c("D", "A"), nrow(Aids2),
        replace = TRUE,
        prob = c(theta_s, 1 - theta_s)
    )
    y_tilde[s,] <- as.numeric(status_new == "D")
}
bayesplot::ppc_stat_grouped(
    as.numeric(Aids2$status == "D"),
```

```
    yrep = y_tilde,
    group = Aids2$state
)
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

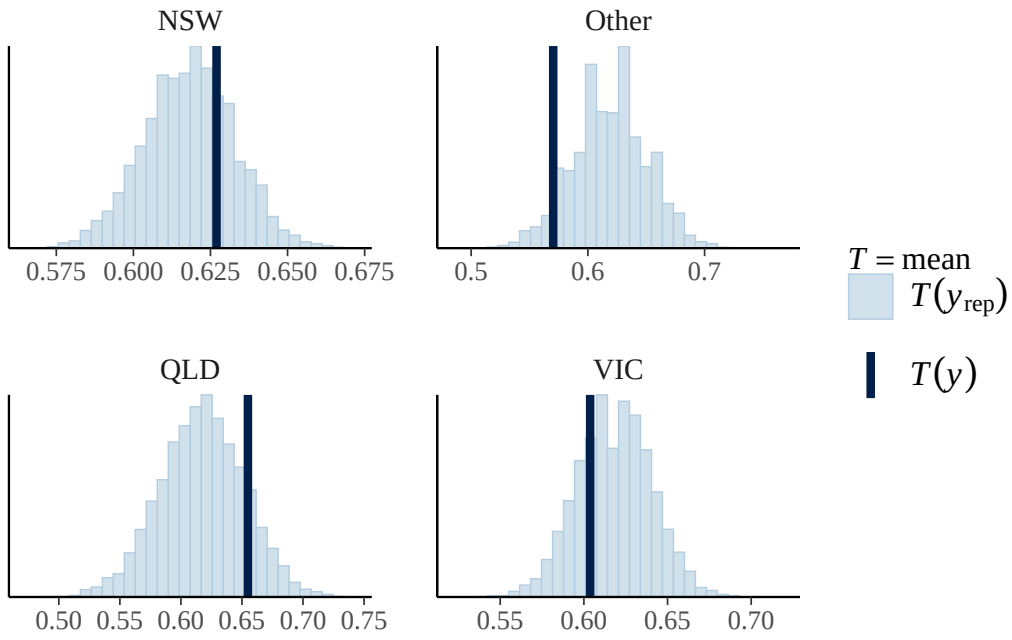


Figure 4.6: Posterior predictive check by states

If the fit is good, the mean, indicated by the darker line, should be within the simulated distribution based on the model. So the model that assumes observations are exchangeable across states is not too off, although it seems fitting less well for `Other` states.

4.2.8.1 Another check on `age`

```
# Create an age group indicator
age50 <- factor(Aids2$age > 50, labels = c("<= 50", "> 50"))
# Draw posterior samples of theta
post_sample <- rbeta(1e4, 1807, 1116)
# Initialize a S by N matrix to store the simulated data
```

```
y_tilde <- matrix(NA,
                  nrow = length(post_sample),
                  ncol = length(Aids2$status))
for (s in seq_along(post_sample)) {
    theta_s <- post_sample[s]
    status_new <- sample(c("D", "A"), nrow(Aids2),
        replace = TRUE,
        prob = c(theta_s, 1 - theta_s)
    )
    y_tilde[s,] <- as.numeric(status_new == "D")
}
bayesplot::ppc_stat_grouped(
    as.numeric(Aids2$status == "D"),
    yrep = y_tilde,
    group = age50
)
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

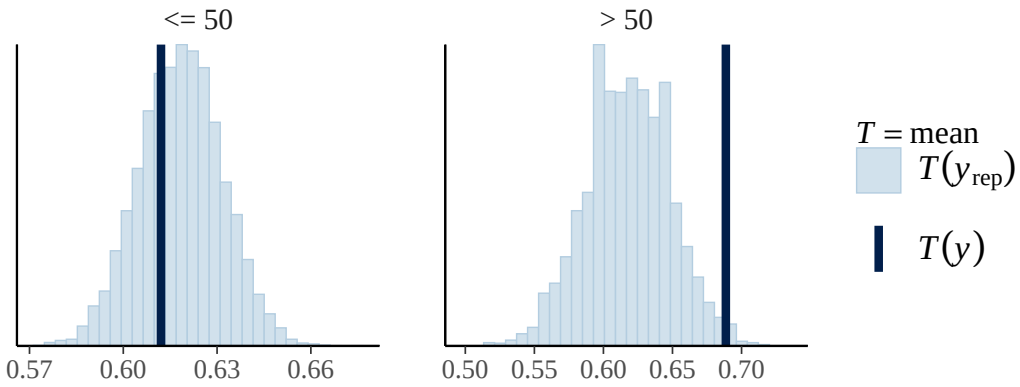


Figure 4.7: Posterior predictive check by age groups (<= 50 vs. > 50)

As can be seen, the model seems off for those aged 50+.

4.2.9 Comparison to frequentist results

Using maximum likelihood, the estimated death rate would be $\hat{\theta} = 1761/2843 = 0.62$, with a standard error (SE) of $\sqrt{0.62(1-0.62)/n} = 0.0091$, with a 90% confidence interval of $[0.6, 0.63]$, which is similar to the interval with Bayesian inference.

4.2.10 Sensitivity to different priors

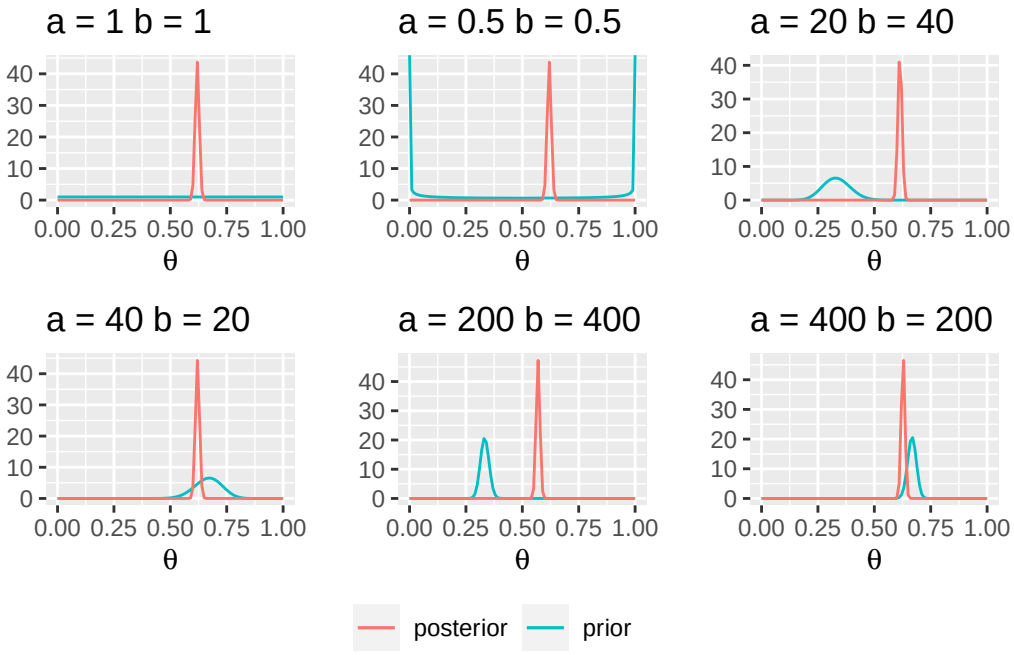


Figure 4.8: Sensitivity of posterior to different priors

You can see one needs (a) a very strong prior (equivalent to 600 data points) and (b) the prior and the data not agreeing to get a substantially different conclusion.

5 Beta-Bernoulli Model With Stan

In the previous lecture, we fitted a Beta-Bernoulli model using Gibbs sampling with our own R code. While this is doable in this relatively simple model (it only has one parameter), for more complex models, Gibbs sampling and other MCMC methods (to be introduced in a later class) require quite a lot of programming. Fortunately for us, we have some readily available software for doing MCMC. While it is probably overkill for the Beta-Bernoulli model, we will learn working with Stan by using it to analyze the Beta-Bernoulli model. Specifically, we will learn to:

1. Install Stan and the R package `cmdstanr` for communicating between R and Stan;
2. Write Stan code for the Beta-Bernoulli model;
3. Draw posterior samples using Stan;
4. Summarize and plot the posterior samples.

We will talk about convergence of MCMC, which is an extremely important topic, in a later class.

5.1 Installing Stan

1. Follow the steps in https://mc-stan.org/cmdstanr/ to install the `cmdstanr` package.
2. Load the `cmdstanr` package, and run `install_cmdstan()`

```
library(cmdstanr)
install_cmdstan()
```

3. If you run into an error in the previous step related to C++ toolchain, follow the directions here: https://mc-stan.org/cmdstanr/articles/cmdstanr.html

5.2 Fitting a Beta-Bernoulli Model in Stan

5.2.1 Data Import

From last class:

```
data("Aids2", package = "MASS")
head(Aids2)
```

```
  state sex  diag death status T.categ age
1   NSW   M 10905 11081      D      hs  35
2   NSW   M 11029 11096      D      hs  53
3   NSW   M  9551  9983      D      hs  42
4   NSW   M  9577  9654      D    haem  44
5   NSW   M 10015 10290      D      hs  39
6   NSW   M  9971 10344      D      hs  36
```

5.2.2 Writing Stan syntax

Stan has its own syntax and is different from R. For example, we want to fit the following Beta-Bernoulli model:

$$y_i \sim \text{Bern}(\theta) \text{ for } i = 1, 2, \ldots, N$$
$$P(\theta) \sim \text{Beta}(2, 2)$$

and the model can be written in Stan as follows:

```
data {
  int<lower=0> N;  // number of observations
  array[N] int<lower=0,upper=1> y;  // y
}
parameters {
  real<lower=0,upper=1> theta;  // theta parameter
}
model {
  theta ~ beta(2,2);  // prior: Beta(2, 2)
  y ~ bernoulli(theta);  // model: Bernoulli
}
```

Save the above model syntax in a separate file ending in `.stan`. For example, I saved the syntax in the file `beta-bernoulli.stan` in a folder named `stan_code`.

In Stan, anything after `//` denotes comments (like `#` in R) and will be ignored by the program. In each block (e.g., `data {}`), a statement should end with a semicolon (`;`). There are several blocks in the above Stan code:

- `data`: The data input for Stan is usually not only an R data frame, but a list that includes other information, such as sample size, number of predictors, and prior scales. Each type of data has an input type, such as
  - `int` = integer,
  - `real` = numbers with decimal places,
  - `matrix` = 2-dimensional data of real numbers,
  - `vector` = 1-dimensional data of real numbers, and
  - `array` = 1- to many-dimensional data. For example, we use `array[N]` for the data type of `y`, because it is a vector, but each element is an integer (and cannot take decimals).

  We can set the lower and upper bounds so that Stan can check the input data. In the above, we used `<lower=0,upper=1>`.
- `parameters`: The parameters to be estimated
- `transformed parameters`: optional variables that are transformations of the model parameters. It is usually used for more advanced models to allow more efficient MCMC sampling.
- `model`: It includes expressions of prior distributions for each parameter and the likelihood for the data. There are many possible distributions that can be used in Stan.
- `generated quantities`: Any quantities that are not part of the model but can be computed from the parameters for every iteration. Examples include posterior generated samples, effect sizes, and log-likelihood (for fit computation). We will see an example later.

5.2.3 Compiling the Stan model from R

To compile the model, we can call the `cmdstan_model` function in `cmdstanr`:

```
bern_mod <- cmdstan_model("stan_code/beta-bernoulli.stan")
```

5.2.4 Posterior Sampling

We need to first prepare the data for input to Stan. In the Stan code, we have two objects in the data block: `N` and `y`, so we need to have a list of two elements in R:

```
Aids2_standata <- list(
    N = nrow(Aids2),
    y = as.integer(Aids2$status == "D")  # integer
)
```

Now we can draw posterior samples:

```
fit <- bern_mod$sample(Aids2_standata)
```

```
Running MCMC with 4 sequential chains...

Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration:  100 / 2000 [  5%]  (Warmup)
Chain 1 Iteration:  200 / 2000 [ 10%]  (Warmup)
Chain 1 Iteration:  300 / 2000 [ 15%]  (Warmup)
Chain 1 Iteration:  400 / 2000 [ 20%]  (Warmup)
Chain 1 Iteration:  500 / 2000 [ 25%]  (Warmup)
Chain 1 Iteration:  600 / 2000 [ 30%]  (Warmup)
Chain 1 Iteration:  700 / 2000 [ 35%]  (Warmup)
Chain 1 Iteration:  800 / 2000 [ 40%]  (Warmup)
Chain 1 Iteration:  900 / 2000 [ 45%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 1 Iteration: 1100 / 2000 [ 55%]  (Sampling)
Chain 1 Iteration: 1200 / 2000 [ 60%]  (Sampling)
Chain 1 Iteration: 1300 / 2000 [ 65%]  (Sampling)
Chain 1 Iteration: 1400 / 2000 [ 70%]  (Sampling)
Chain 1 Iteration: 1500 / 2000 [ 75%]  (Sampling)
Chain 1 Iteration: 1600 / 2000 [ 80%]  (Sampling)
Chain 1 Iteration: 1700 / 2000 [ 85%]  (Sampling)
Chain 1 Iteration: 1800 / 2000 [ 90%]  (Sampling)
Chain 1 Iteration: 1900 / 2000 [ 95%]  (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 1 finished in 0.0 seconds.
Chain 2 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 2 Iteration:  100 / 2000 [  5%]  (Warmup)
Chain 2 Iteration:  200 / 2000 [ 10%]  (Warmup)
```

```
Chain 2 Iteration:  300 / 2000 [ 15%]  (Warmup)
Chain 2 Iteration:  400 / 2000 [ 20%]  (Warmup)
Chain 2 Iteration:  500 / 2000 [ 25%]  (Warmup)
Chain 2 Iteration:  600 / 2000 [ 30%]  (Warmup)
Chain 2 Iteration:  700 / 2000 [ 35%]  (Warmup)
Chain 2 Iteration:  800 / 2000 [ 40%]  (Warmup)
Chain 2 Iteration:  900 / 2000 [ 45%]  (Warmup)
Chain 2 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 2 Iteration: 1100 / 2000 [ 55%]  (Sampling)
Chain 2 Iteration: 1200 / 2000 [ 60%]  (Sampling)
Chain 2 Iteration: 1300 / 2000 [ 65%]  (Sampling)
Chain 2 Iteration: 1400 / 2000 [ 70%]  (Sampling)
Chain 2 Iteration: 1500 / 2000 [ 75%]  (Sampling)
Chain 2 Iteration: 1600 / 2000 [ 80%]  (Sampling)
Chain 2 Iteration: 1700 / 2000 [ 85%]  (Sampling)
Chain 2 Iteration: 1800 / 2000 [ 90%]  (Sampling)
Chain 2 Iteration: 1900 / 2000 [ 95%]  (Sampling)
Chain 2 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 2 finished in 0.0 seconds.
Chain 3 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 3 Iteration:  100 / 2000 [  5%]  (Warmup)
Chain 3 Iteration:  200 / 2000 [ 10%]  (Warmup)
Chain 3 Iteration:  300 / 2000 [ 15%]  (Warmup)
Chain 3 Iteration:  400 / 2000 [ 20%]  (Warmup)
Chain 3 Iteration:  500 / 2000 [ 25%]  (Warmup)
Chain 3 Iteration:  600 / 2000 [ 30%]  (Warmup)
Chain 3 Iteration:  700 / 2000 [ 35%]  (Warmup)
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Chain 3 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 3 Iteration: 1100 / 2000 [ 55%]  (Sampling)
Chain 3 Iteration: 1200 / 2000 [ 60%]  (Sampling)
Chain 3 Iteration: 1300 / 2000 [ 65%]  (Sampling)
Chain 3 Iteration: 1400 / 2000 [ 70%]  (Sampling)
Chain 3 Iteration: 1500 / 2000 [ 75%]  (Sampling)
Chain 3 Iteration: 1600 / 2000 [ 80%]  (Sampling)
Chain 3 Iteration: 1700 / 2000 [ 85%]  (Sampling)
Chain 3 Iteration: 1800 / 2000 [ 90%]  (Sampling)
Chain 3 Iteration: 1900 / 2000 [ 95%]  (Sampling)
Chain 3 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 3 finished in 0.0 seconds.
```

```
Chain 4 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 4 Iteration:  100 / 2000 [  5%]  (Warmup)
Chain 4 Iteration:  200 / 2000 [ 10%]  (Warmup)
Chain 4 Iteration:  300 / 2000 [ 15%]  (Warmup)
Chain 4 Iteration:  400 / 2000 [ 20%]  (Warmup)
Chain 4 Iteration:  500 / 2000 [ 25%]  (Warmup)
Chain 4 Iteration:  600 / 2000 [ 30%]  (Warmup)
Chain 4 Iteration:  700 / 2000 [ 35%]  (Warmup)
Chain 4 Iteration:  800 / 2000 [ 40%]  (Warmup)
Chain 4 Iteration:  900 / 2000 [ 45%]  (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 4 Iteration: 1100 / 2000 [ 55%]  (Sampling)
Chain 4 Iteration: 1200 / 2000 [ 60%]  (Sampling)
Chain 4 Iteration: 1300 / 2000 [ 65%]  (Sampling)
Chain 4 Iteration: 1400 / 2000 [ 70%]  (Sampling)
Chain 4 Iteration: 1500 / 2000 [ 75%]  (Sampling)
Chain 4 Iteration: 1600 / 2000 [ 80%]  (Sampling)
Chain 4 Iteration: 1700 / 2000 [ 85%]  (Sampling)
Chain 4 Iteration: 1800 / 2000 [ 90%]  (Sampling)
Chain 4 Iteration: 1900 / 2000 [ 95%]  (Sampling)
Chain 4 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 4 finished in 0.0 seconds.

All 4 chains finished successfully.
Mean chain execution time: 0.0 seconds.
Total execution time: 0.7 seconds.
```

For this simple model, this takes less than a second.

5.2.5 Summarizing and plotting the posterior samples

```r
# Actual posterior samples
fit$draws("theta", format = "draws_df")
```

```
# A draws_df: 1000 iterations, 4 chains, and 1 variables
   theta
1   0.63
2   0.63
3   0.62
```

```
4   0.63
5   0.62
6   0.62
7   0.62
8   0.62
9   0.64
10  0.63
# ... with 3990 more draws
# ... hidden reserved variables {'.chain', '.iteration', '.draw'}
```

```
# Summary table
fit$summary()
```

```
# A tibble: 2 x 10
  variable      mean    median      sd     mad        q5      q95  rhat ess_bulk
  <chr>        <dbl>     <dbl>   <dbl>   <dbl>     <dbl>    <dbl> <dbl>    <dbl>
1 lp__     -1892.    -1892.    0.698   0.326   -1894.    -1.89e+3  1.00    1598.
2 theta        0.619     0.619 0.00920 0.00930     0.604  6.34e-1  1.00    1390.
# i 1 more variable: ess_tail <dbl>
```

```
# Histogram
fit$draws("theta") |>
    mcmc_hist()
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

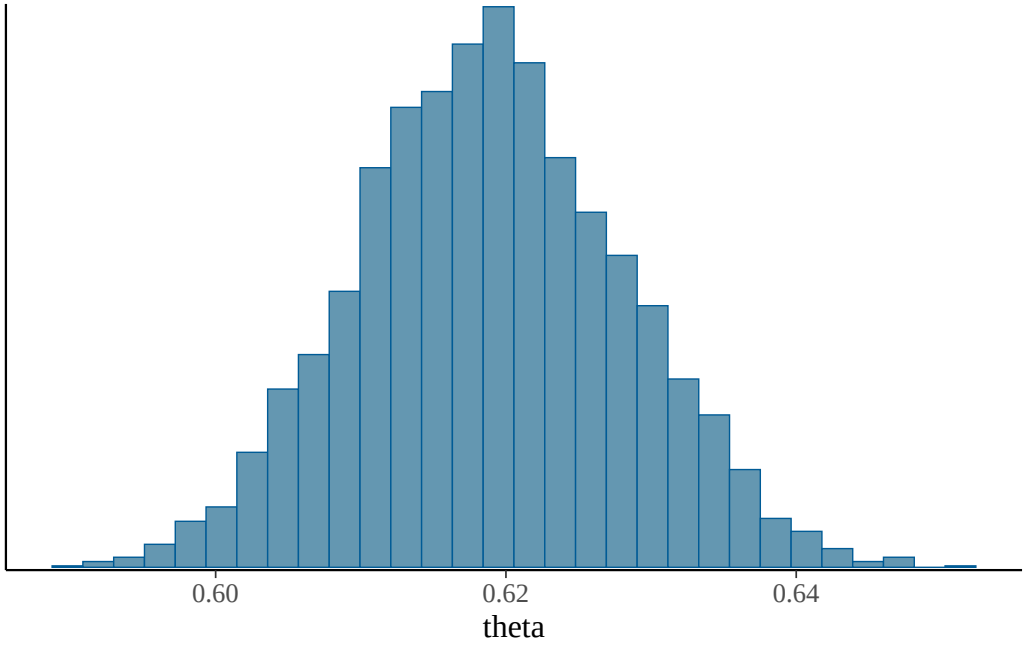


Figure 5.1: Posterior distribution of the parameter.

The results are similar to those in last class.

5.3 Prior Predictive Check

In Bayesian analyses, it is recommended to check both the prior and the model. This can be done by

1. Prior predictive check: Simulating data from the prior distribution, and see if the simulated data fit our prior belief.
2. Posterior predictive check: Simulating data from the posterior distribution, and see if the simulated data are comparable to the observed data.

We will use the following Stan code to do prior and posterior predictive checks, which has an additional generated quantity block to obtain

a. `prior_theta`: simulated values of θ based on the prior distribution
b. `prior_ytilde`: simulated data based on the prior distribution of θ
c. `ytilde`: simulated data based on the posterior distribution of θ

```
data {
  int<lower=0> N;  // number of observations
  array[N] int<lower=0,upper=1> y;  // y
}
parameters {
  real<lower=0,upper=1> theta;  // theta parameter
}
model {
  theta ~ beta(2, 2);  // prior: Beta(2, 2)
  y ~ bernoulli(theta);  // model: Bernoulli
}
generated quantities {
  real prior_theta = beta_rng(2, 2);
  array[N] int prior_ytilde;
  array[N] int ytilde;
  for (i in 1:N) {
    ytilde[i] = bernoulli_rng(theta);
    prior_ytilde[i] = bernoulli_rng(prior_theta);
  }
}
```

```
bern_pp_mod <- cmdstan_model("stan_code/beta-bernoulli-pp.stan")
bern_pp_fit <- bern_pp_mod$sample(
    Aids2_standata,
    refresh = 500  # show progress every 500 iterations
)
```

```
Running MCMC with 4 sequential chains...

Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration:  500 / 2000 [ 25%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 1 Iteration: 1500 / 2000 [ 75%]  (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 1 finished in 0.9 seconds.
Chain 2 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 2 Iteration:  500 / 2000 [ 25%]  (Warmup)
Chain 2 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 2 Iteration: 1500 / 2000 [ 75%]  (Sampling)
Chain 2 Iteration: 2000 / 2000 [100%]  (Sampling)
```

```
Chain 2 finished in 0.9 seconds.
Chain 3 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 3 Iteration:  500 / 2000 [ 25%]  (Warmup)
Chain 3 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 3 Iteration: 1500 / 2000 [ 75%]  (Sampling)
Chain 3 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 3 finished in 0.8 seconds.
Chain 4 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 4 Iteration:  500 / 2000 [ 25%]  (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 4 Iteration: 1500 / 2000 [ 75%]  (Sampling)
Chain 4 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 4 finished in 0.9 seconds.

All 4 chains finished successfully.
Mean chain execution time: 0.9 seconds.
Total execution time: 3.8 seconds.
```

With Stan, because we obtained 4,000 prior/posterior draws (the software default) of θ, we also obtained 4,000 simulated data sets. We can see the first one, based on only the prior distribution (i.e., $\theta \sim \text{Beta}(2, 2)$):

```
bern_pp_fit$draws("prior_ytilde", format = "draws_df")[1, ] |>
    as.numeric() |>
    table()
```

```
   0    1
1109 1737
```

> Note that the data set has more 1's than 0's. Our prior is weak, which means that it allows for a lot of variation in how the data would look.

The distribution of simulated *data* based on the prior distribution of the parameters is called the *prior predictive distribution*. Mathematically, we write it as

$$P(\tilde{y}) = \int P(\tilde{y}|\theta)P(\theta)\,\mathrm{d}\theta$$

Because we have 4,000 data sets, it is not easy to visualize all individual data points. Instead, we can visualize some summary statistics of the simulated data. Here, we will choose the proportion of deaths (i.e., the mean of the variable) in each simulated data set:

```
bern_pp_fit$draws("prior_ytilde", format = "draws_matrix") |>
    ppd_stat(stat = "mean")
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

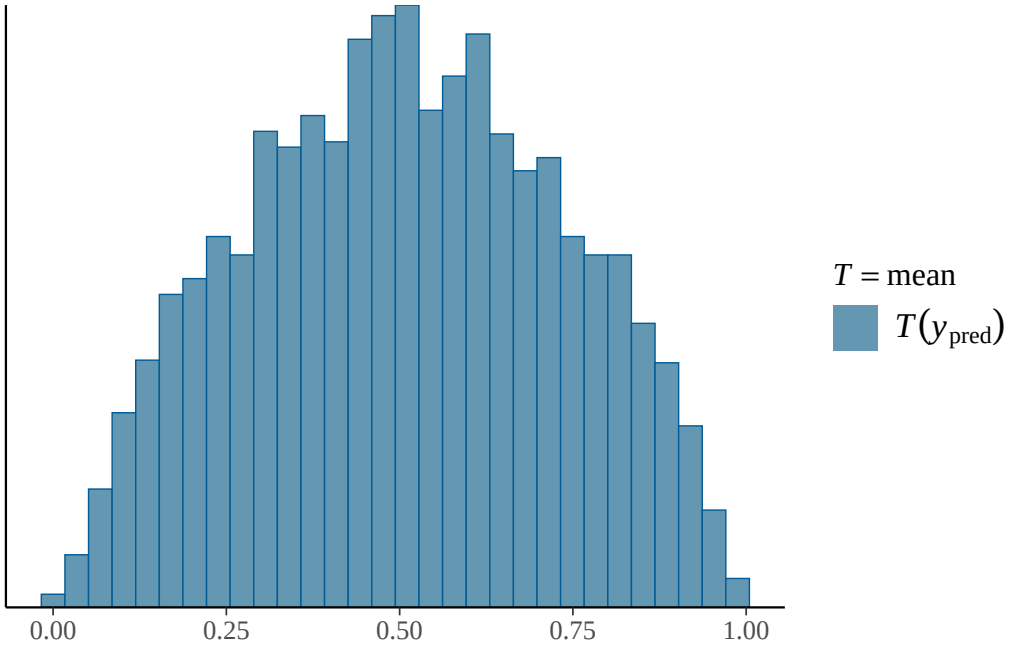


Figure 5.2: Prior predictive distribution of the sample mean.

This represents our prior belief about the proportion of deaths without looking at the actual data. If this doesn't seem to match our belief, we may want to modify our prior distribution and do the prior predictive check again, until the simulated data matches our actual prior belief.

5.4 Posterior Predictive Check

5.4.1 Check 1: Sample Mean

$$P(\tilde{y}|y) = \int P(\tilde{y}|\theta, y)P(\theta|y)\ \mathrm{d}\theta$$

The difference here is that we use the posterior distribution $P(\theta|y)$ instead of the prior distribution $P(\theta)$. We can obtain the posterior predictive distribution of the death rate, and indicate the actual data in the plot:

```
bern_pp_fit$draws("ytilde", format = "draws_matrix") |>
    ppc_stat(y = Aids2_standata$y, stat = "mean")
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

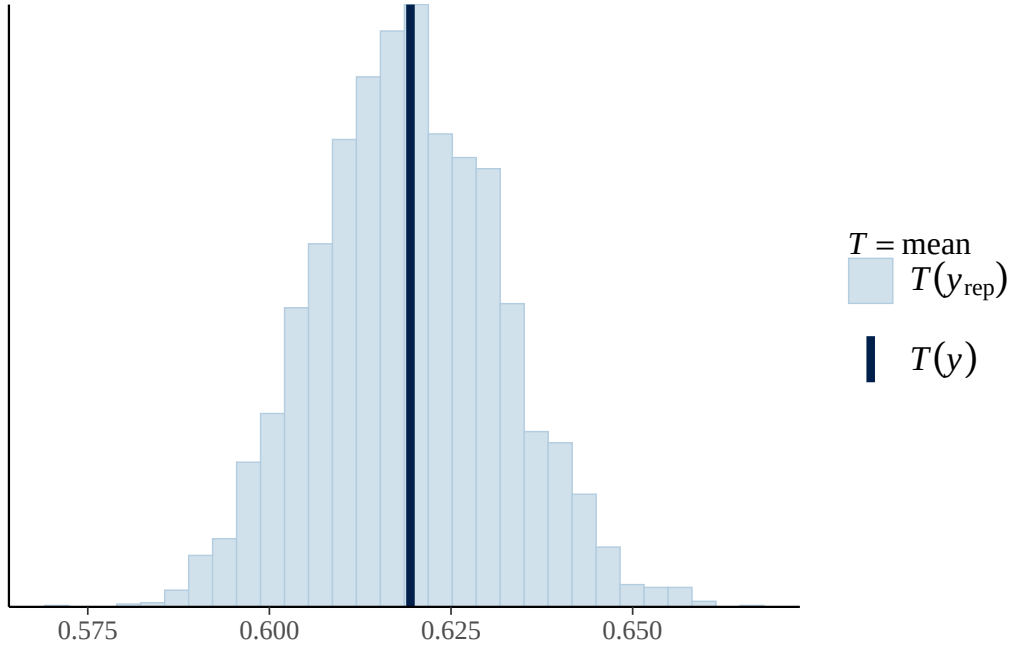


Figure 5.3: Posterior predictive distribution of the sample mean.

5.4.2 Check 2: Sample Mean by Age Group

```
# Create binary indicator of two age groups
age50 <- factor(Aids2$age > 50, labels = c("<= 50", "> 50"))
bern_pp_fit$draws("ytilde", format = "draws_matrix") |>
    ppc_stat_grouped(y = Aids2_standata$y, group = age50,stat = "mean")
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

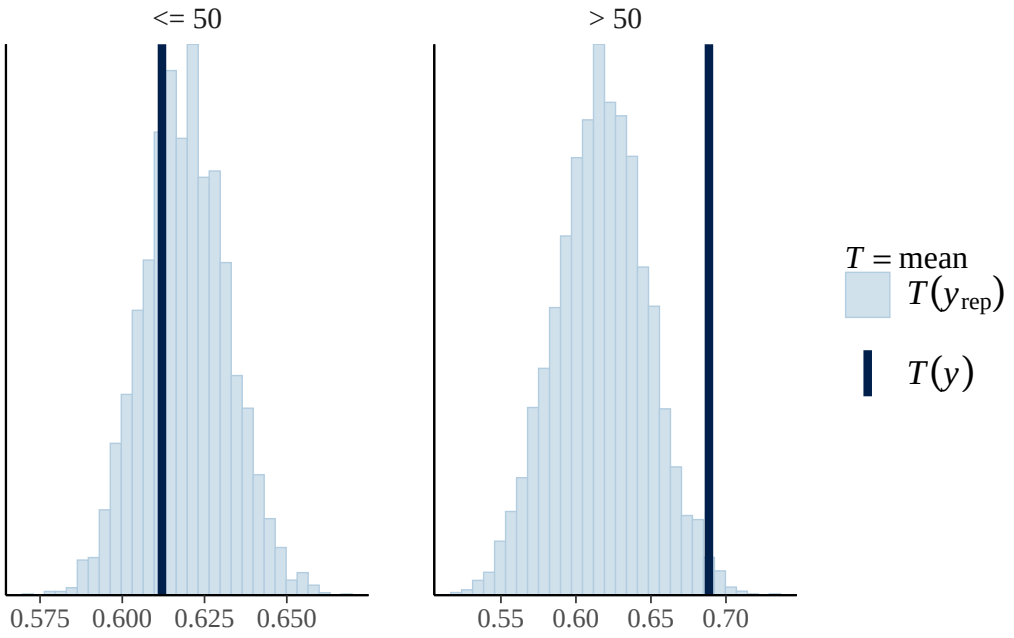


Figure 5.4: Posterior predictive distribution of the sample mean by age group.

6 Poisson Model

> Please note: This document uses count data on fatal police shootings.

I came across this data set from https://andrewpwheeler.com/2021/01/11/checking-a-poisson-distribution-fit-an-example-with-officer-involved-shooting-deaths-wapo-data-r-functions/

As explained here, the data are by the Washington Post in an effort to record every fatal shooting in the United States by a police officer since January 1, 2015.

6.1 Research Question

What's the rate of fatal police shootings in the United States per year?

6.2 Data Import and Pre-Processing

```
# Import data
fps_dat <- read_csv(
    "https://github.com/washingtonpost/data-police-shootings/raw/master/v2/fatal-police-shoot
)
```

We first count the data by year

```
# Create a year column
fps_dat <- fps_dat |>
    mutate(year = format(date, format = "%Y"))
# Filter out the latest year
fps_1523 <- filter(fps_dat, year != max(year))
count(fps_1523, year)
```

```
# A tibble: 9 x 2
  year      n
  <chr> <int>
1 2015    995
2 2016    959
3 2017    984
4 2018    992
5 2019    994
6 2020   1021
7 2021   1050
8 2022   1097
9 2023   1164
```

Our interest is the rate of occurrence of fatal police shootings per year. Denote this as θ. The *support* of θ is $[0, \infty)$.

A *Poisson model* is usually a starting point for analyzing count data in a fixed amount of time. It assumes that the data follow a Poisson distribution with a fixed rate parameter:

$$P(y \mid \theta) \propto \theta^y \exp(-\theta),$$

where the data can be any non-negative integers (no decimals).

6.3 Choosing a Prior

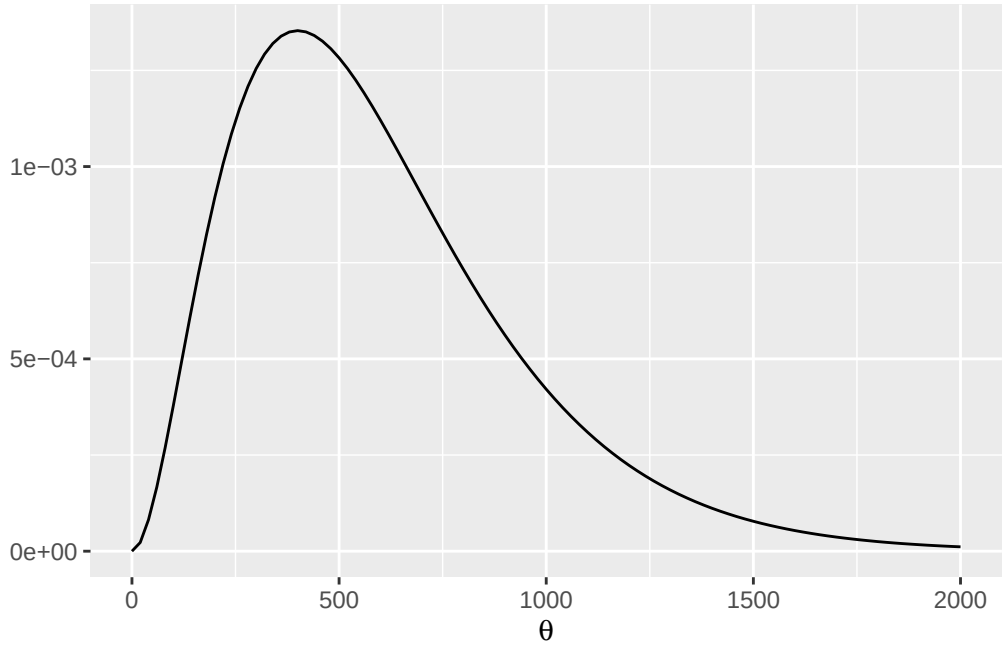
The Gamma distribution has support: $[0, \infty)$, and is a conjugate family to the Poisson model. The Gamma distribution has the form

$$P(\theta) \propto \theta^{a-1} \exp(-b\theta),$$

where a is the prior incidence rate, and b is the number of prior data points to control for the prior strength. Here, without much prior knowledge, I would simply guess there is one fatal shooting per state per month, so 600 shootings per year, but my belief is pretty weak, so I will assume a prior b of 1 / 200 (one observation is one year). The a will be 600 * b = 3.

Here's a plot:

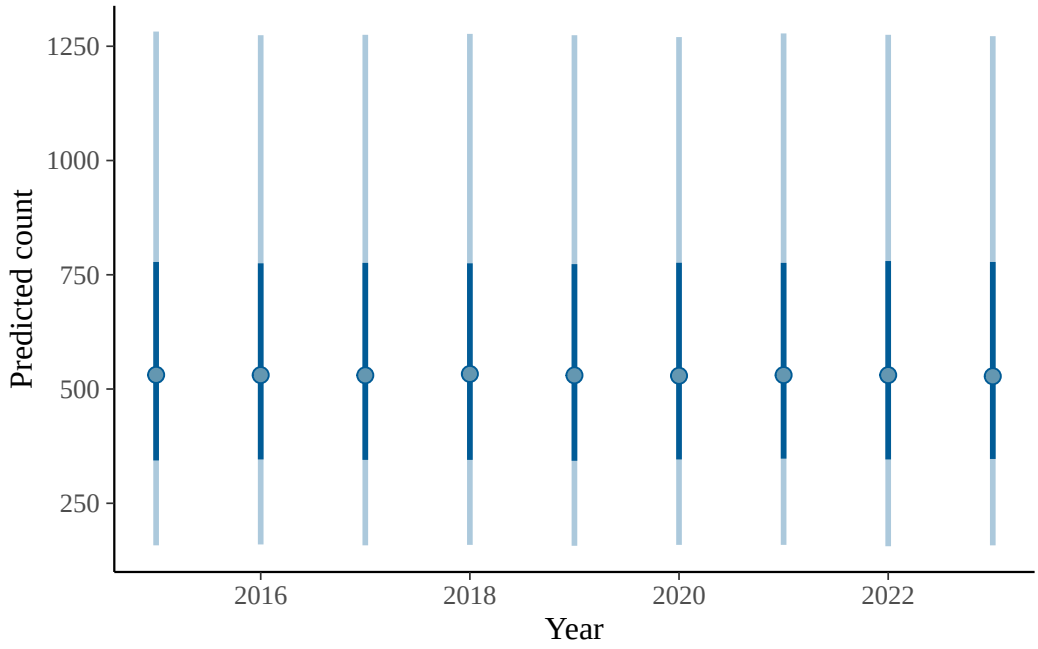
```
ggplot(data.frame(th = c(0, 2000)), aes(x = th)) +
    stat_function(fun = dgamma,
    args = list(shape = 3, rate = 1 / 200)) +
    labs(y = "", x = expression(theta))
```


1e−03
5e−04
0e+00
0
500
1000
1500
2000
θ

6.3.4 Prior predictive check

Here I plot simulated trends from the prior distribution.

```
# Extract predicted y from prior
fit$draws("prior_ytilde", format = "draws_matrix") |>
    ppd_intervals(x = 2015:2023) +
    labs(x = "Year", y = "Predicted count")
```

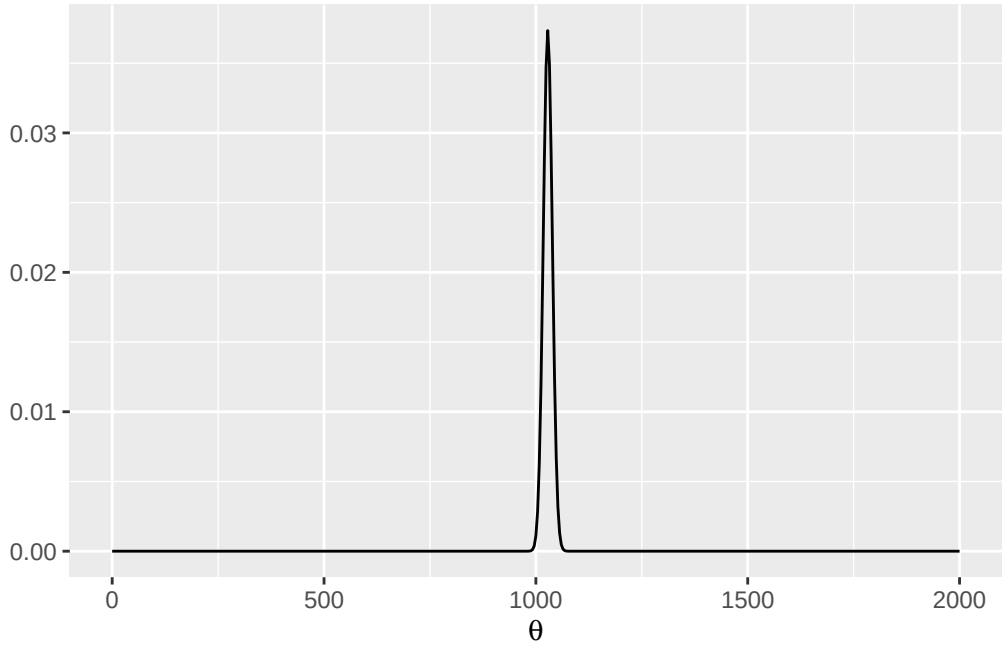


The check is on whether the numbers seem reasonably reflective of my knowledge.

6.4 Posterior

With a conjugate prior, the posterior distribution is Gamma$(a + \sum_{i=1}^{N} y_i, b + N)$.

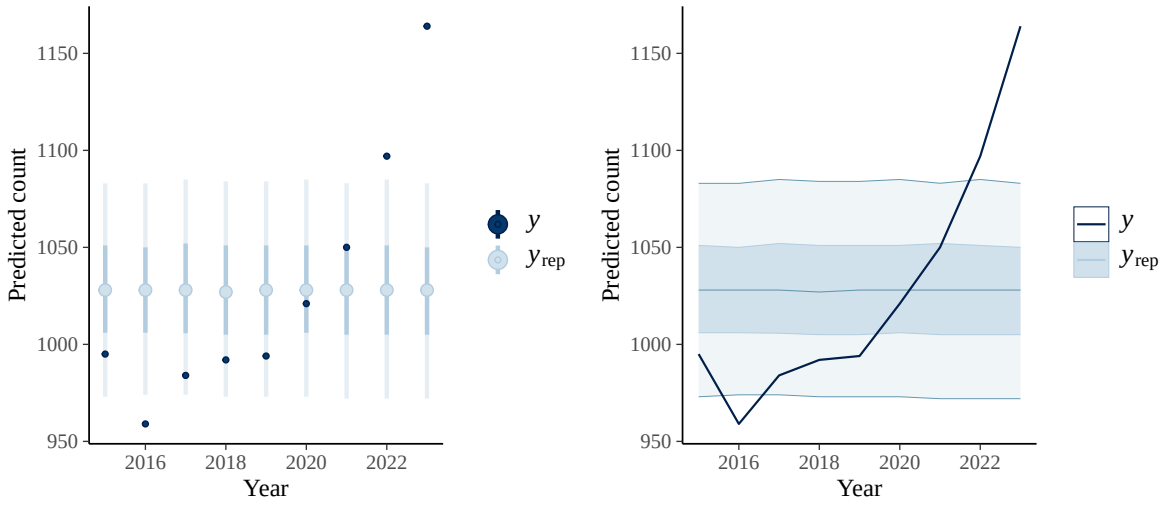
```
ggplot(data.frame(th = c(0, 2000)), aes(x = th)) +
    stat_function(fun = dgamma,
    args = list(shape = 3 + nrow(fps_1523),
                rate = 1 / 200 + fps_standata$N), n = 501) +
    labs(y = "", x = expression(theta))
```



6.5 Posterior Predictive Check

Plot predicted data from the posterior against observed data

```
# Extract predicted y from posterior
fit$draws("ytilde", format = "draws_matrix") |>
    ppc_intervals(
        y = fps_standata$y,
        x = 2015:2023
    ) +
    labs(x = "Year", y = "Predicted count")
# We can also use `bayesplot::ppc_ribbon()`
fit$draws("ytilde", format = "draws_matrix") |>
    ppc_ribbon(
        y = fps_standata$y,
        x = 2015:2023
    ) +
    labs(x = "Year", y = "Predicted count")
```



(a) Interval plots.

(b) Ribbon plots.

Figure 6.1: Posterior predictive check.

From Figure 6.1, one can see that the fit is not good, as there is a large gap between the model prediction and the observed data from recent years. This suggests a need to incorporate the time trend in the model.

6.6 Summary of Posterior

For now, we will proceed with interpreting the posterior distribution, despite the apparent misfit.

```
(summ_theta <- fit$summary("theta"))
```

```
# A tibble: 1 x 10
  variable  mean median    sd   mad    q5   q95  rhat ess_bulk ess_tail
  <chr>    <dbl>  <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
1 theta    1028.  1028.  10.5  10.8 1011. 1045.  1.00    1164.    1960.
```

So the estimated rate is 1,028 per year, with a 90% CI [1,011, 1,045].

Part IV

Week 4

7 Hierarchical Models

Although many statistical models can be fitted using Bayesian or frequentist methods, some models are more naturally used in the Bayesian framework. One class of such models is the family of **hierarchical models.** Consider situations when the data contain *clusters*, such as multiple data points in each of many participants, or multiple participants in each of several treatment conditions. While it is possible to run J Bayesian analyses for the J subsets of the data, it is usually more efficient to pool the data together. In this approach, each cluster j has some parameters θ_j, and these J θ values themselves come from a common distribution. Figure 7.1 shows a graphical representation of the concept of pooling. This is the same idea as multilevel modeling, a topic we will discuss more later in the course.

> **!** A hierarchical model is one in which some higher-level distributions govern one or more parameters, and those higher-level distributions are characterized by *hyperparameters* and can be assigned *hyperpriors*.
> Hierarchical models are commonly used to study and account for individual differences in some model parameters.

In this note, you will see two examples, one from a textbook (Kruschke, 2015) with a hierarchical Bernoulli/binomial model, and another from a classic data set with eight schools, modelled by a hierarchical normal model.

7.1 Hierarchical Bernoulli/Binomial

We will first consider a therapeutic touch example (Kruschke, 2015, Chapter 9). Therapeutic touch is a technique in alternative medicine to relieve pain, but scientific evidence does not support its effectiveness. The data here are from an experiment where the experimenter randomly hovered their hand over either the participant's left or right hand, and the participant had to guess which hand was being hovered without seeing. This is repeated 10 times for each participant. There are a total of 28 participants in the dataset.

Previously, we have seen the Bernoulli model for N outcomes (i.e., whether the guess is correct):

$$y_i \sim \text{Bern}(\theta), \text{for } i = 1, \ldots, N$$

We assumed exchangeability with θ being the participant's "ability" to guess correctly.

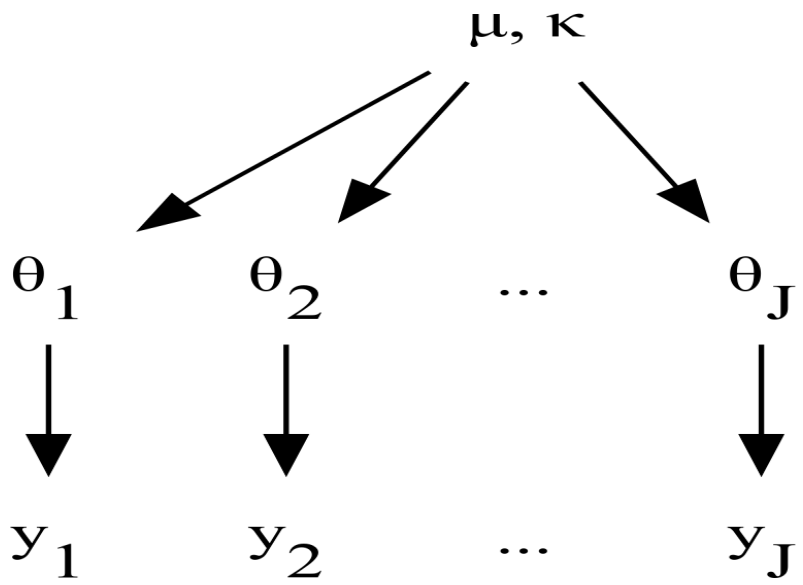


Figure 7.1: A graphical representation of a hierarchical binomial model.

Alternative Parameterization of Beta

In the last class, we have used the Beta(a, b) prior for a Bernoulli outcome, such that

$$P(\theta \mid a, b) \propto \theta^{a-1}(1-\theta)^{b-1}.$$

However, in hierarchical models to be discussed later, it is beneficial to consider another way to express the Beta distribution, in terms of the *prior mean*, $\mu = a/(a+b)$, $\mu \in [0, 1]$, and the concentration, $\kappa = a + b$, $\kappa \in [0, \infty)$. So, instead of the above formula, we can write

$$P(\theta \mid \mu, \kappa) \propto \theta^{\mu\kappa-1}(1-\theta)^{(1-\mu)\kappa-1}.$$

The two expressions represent exactly the same distribution, but just in terms of parameters of different meanings. Therefore, they are referred to as **different parameterization** of the Beta distribution.

7.1.1 Multiple Bernoulli = Binomial

With N exchangeable Bernoulli observations, an equivalent but more efficient way to code the model is to use the *binomial* distribution. Let $z = \sum_{i=1}^{N} y_i$, then

$$z \sim \text{Bin}(N, \theta)$$

7.1.2 Multiple Binomial Observations

Now, because we have multiple participants, we could study whether each participant had noticeable differences in their guessing ability. We can use a binomial model for each participant, from participant 1 to participant J:

$$\begin{aligned} z_1 &\sim \text{Bin}(N_1, \theta_1) \\ z_2 &\sim \text{Bin}(N_2, \theta_2) \\ &\vdots \\ z_J &\sim \text{Bin}(N_J, \theta_J) \end{aligned}$$

Or instead of writing J equations, we can use the subscript j to refer to each participant:

$$z_j \sim \text{Bin}(N_j, \theta_j)$$

If we believe that all participants have the same ability, then we could consider the model

$$z_j \sim \text{Bin}(N_j, \theta),$$

which still contains only one parameter, θ. However, if we have reason to believe that the coins have different biases, then we should have

$$z_j \sim \text{Bin}(N_j, \theta_j),$$

with parameters $\theta_1, \ldots, \theta_j$.

We can assign priors to each θ_j. However, suppose our prior belief is that there's something common among the different participants (e.g., they're all human beings), so they come from a common distribution. In that case, we can have common parameters for the prior distributions of the θs:

$$\theta_j \sim \text{Beta\_Proportion}(\mu, \kappa),$$

note I use Beta_Proportion to denote the mean parameterization. Here, we express the prior belief that the **mean ability** of the different participants is μ, and how each participant differs from the mean depends on κ. Now, μ and κ are hyperparameters. We can assign some fixed values to μ and κ, as if we know what the average ability is. However, the power of the

hierarchical model is that we can put priors (or hyper priors) on μ and κ, and obtain posterior distributions of them, based on what the data say.

What priors to use for μ and κ? μ is relatively easy because it is the mean ability; if we put a Beta prior for each participant's ability, we can again use a Beta prior for the mean ability. κ is more challenging. A larger κ means that the participants' abilities are more similar to each other. We can perform a prior predictive check to see what the data look like. As a starting point, some textbook (e.g., chapter 9 of Kruschke, 2015) suggested using Gamma(0.01, 0.01). So the full model in our case, with a weak Beta(1.5, 1.5) prior on μ, is

Model:

$$z_j \sim \text{Bin}(N_j, \theta_j)$$
$$\theta_j \sim \text{Beta2}(\mu, \kappa)$$

Prior:

$$\mu \sim \text{Beta}(1.5, 1.5)$$
$$\kappa \sim \text{Gamma}(0.01, 0.01)$$

We will import the data and fit the model

```
# Data file from GitHub
tt_url <- paste0(
    "https://github.com/boboppie/kruschke-doing_bayesian_data_analysis/",
    "raw/master/2e/TherapeuticTouchData.csv"
)
tt_dat <- read.csv(tt_url)
# Get aggregated data by summing the counts
tt_agg <- tt_dat |>
    group_by(s) |>
    summarise(y = sum(y),  # total number of correct
              n = n())
# Plot proportion correct distribution
p1 <- ggplot(tt_agg, aes(x = y / n)) +
    geom_histogram(binwidth = .1) +
    labs(x = "Proportion Correct")
```

7.1.3 Stan Code

```
data {
  int<lower=0> J;  // number of clusters (e.g., studies, persons)
  array[J] int y;  // number of "1"s in each cluster
```

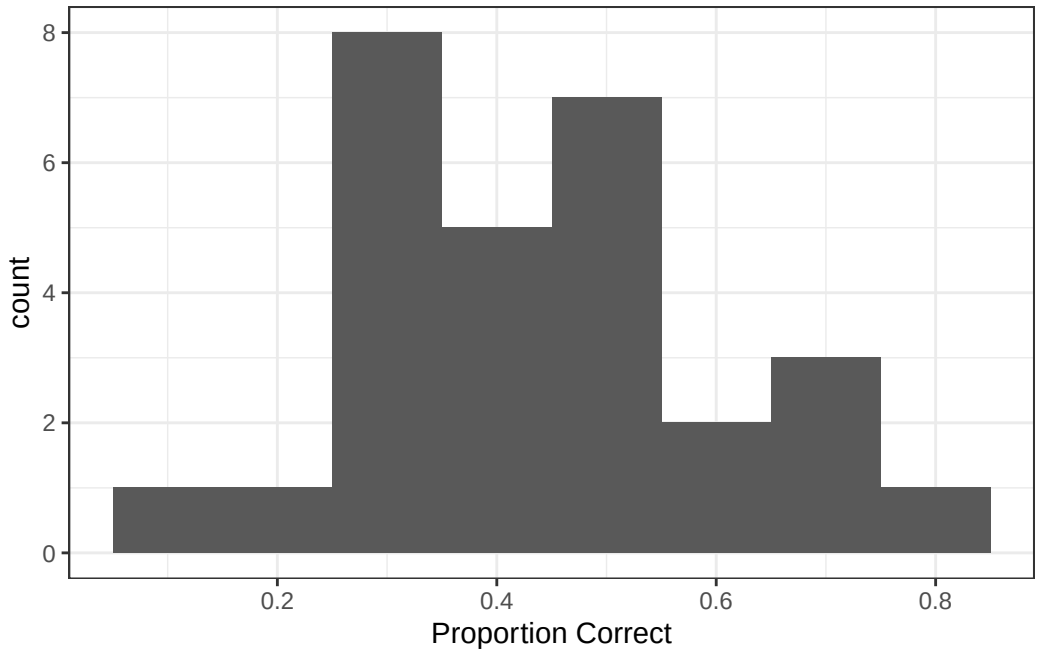


Figure 7.2: Distribution of proportions of correct responses across participants.

```
  array[J] int N;  // sample size for each cluster
}
parameters {
  // cluster-specific probabilities
  vector<lower=0, upper=1>[J] theta;
  real<lower=0, upper=1> mu;  // overall mean probability
  real<lower=0> kappa;        // overall concentration
}
model {
  y ~ binomial(N, theta);  // each observation is binomial
  // Priors
  theta ~ beta_proportion(mu, kappa);
  mu ~ beta(1.5, 1.5);      // weak prior
  kappa ~ gamma(.1, .1);  // prior recommended by Kruschke
}
generated quantities {
  // Prior and posterior predictive
  real<lower=0, upper=1> prior_mu = beta_rng(1.5, 1.5);
  real<lower=0> prior_kappa = gamma_rng(.1, .1);
  vector<lower=0, upper=1>[J] prior_theta;
```

```
  for (j in 1:J) {
    prior_theta[j] = beta_proportion_rng(prior_mu, prior_kappa);
  }
  array[J] int prior_ytilde = binomial_rng(N, prior_theta);
  // Posterior predictive
  array[J] int ytilde = binomial_rng(N, theta);
}
```

```
hbin_mod <- cmdstan_model("stan_code/hierarchical-binomial.stan")
```

7.1.4 Prior predictive

You can use Stan to sample the prior and obtain the prior predictive distribution; here, I show how to do it in R, with a Gamma(.01, .01) prior on κ:

```
set.seed(1706)
plist <- vector("list", 12L)
plist[[1]] <- p1 +
    labs(x = "Observed data") +
    theme(axis.title.x = element_text(color = "red"))
num_subjects <- 28
for (s in 1:11) {
    # Get prior values of mu and kappa
    mu_s <- rbeta(1, shape1 = 1.5, shape2 = 1.5)
    kappa_s <- rgamma(1, shape = 0.01, rate = 0.01)
    # Generate theta
    theta <- rbeta(num_subjects,
                   shape1 = mu_s * kappa_s,
                   shape2 = (1 - mu_s) * kappa_s)
    # Generate data
    new_y <- rbinom(num_subjects, size = tt_agg$n, prob = theta)
    plist[[s + 1]] <-
        p1 %+% mutate(tt_agg, y = new_y) +
        labs(x = paste("Simulated data", s)) +
        theme(axis.title.x = element_text(color = "black"))
}
gridExtra::grid.arrange(grobs = plist, nrow = 3)
```

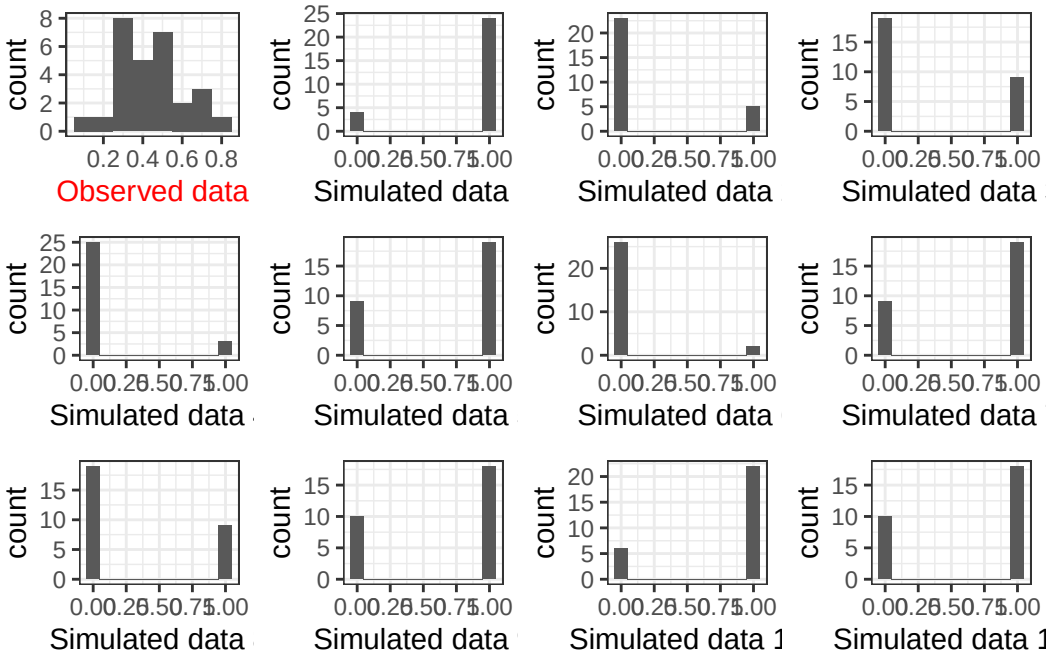


Figure 7.3: Prior predictive distribution.

The prior on κ is not very realistic because it pushes the bias to either 0 or 1. Using something like Gamma(0.1, 0.1) or Gamma(2, 0.01) may be more reasonable (you can try it out yourself).

7.1.5 Calling Stan

```
tt_fit <- hbin_mod$sample(
    data = list(J = nrow(tt_agg),
                y = tt_agg$y,
                N = tt_agg$n),
    seed = 1716,  # for reproducibility
    refresh = 1000
)
```

```
Running MCMC with 4 sequential chains...

Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
```

```
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 1 finished in 0.1 seconds.
Chain 2 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 2 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]  (Sampling)

Chain 2 Informational Message: The current Metropolis proposal is about to be rejected becaus

Chain 2 Exception: beta_proportion_lpdf: Location parameter is 1, but must be less than 1.000

Chain 2 If this warning occurs sporadically, such as for highly constrained variable types li

Chain 2 but if this warning occurs often then your model may be either severely ill-condition

Chain 2

Chain 2 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 2 finished in 0.1 seconds.
Chain 3 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 3 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 3 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 3 finished in 0.1 seconds.
Chain 4 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]  (Sampling)

Chain 4 Informational Message: The current Metropolis proposal is about to be rejected becaus

Chain 4 Exception: beta_proportion_lpdf: Location parameter is 0, but must be positive! (in

Chain 4 If this warning occurs sporadically, such as for highly constrained variable types li

Chain 4 but if this warning occurs often then your model may be either severely ill-condition

Chain 4
```

```
Chain 4 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 4 finished in 0.2 seconds.

All 4 chains finished successfully.
Mean chain execution time: 0.1 seconds.
Total execution time: 1.0 seconds.
```

You can explore the convergence and posterior distributions using the `shinystan` package

```
shinystan::launch_shinystan(tt_fit)
```

7.1.6 Table of coefficients

```
tt_fit$summary(c("theta", "mu", "kappa")) |>
    # Use `knitr::kable()` for tabulation
    knitr::kable(digits = 2)
```

Table 7.1: Posterior summary of hierarchical binomial model for the therapeutic touch example.

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
theta[1]	0.31	0.31	0.10	0.10	0.15	0.47	1	3268.39	2404.91
theta[2]	0.35	0.35	0.10	0.10	0.19	0.51	1	3741.46	2422.69
theta[3]	0.39	0.39	0.10	0.10	0.23	0.55	1	4744.99	2794.69
theta[4]	0.39	0.39	0.10	0.10	0.23	0.55	1	4859.60	3056.80
theta[5]	0.39	0.39	0.10	0.10	0.22	0.55	1	4817.40	2485.43
theta[6]	0.39	0.38	0.10	0.10	0.23	0.55	1	5260.92	2493.09
theta[7]	0.39	0.38	0.10	0.10	0.23	0.55	1	5586.84	2968.73
theta[8]	0.39	0.39	0.10	0.10	0.23	0.55	1	4926.08	3008.76
theta[9]	0.39	0.39	0.10	0.10	0.23	0.55	1	4802.85	2558.79
theta[10]	0.39	0.39	0.10	0.10	0.22	0.55	1	4743.85	2910.25
theta[11]	0.43	0.42	0.10	0.09	0.27	0.59	1	5041.77	3066.93
theta[12]	0.42	0.42	0.09	0.10	0.27	0.58	1	6055.56	2896.89
theta[13]	0.43	0.42	0.10	0.10	0.27	0.59	1	4898.48	3112.24
theta[14]	0.43	0.42	0.10	0.10	0.27	0.59	1	5909.48	3065.15
theta[15]	0.43	0.42	0.10	0.10	0.27	0.59	1	6304.56	3049.53
theta[16]	0.46	0.46	0.10	0.10	0.31	0.62	1	5642.01	3230.67
theta[17]	0.46	0.46	0.10	0.10	0.30	0.63	1	5517.58	3108.00
theta[18]	0.46	0.46	0.10	0.10	0.30	0.63	1	5622.46	2837.76

Table 7.1: Posterior summary of hierarchical binomial model for the therapeutic touch example.

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
theta[19]	0.46	0.46	0.10	0.09	0.31	0.63	1	6228.82	3062.79
theta[20]	0.46	0.46	0.10	0.10	0.30	0.63	1	4758.62	2538.88
theta[21]	0.46	0.46	0.10	0.10	0.30	0.62	1	5922.64	2921.96
theta[22]	0.46	0.46	0.10	0.10	0.31	0.62	1	5218.69	3180.07
theta[23]	0.50	0.50	0.10	0.10	0.34	0.67	1	5424.13	2936.72
theta[24]	0.50	0.50	0.10	0.10	0.34	0.67	1	5321.61	2733.91
theta[25]	0.54	0.54	0.10	0.10	0.38	0.71	1	3861.44	2248.48
theta[26]	0.54	0.54	0.10	0.10	0.37	0.72	1	3808.59	2430.69
theta[27]	0.54	0.54	0.10	0.10	0.38	0.71	1	3679.86	2556.84
theta[28]	0.58	0.57	0.10	0.11	0.41	0.75	1	3005.40	2460.66
mu	0.44	0.44	0.04	0.04	0.38	0.50	1	2482.91	2932.61
kappa	18.65	16.37	9.63	7.92	7.49	36.92	1	992.72	1793.53

7.1.7 Posterior Predictive Check

With hierarchical models, there are two types of posterior predictive distributions:

1. *Same participants but new observations.* We can use the model to generate new observations, but the individual parameters (e.g., θ_j) remain the same. In our example, this would be the situation where we ask **the same 28 participants** to each do 10 more trials.
2. *New participants and new observations.* We can use the model to generate new observations with new parameters from the higher-order distribution (e.g., the Beta distribution for θ_j). In our example, this would be the situation where we ask **a new set of 28 participants** to each do 10 more trials.

In our Stan code, I used (1) to check the fit of the observed data. However, (2) can be helpful when one wants to use the model to make predictions of future data, as future data are unlikely to concern exactly the same participants.

```
# The bayesplot::ppc_bars() unfortunately contains a bug
# (https://github.com/stan-dev/bayesplot/issues/266) at
# the time when I wrote this, so I'll use my own code.
# tt_fit$draws("ytilde", format = "draws_matrix") |>
#     ppc_bars(y = tt_agg$y)
yrep <- tt_fit$draws("ytilde", format = "draws_matrix")
yrep_intervals <- apply(
```

```
    yrep, MARGIN = 1, FUN = \(x) table(factor(x, levels = 0:10))
    ) |>
    apply(MARGIN = 1, FUN = \(x) {
        c(
            lo = quantile(x, .05)[[1]],
            me = median(x),
            hi = quantile(x, .95)[[1]]
        )
    })
data.frame(
    y = table(factor(tt_agg$y, levels = 0:10))
) |>
    setNames(c("x", "y")) |>
    cbind(t(yrep_intervals)) |>
    ggplot(aes(x = x, y = y)) +
    geom_col(alpha = 0.5) +
    geom_pointrange(aes(y = me, ymin = lo, ymax = hi)) +
    labs(y = "count", x = NULL)
```

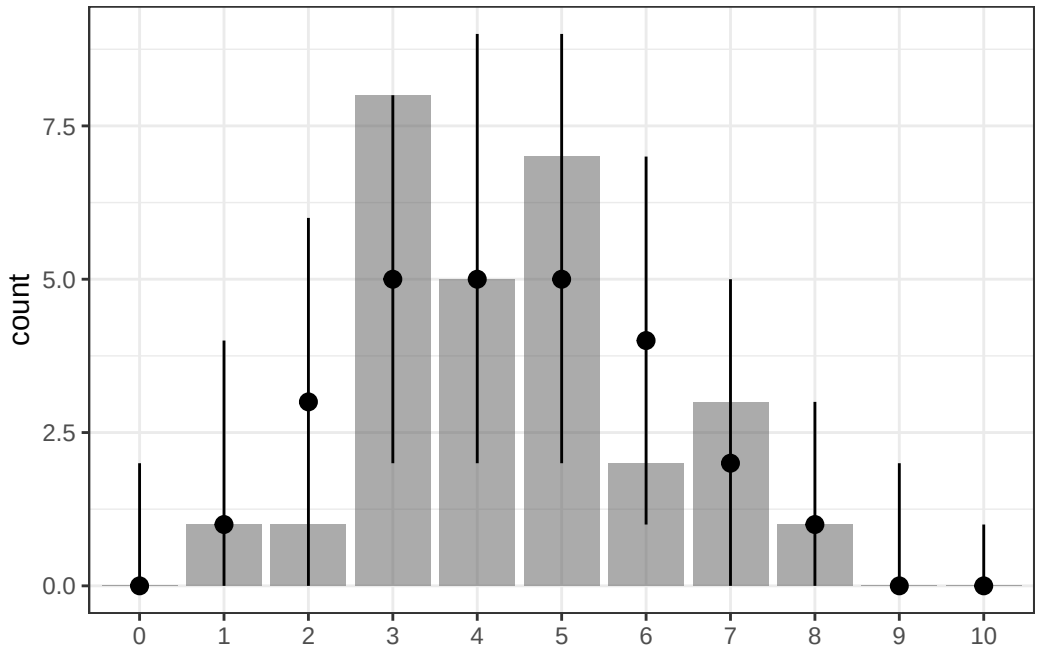


Figure 7.4: Posterior predictive check. The bar graph shows the observed data, and the error bars show the 90% posterior predictive interval in replicated data. The dots are the medians in the posterior predictive distribution.

7.1.8 Derived coefficients

One nice thing about MCMC is that it is straightforward to obtain posterior distributions that are functions of the parameters. For example, even though we only sampled from the posteriors of the θs, we can ask questions like whether there is evidence for a nonzero *difference* in θ between person 1 and person 28.

```
tt_fit$draws() |>
    mutate_variables(
        theta1_minus14 = `theta[1]` - `theta[14]`,
        theta1_minus28 = `theta[1]` - `theta[28]`,
        theta14_minus28 = `theta[14]` - `theta[28]`
    ) |>
    subset(variable = c("theta1_minus14", "theta1_minus28",
                        "theta14_minus28")) |>
    summarise_draws() |>
    knitr::kable(digits = 2)
```

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
theta1_minus14	-0.11	-0.11	0.13	0.13	-0.34	0.09	1	4950.80	2632.63
theta1_minus28	-0.27	-0.26	0.15	0.16	-0.53	-0.03	1	2312.44	3115.27
theta14_minus28	-0.15	-0.15	0.14	0.14	-0.38	0.06	1	4309.81	3013.97

7.1.9 Conclusion

As 0.5 is included in the 95% CI of θ for all participants, there is insufficient evidence that people can sense "therapeutic touch."

7.1.10 Shrinkage

```
mcmc_intervals(tt_fit$draws(),
               # plot only parameters matching "theta"
               regex_pars = "^theta") +
    geom_point(
        data = tibble(
            parameter = paste0("theta[", 1:28, "]"),
            x = tt_agg$y / tt_agg$n
        ),
```

```
        aes(x = x, y = parameter),
        col = "red"
    ) +
    xlim(0, 1)
```

```
Scale for x is already present.
Adding another scale for x, which will replace the existing scale.
```

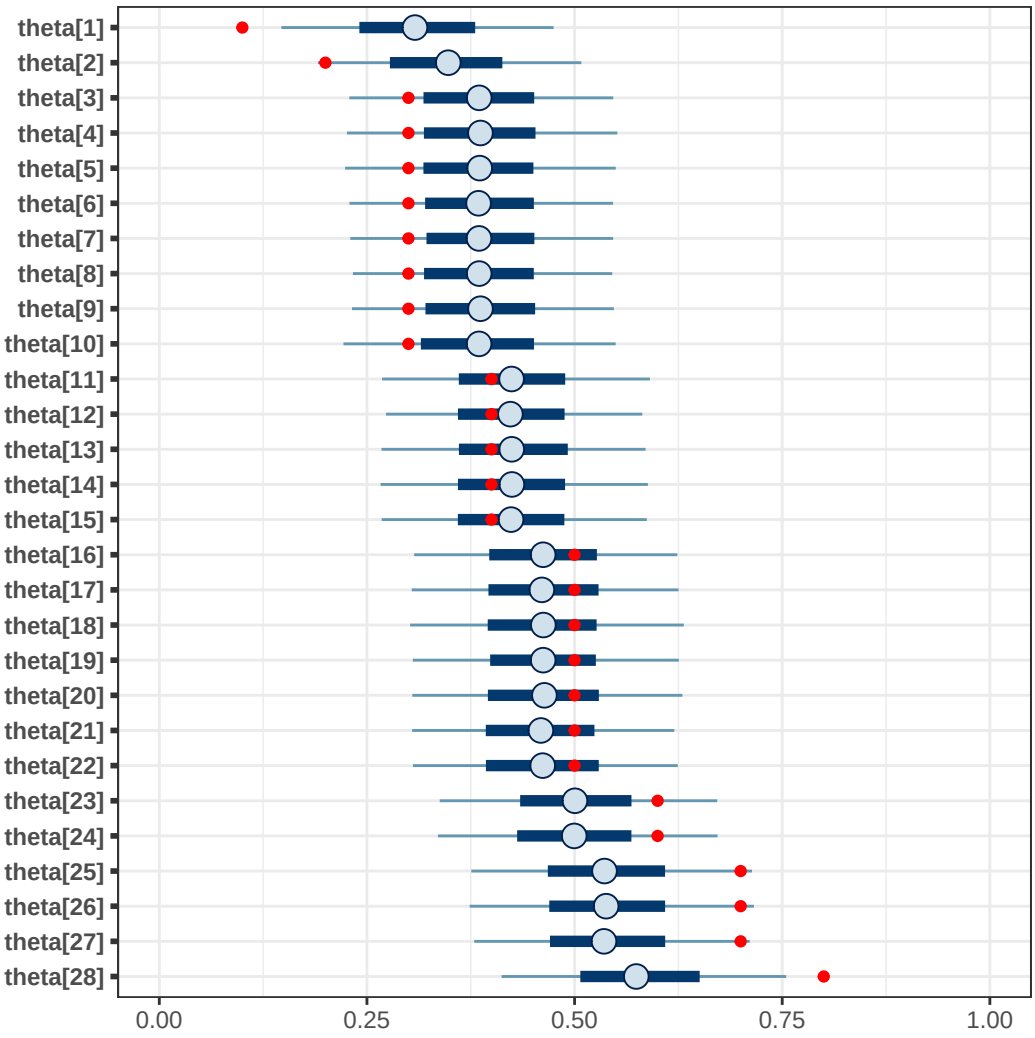


Figure 7.5: Shrinkage effect in a hierarchical model.

As can be seen, the posterior distributions are closer to the center than the data (in red). This

pooling results from the belief that the participants have something in common.

7.1.11 Multiple Comparisons?

Another benefit of a Bayesian hierarchical model is that *you don't need to worry about multiple comparisons*. There are multiple angles on why this is the case, but the basic answer is that the use of common prior distributions builds in the prior belief that the clusters/groups are likely to be equal. See discussion here and here.

7.2 Hierarchical Normal Model

7.2.1 Eight Schools Example

This is a classic data set first analyzed by Rubin (1981). It is also the example used in the RStan Getting Started page. The data contains the effect of coaching from randomized experiments in eight schools. The numbers shown (labelled as `y`) are the mean difference (i.e., effect size) in performance between the treatment and control groups on SAT-V scores.

```
schools_dat <- list(
    J = 8,
    y = c(28, 8, -3, 7, -1, 1, 18, 12),
    sigma = c(15, 10, 16, 11, 9, 11, 10, 18)
)
```

In the above data, some numbers are positive, and some are negative. Because the sample sizes are different, the data also contained the standard errors (labelled as `sigma`) of the effect sizes. Generally speaking, a larger sample size corresponds to a smaller standard error. The research question is

1. What is the average treatment effect of coaching?
2. Are the treatment effects similar across schools?

7.2.2 Model

Model:

$$d_j \sim N(\theta_j, s_j)$$
$$\theta_j \sim N(\mu, \tau)$$

Prior:

$$\mu \sim N(0, 100)$$
$$\tau \sim t_4^+(0, 100)$$

Given the SAT score range, it is unlikely that a coaching program will improve scores by 100 or so, so we use a prior of $\mu \sim N(0, 100)$ and $\tau \sim t_4^+(0, 100)$.

> The model above is the same as one used in a *random-effect meta-analysis*. See this paper for an introduction.

7.2.3 Non-Centered Parameterization

The hierarchical model is known to create issues in MCMC sampling, such that the posterior draws tend to be highly correlated even with more advanced techniques like HMC. One way to alleviate that is to reparameterize the model using what is called the **non-centered parameterization**. The basic idea is that, instead of treating the θs as parameters, one uses the **standardized deviation** from the mean to be parameters. You can think about it as converting the θs into z scores, and then sample the z scores instead of the original θs.

Model:

$$
\begin{aligned}
d_j &\sim N(\theta_j, s_j) \\
\theta_j &= \mu + \tau\eta_j \\
\eta_j &\sim N(0, 1)
\end{aligned}
$$

```
data {
  int<lower=0> J;            // number of schools
  vector[J] y;               // estimated treatment effects
  vector<lower=0>[J] sigma;  // s.e. of effect estimates
}
parameters {
  real mu;                   // overall mean
  real<lower=0> tau;         // between-school SD
  vector[J] eta;             // standardized deviation (z score)
}
transformed parameters {
  vector[J] theta;
  theta = mu + tau * eta;    // non-centered parameterization
}
model {
  eta ~ std_normal();        // same as eta ~ normal(0, 1);
  y ~ normal(theta, sigma);
  // priors
  mu ~ normal(0, 100);
  tau ~ student_t(4, 0, 100);
}
```

```r
hnorm_mod <- cmdstan_model("stan_code/hierarchical-normal.stan")
```

```r
fit <- hnorm_mod$sample(
    data = schools_dat,
    seed = 1804,  # for reproducibility
    refresh = 1000,
    adapt_delta = 0.9  # to improve convergence
)
```

```
Running MCMC with 4 sequential chains...

Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 1 finished in 0.0 seconds.
Chain 2 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 2 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 2 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 2 finished in 0.0 seconds.
Chain 3 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 3 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 3 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 3 finished in 0.0 seconds.
Chain 4 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 4 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 4 finished in 0.0 seconds.

All 4 chains finished successfully.
Mean chain execution time: 0.0 seconds.
Total execution time: 0.5 seconds.
```

Treatment effect estimates of individual schools (θ), average treatment effect (μ), and treatment effect heterogeneity (τ).

```r
fit$summary(c("theta", "mu", "tau")) |>
    knitr::kable(digits = 2)
```

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
theta[1]	11.70	10.60	8.69	7.38	-0.20	27.60	1.00	3475.69	3347.72
theta[2]	7.98	7.93	6.31	5.82	-2.18	18.34	1.00	5870.22	3353.39
theta[3]	6.13	6.77	7.97	6.50	-7.14	17.85	1.00	4318.80	2941.48
theta[4]	7.69	7.75	6.75	6.15	-3.43	18.53	1.00	5452.05	3268.65
theta[5]	5.22	5.53	6.22	5.82	-5.64	14.70	1.00	4118.93	3165.15
theta[6]	6.15	6.52	6.87	6.15	-5.19	16.86	1.00	4526.45	3352.39
theta[7]	10.80	10.14	6.78	6.32	0.88	23.09	1.00	4445.48	3533.95
theta[8]	8.55	8.33	7.74	6.42	-3.59	21.11	1.00	4978.08	3232.97
mu	7.95	8.00	5.26	4.97	-0.43	16.20	1.00	2917.45	1987.36
tau	6.75	5.31	5.91	4.84	0.55	17.53	1.01	1316.86	1673.79

On average, based on the 90% CI, coaching seemed to improve SAT-V by -0.43 to 16.2 points. There was substantial heterogeneity across schools.

We can also get the probability that the treatment effect was > 0:

```
# Obtain draws
draws_mu <- fit$draws("mu", format = "draws_matrix")
mean(draws_mu > 0)
```

```
[1] 0.93975
```

Here are the individual-school treatment effects:

```
mcmc_areas_ridges(fit$draws(), regex_pars = "theta")
```

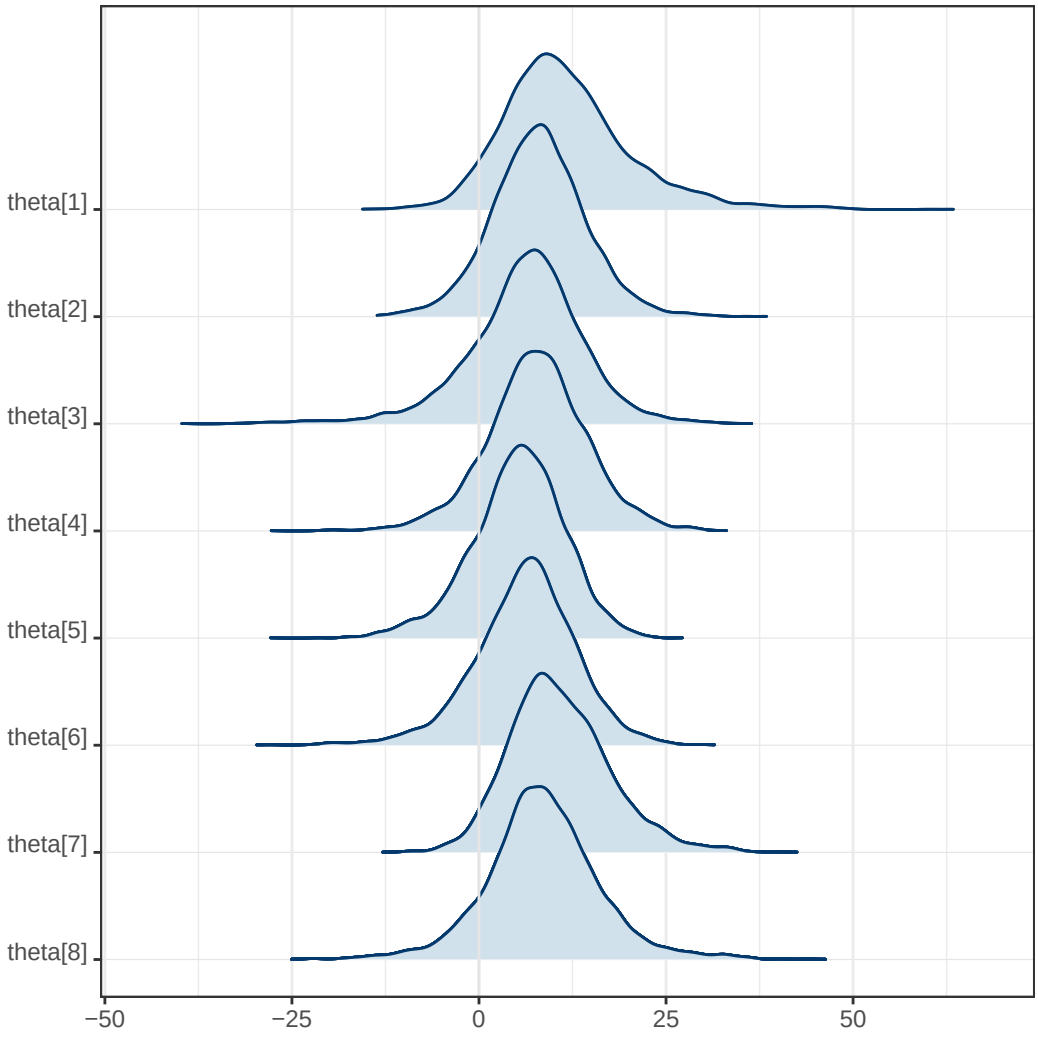


Figure 7.6: Posterior distribution of the true effect size in the eight schools example.

7.2.4 Prediction Interval

Posterior distribution of the true effect size of a new study, $\tilde{\theta}$

```
# Prediction Interval
# (can also be done in Stan, as in the previous example)
fit$draws(c("mu", "tau")) |>
```

```
    mutate_variables(
        theta_tilde = rnorm(4000, mean = mu, sd = tau)) |>
    summarise_draws() |>
    knitr::kable(digits = 2)
```

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
mu	7.95	8.00	5.26	4.97	-0.43	16.20	1.00	2917.45	1987.36
tau	6.75	5.31	5.91	4.84	0.55	17.53	1.01	1316.86	1673.79
theta_tilde	8.03	7.87	10.19	7.00	-6.69	22.89	1.00	3947.08	3042.56

The posterior interval for $\tilde{\theta}$ indicates a range of the treatment effect for a new study.

Part V

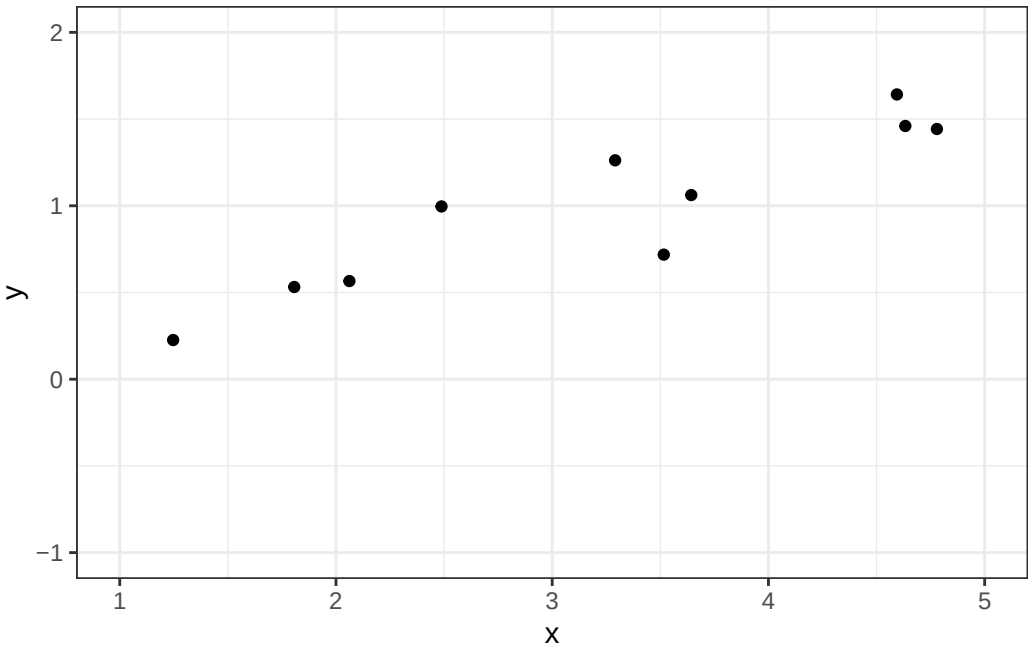
Week 5–6

8 Linear Models

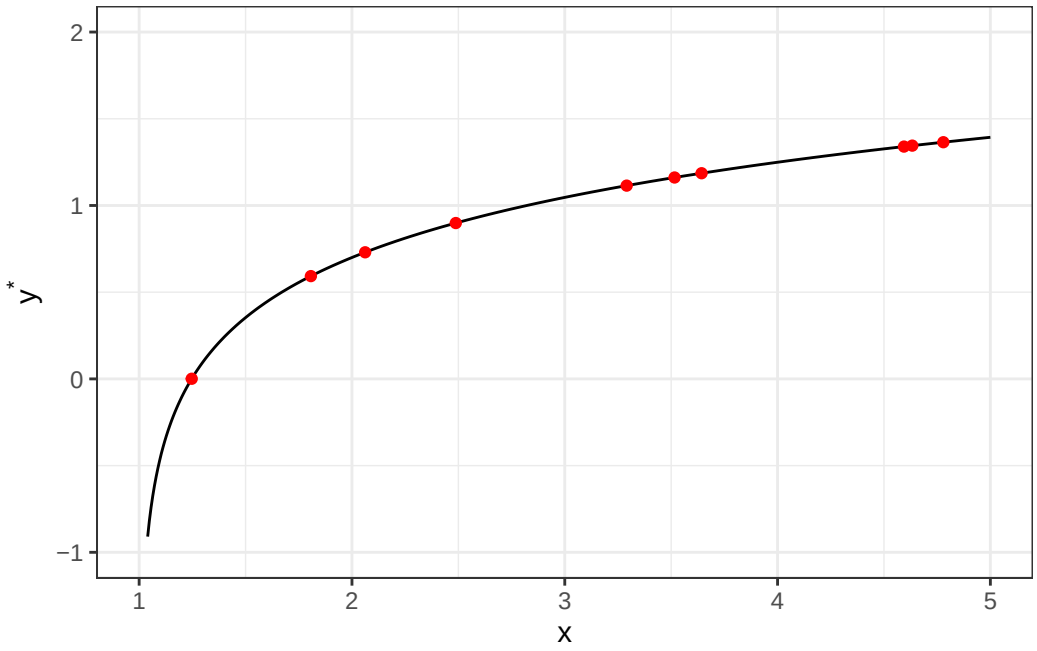
8.1 What is Regression?

Regression is a class of statistical techniques to understand the relationship between an outcome variable (also called a criterion/response/dependent variable) and one or more predictor variables (also called explanatory/independent variables). For example, if we have the following scatter plot between two variables (Y and X):

```
set.seed(1)
x <- round(runif(10, 1, 5), 3)
y <- 0.7 + 0.5 * log(x - 1) + rnorm(10, sd = 0.2)
df <- data.frame(x, y)
ggplot(df, aes(x, y)) +
    geom_point() +
    xlim(1, 5) +
    ylim(-1, 2)
```



We want to find some pattern in this relationship. In conventional regression, we model the conditional distribution of Y given X, $P(Y \mid X)$, by separating the outcome variable Y into (a) a *systematic component* that depends on the predictor, and (b) a *random/probabilistic* component that does not depend on the predictor. For example, we can start with a systematic component which only depends on the predictor:

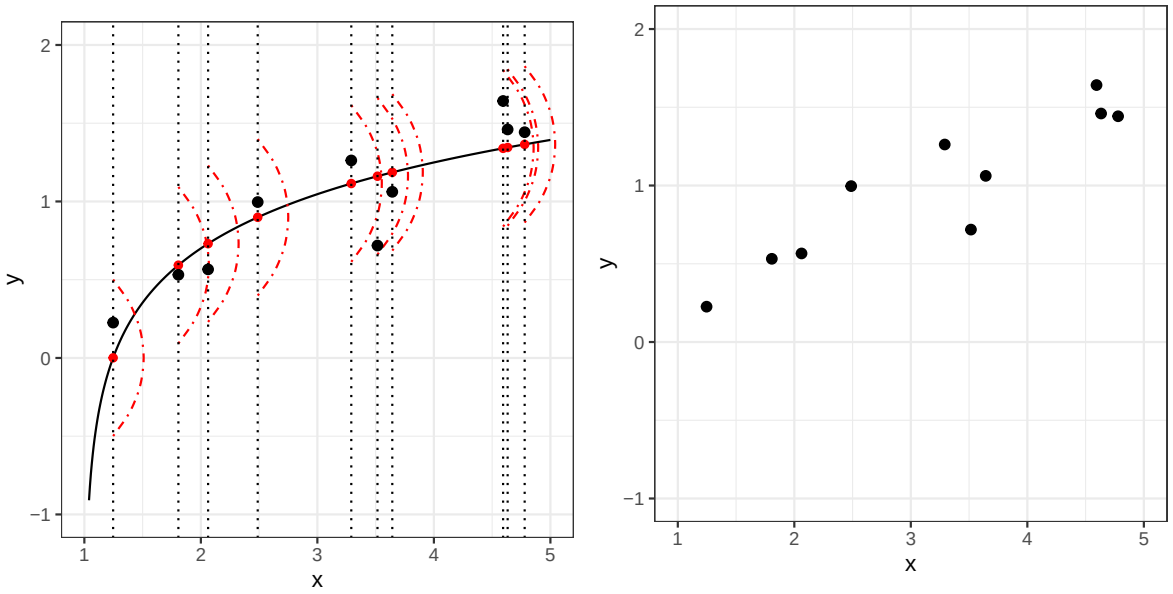


As you can see, all the red dots fall exactly on the curve in the graph above, meaning that as long as one knows the X value, one can predict the Y value with 100% accuracy. We can thus write $Y^* = f(X)$ (where Y^* is the systematic component of Y).

However, in almost all scientific inquiries, one can never predict with 100% certainty (e.g., there are measurement errors and college randomness in physics). The uncertainty stems from the fact that we rarely measure all the factors that determine Y, and there are genuinely random things (as in quantum physics). Therefore, we need to expand our model to incorporate this randomness by adding a probabilistic component. Therefore, instead of saying that Y depends just on X, we say Y is random, but the information about X provides information about how Y is distributed. In regression, one studies the conditional distribution $P(Y \mid X)$ such that the conditional expectation, $E(Y \mid X)$, is determined by X; on top of the conditional expectation, we assume that the observed Y values scatter around the conditional expectations, like the graph on the left below:

```
ggplot(df, aes(x, yhat)) +
    stat_function(fun = function(x) 0.7 + 0.5 * log(x - 1), n = 501) +
    geom_point(col = "red") +
```

```
    xlim(1, 5) +
    ylim(-1, 2) +
    ylab("y") +
    geom_curve(aes(x = x, y = yhat + 0.5, xend = x, yend = yhat - 0.5),
        curvature = -0.4, col = "red", linetype = "dotdash"
    ) +
    geom_vline(aes(xintercept = x), linetype = "dotted") +
    geom_point(aes(x, y), size = 2)
ggplot(df, aes(x, y)) +
    geom_point(size = 2) +
    xlim(1, 5) +
    ylim(-1, 2)
```



(a) With the true underlying relationship shown

(b) With the true underlying relationship hidden, as is always the case in real life

Figure 8.1: Sample regression function.

We can write the systematic part as:

$$E(Y \mid X) = f(X; \beta_1, \beta_2, ...),$$

where β_1, β_2, ... are the parameters for some arbitrary function $f(\cdot)$. The random part is about $P(Y \mid X)$, which can take some arbitrary distributions. In reality, even if such a model holds,

we do not know what $f(\cdot)$ and the true distribution of $Y \mid X$ are, as we only have data like those illustrated in the graph on the right above.

8.2 Linear Regression

The linear regression model assumes that

(a) the function for the systematic component, $f(\cdot)$, is a linear function (in the βs),
(b) $Y \mid X$ is normally distributed, and
(c) Y_i's are conditionally exchangeable given X with equal variance σ^2 (which can be relaxed).

Under these conditions, we have a model

$$
\begin{aligned}
Y_i &\sim N(\mu_i, \sigma) \\
\mu_i &= \eta_i \\
\eta_i &= \beta_0 + \beta_1 X_i
\end{aligned}
$$

With parameters:

- β_0: regression intercept; predicted Y value for observations with $X = 0$
- β_1: regression slope/coefficient; predicted difference in Y for one unit difference in X
- σ: standard deviation of prediction error; roughly speaking, the margin of error in prediction

8.2.1 Example

We will use an example based on the "bread and peace" model by political scientist Douglas Hibbs, which can be used to forecast the U.S. presidential election outcome based on some weighted metric of personal income growth. The example is taken from chapter 7 of the book Regression and Other Stories.[1]

Figure 8.2 is a graph showing the data from 1952 to 2012, with one variable being personal income growth in the four years prior to an election, and the other being the vote share (in %) of the incumbent's party.

[1] See https://douglas-hibbs.com/background-information-on-bread-and-peace-voting-in-us-presidential-elections/ for more information on the "bread and peace" model.

```
# Economy and elections data
if (!file.exists("data/hibbs.dat")) {
    download.file(
        "https://github.com/avehtari/ROS-Examples/raw/master/ElectionsEconomy/data/hibbs.dat"
        "data/hibbs.dat"
    )
}
hibbs <- read.table("data/hibbs.dat", header = TRUE)
```

```
ggplot(hibbs, aes(x = growth, y = vote, label = year)) +
    geom_point() +
    ggrepel::geom_text_repel() +
    labs(x = "Average recent growth in personal income",
         y = "Incumbent party's vote share (%)")
```

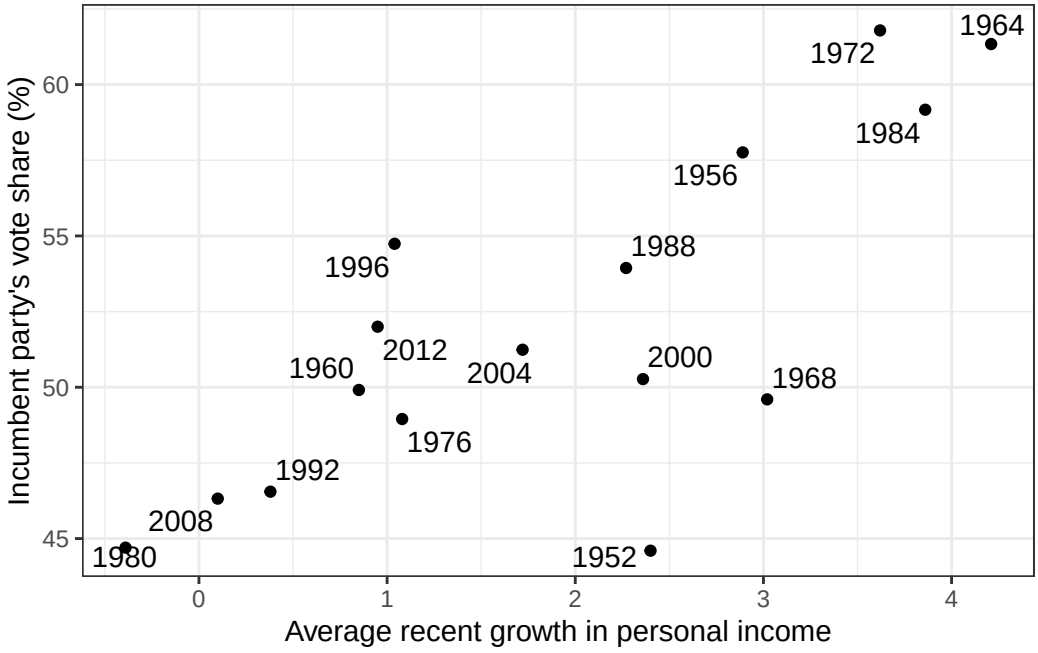


Figure 8.2: Scatter plot of personal income growth and vote share.

8.3 Model and Priors

Model:

$$\begin{aligned}\text{vote}_i &\sim N(\mu_i, \sigma) \\ \mu_i &= \beta_0 + \beta_1 \text{growth}_i\end{aligned}$$

σ: SD (margin) of prediction error

Priors:

$$\begin{aligned}\beta_0 &\sim N(45, 10) \\ \beta_1 &\sim N(0, 10) \\ \sigma &\sim t_4^+(0, 5)\end{aligned}$$

8.4 Model Fitting With Stan

Once you've written the model, it's straightforward to code the model in Stan to perform MCMC sampling, like the code below.

```
data {
  int<lower=0> N;  // number of observations
  vector[N] y;  // outcome;
  vector[N] x;  // predictor;
  int<lower=0,upper=1> prior_only;  // whether to sample prior only
}
parameters {
  real beta0;  // regression intercept
  real beta1;  // regression coefficient
  real<lower=0> sigma;  // SD of prediction error
}
model {
  // model
  if (!prior_only) {
    y ~ normal(beta0 + beta1 * x, sigma);
  }
  // prior
  beta0 ~ normal(45, 10);
  beta1 ~ normal(0, 10);
  sigma ~ student_t(4, 0, 5);
}
generated quantities {
  // Prior/posterior predictive
```

```
  array[N] real ytilde = normal_rng(beta0 + beta1 * x, sigma);
}
```

```
linear_reg <- cmdstan_model("stan_code/linear_reg.stan")
```

8.4.1 Prior Predictive

```
m1_prior <- linear_reg$sample(
    data = list(N = nrow(hibbs),
                y = hibbs$vote,
                x = hibbs$growth,
                prior_only = TRUE),
    seed = 1227,  # for reproducibility
    refresh = 1000
)
```

```
Running MCMC with 4 sequential chains...

Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 1 finished in 0.0 seconds.
Chain 2 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 2 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 2 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 2 finished in 0.0 seconds.
Chain 3 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 3 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 3 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 3 finished in 0.0 seconds.
Chain 4 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 4 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 4 finished in 0.0 seconds.
```

```
All 4 chains finished successfully.
Mean chain execution time: 0.0 seconds.
Total execution time: 0.5 seconds.
```

```
m1_prior$draws("ytilde", format = "matrix") |>
    ppc_ribbon(y = hibbs$vote, x = hibbs$growth,
               y_draw = "points") +
    labs(x = "Average recent growth in personal income",
         y = "Incumbent party's vote share (%)") +
    coord_cartesian(ylim = c(0, 100))
```

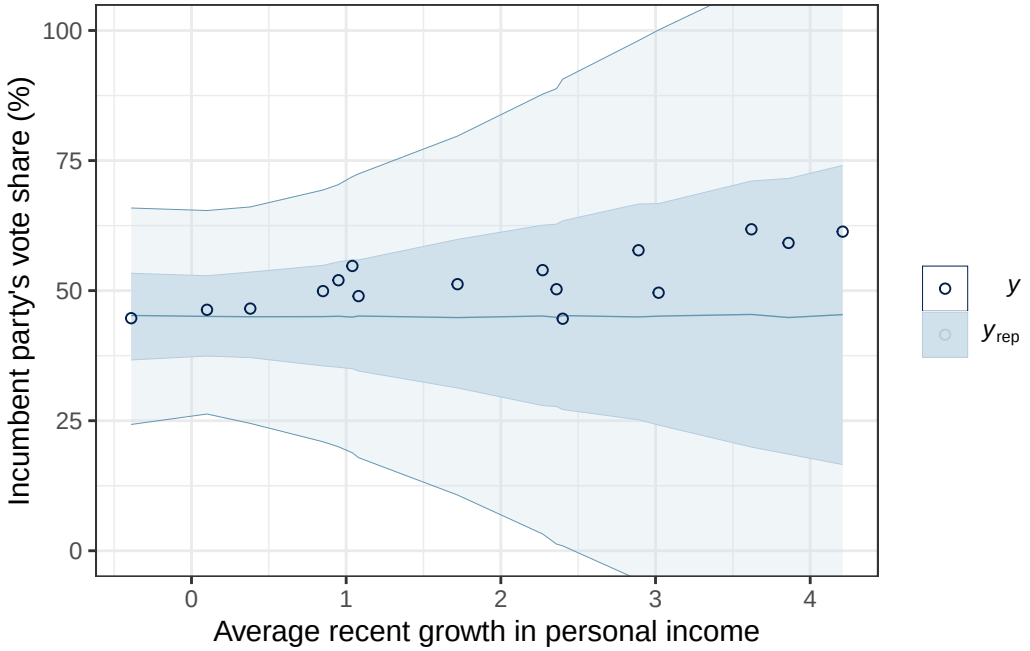


Figure 8.3: Prior predictive distribution of the linear regression model for vote share against personal income.

We can also visualize the prior regression lines based on the prior distributions:

```
prior_draws_beta <- m1_prior$draws(c("beta0", "beta1"), format = "data.frame")
ggplot(hibbs, aes(x = growth, y = vote, label = year)) +
    geom_point() +
    geom_abline(data = prior_draws_beta, aes(intercept = beta0, slope = beta1),
    linewidth = 0.1, alpha = 0.1) +
    ggrepel::geom_text_repel() +
```

```
    labs(x = "Average recent growth in personal income",
         y = "Incumbent party's vote share (%)") +
    coord_cartesian(ylim = c(0, 100))
```

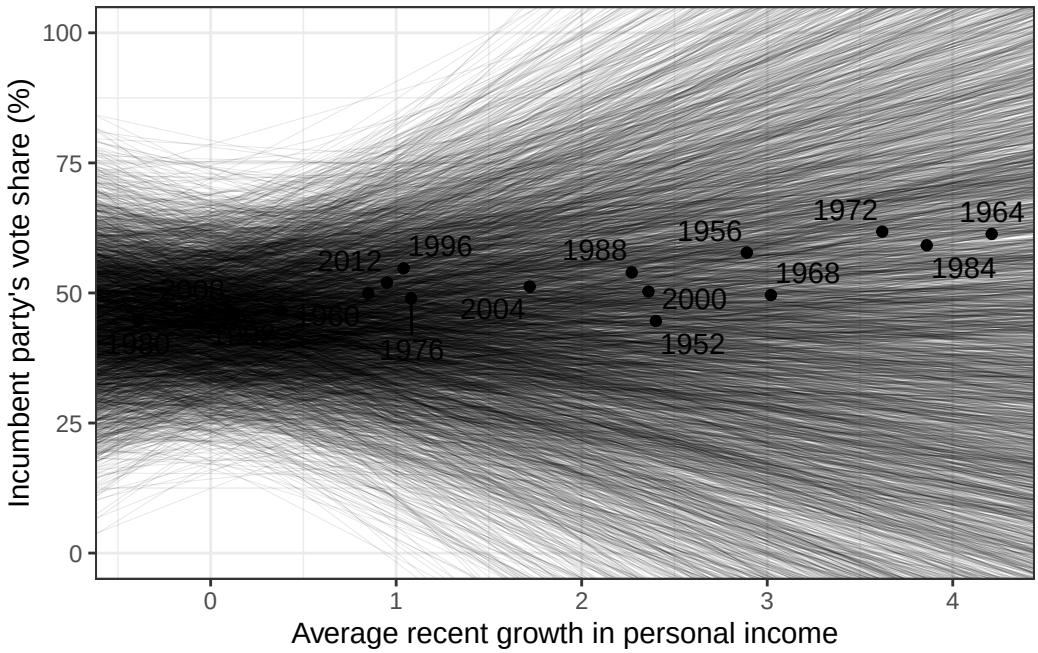


Figure 8.4: Prior predictive distribution of the regression lines.

8.4.2 Results

We'll now fit the model (without `prior_only = TRUE`).

```
m1_post <- linear_reg$sample(
    data = list(N = nrow(hibbs),
                y = hibbs$vote,
                x = hibbs$growth,
                prior_only = FALSE),
    seed = 1227,  # for reproducibility
    refresh = 1000
)
```

```
Running MCMC with 4 sequential chains...
```

```
Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 1 finished in 0.0 seconds.
Chain 2 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 2 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 2 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 2 finished in 0.0 seconds.
Chain 3 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 3 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 3 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 3 finished in 0.0 seconds.
Chain 4 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 4 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 4 finished in 0.0 seconds.

All 4 chains finished successfully.
Mean chain execution time: 0.0 seconds.
Total execution time: 0.5 seconds.
```

```r
m1_summ <- m1_post$summary(c("beta0", "beta1", "sigma"))
# Use `knitr::kable()` for tabulation
knitr::kable(m1_summ, digits = 2)
```

Table 8.1: Posterior summary of linear regression model.

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
beta0	46.25	46.26	1.73	1.66	43.42	49.06	1	1582.97	1590.35
beta1	3.05	3.06	0.75	0.71	1.83	4.26	1	1605.18	1745.88
sigma	4.03	3.91	0.78	0.70	2.97	5.48	1	2047.68	2056.33

The parameter estimates are shown in Table 13.3. Here's a paragraph for the results:

The model predicts that when personal income growth is 0, the vote share for the incumbent party is 46%, 90% CI [43%, 49%]. A 1-unit difference in personal income growth corresponds to a difference in vote share by 3 percentage points, 90% CI [1.8, 4.3].

8.4.3 Convergence

We will talk about convergence more in a future week. For now, you want to see that

- The chains mix well
- the rank histograms are close to uniform distributions

```
m1_post_draws <- m1_post$draws(c("beta0", "beta1", "sigma"))
mcmc_trace(m1_post_draws)
mcmc_rank_hist(m1_post_draws)
```

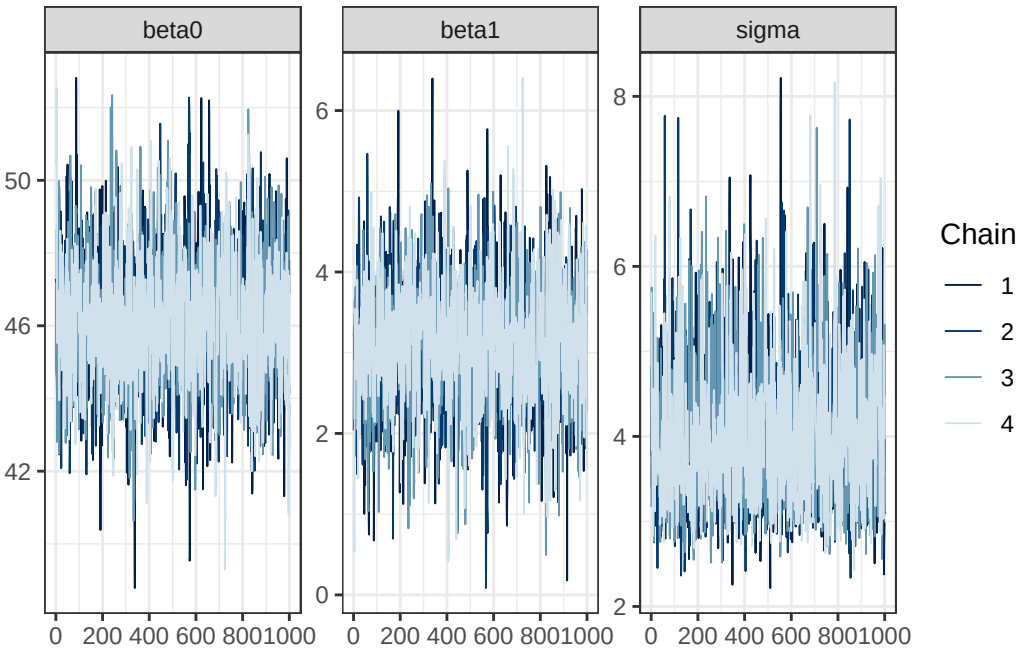
8.4.4 Posterior plots

There are many ways to visualize the results of a regression model. **The most important thing is to be as familiar with what the results mean as possible.** Statistics is not magic that gives you numbers that either support or do not support your theory or hypothesis. It is a way to describe your data. **If you do not want to do the work to understand what your data tell you, why bother to collect the data in the first place?**

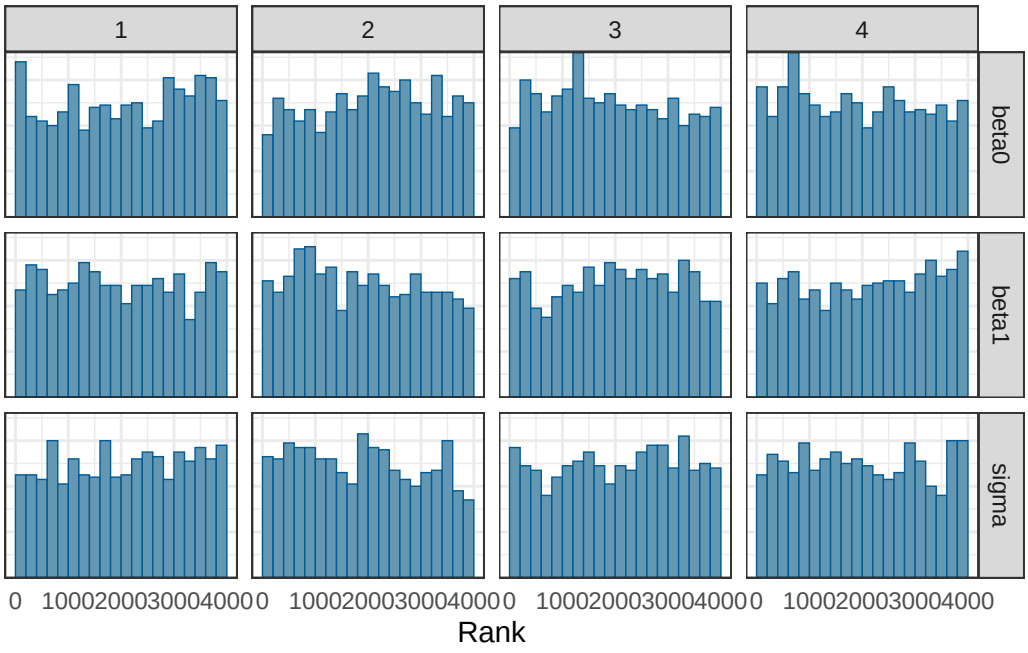
8.4.4.1 Posterior density

Posterior distributions of the three parameters

```
mcmc_dens(m1_post_draws)
```



(a) Trace plot



(b) Rank histogram

Figure 8.5: Convergence diagnostics for the linear regression model.

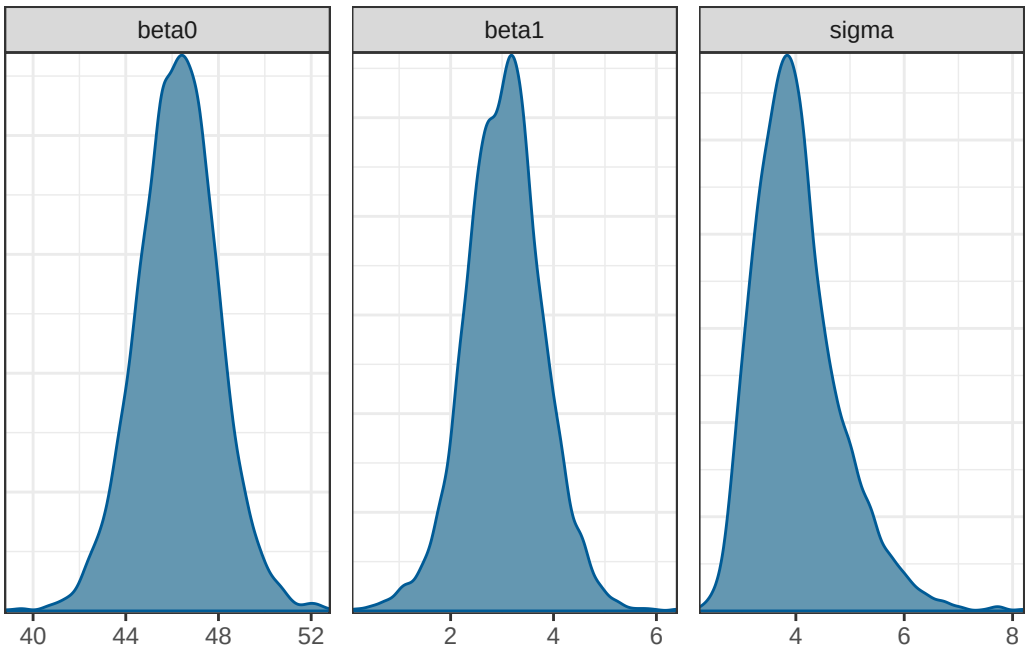


Figure 8.6: Posterior density plots for β_0, β_1, and σ in the linear regression model.

You can also combine the density plot and the trace plot

```
mcmc_combo(m1_post_draws)
```

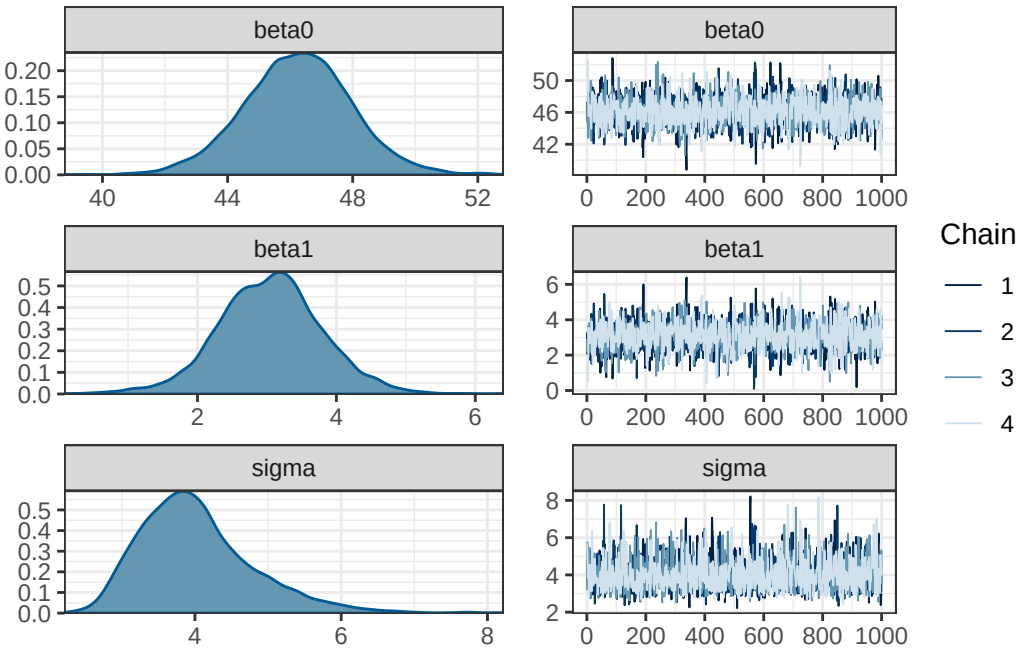


Figure 8.7: Diagnostic plots for MCMC sampling.

8.4.4.2 Plot regression prediction

Figure 13.4 shows the 50% and 90% prediction intervals based on the posterior samples and the model. For example, with the 90% intervals, one expects 90% of the data should be within those intervals. If many data points lie outside the intervals, the linear model is not a good fit.

```
m1_post$draws("ytilde", format = "matrix") |>
    ppc_intervals(y = hibbs$vote, x = hibbs$growth) +
    labs(x = "Average recent growth in personal income",
         y = "Predicted incumbent party's vote share (%)") +
    ggrepel::geom_label_repel(
        aes(y = hibbs$vote, label = hibbs$year)
    )
```

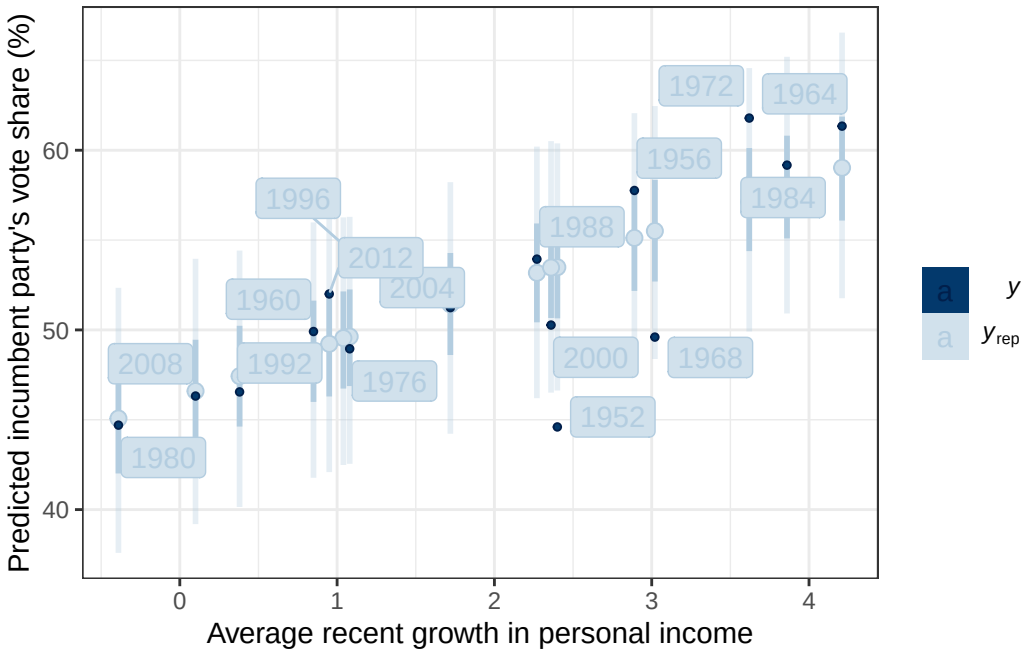


Figure 8.8: Posterior predictive intervals of vote share against personal income growth.

8.5 Predicting a New Data Point

In the four years before 2016, the weighted average personal income growth was 2.0 (based on Hibbs' calculation). So, based on the model, we can obtain a posterior distribution for the predicted vote share of the Democratic Party, which is the incumbent party prior to the 2016 presidential election.

```
linear_pred <- cmdstan_model("stan_code/linear_reg_pred.stan")
```

```
m1_pred <- linear_pred$sample(
    data = list(N = nrow(hibbs),
                y = hibbs$vote,
                x = hibbs$growth,
                prior_only = FALSE,
                xpred = 2),
    seed = 1227,  # for reproducibility
    refresh = 1000
)
```

```
Running MCMC with 4 sequential chains...

Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 1 finished in 0.0 seconds.
Chain 2 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 2 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 2 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 2 finished in 0.0 seconds.
Chain 3 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 3 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 3 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 3 finished in 0.0 seconds.
Chain 4 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 4 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 4 finished in 0.0 seconds.

All 4 chains finished successfully.
Mean chain execution time: 0.0 seconds.
Total execution time: 0.5 seconds.
```

```
m1_pred$draws("ypred") |>
    mcmc_dens()
```

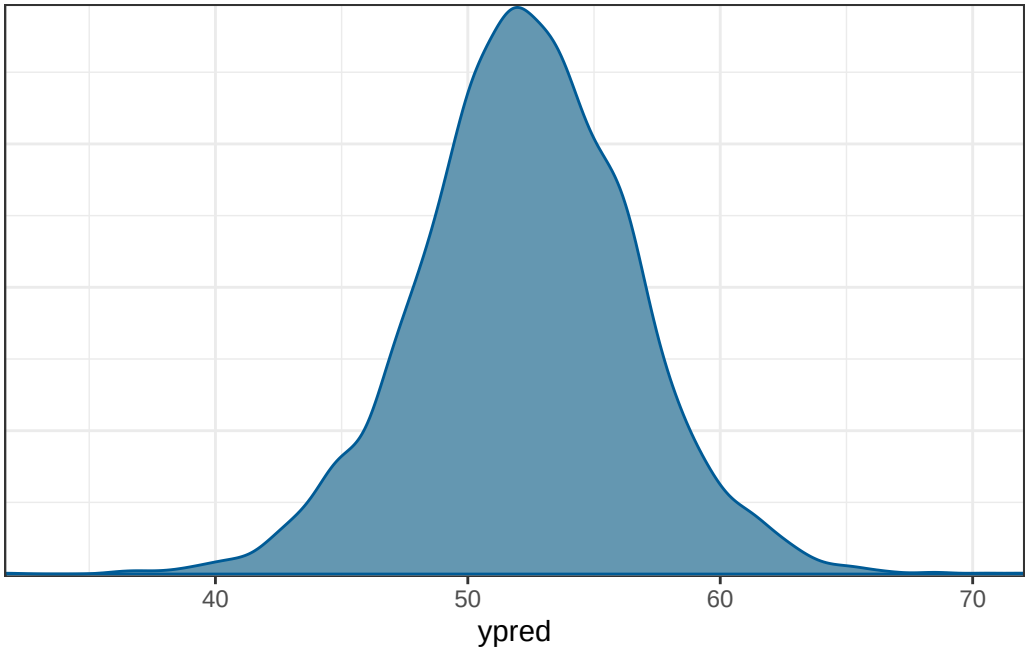


Figure 8.9: Posterior predictive distribution of predicted vote share when growth = 2.

The mean of the incumbent's predicted vote share with average income growth = 2 is 52.3006575. The actual outcome of the election was that the Democratic Party received about 51.1% of the votes among the two parties, so it was below the posterior predictive mean but within the range of possible outcomes. Of course, we know that the actual election outcome is based on the Eelectoral College, not the majority vote.

8.6 Robust Regression

The linear model assuming normally distributed errors is not robust to outliers or influential observations. It can be robustified by assuming a more heavy-tailed distribution, such as the t distribution:

$$\text{vote}_i \sim t_\nu(\mu_i, \sigma),$$

where ν is an additional degrees of freedom parameter controlling for the "heaviness" of the tails. When ν is close to 0 (e.g., 3 or 4), the outliers/influential cases are weighed less; when ν is close to infinity, the t distribution becomes a normal distribution.

With Bayesian methods, we can let the model learn from the data about the ν parameter. In this case, we assume a *hyperprior* for ν; Gamma$(2, 0.1)$ is something recommended in the literature.

```
data {
  int<lower=0> N;  // number of observations
  vector[N] y;  // outcome;
  vector[N] x;  // predictor;
  int<lower=0,upper=1> prior_only;  // whether to sample prior only
}
parameters {
  real beta0;  // regression intercept
  real beta1;  // regression coefficient
  real<lower=0> sigma;  // SD of prediction error
  real<lower=1> nu;  // df parameter
}
model {
  // model
  if (!prior_only) {
    y ~ student_t(nu, beta0 + beta1 * x, sigma);
  }
  // prior
  beta0 ~ normal(45, 10);
  beta1 ~ normal(0, 10);
  sigma ~ student_t(4, 0, 5);
  nu ~ gamma(2, 0.1); // prior for df parameter
}
generated quantities {
  vector[N] ytilde;  // place holder
  for (i in 1:N)
    ytilde[i] = normal_rng(beta0 + beta1 * x[i], sigma);
}
```

```
robust_reg <- cmdstan_model("stan_code/robust_reg.stan")
```

```
m1_robust <- robust_reg$sample(
    data = list(N = nrow(hibbs),
                y = hibbs$vote,
                x = hibbs$growth,
                prior_only = FALSE),
    seed = 1227,  # for reproducibility
    refresh = 0
```

```
)
```

```
Running MCMC with 4 sequential chains...

Chain 1 finished in 0.0 seconds.
Chain 2 finished in 0.0 seconds.
Chain 3 finished in 0.0 seconds.
Chain 4 finished in 0.0 seconds.

All 4 chains finished successfully.
Mean chain execution time: 0.0 seconds.
Total execution time: 0.5 seconds.
```

```
m1r_summ <- m1_robust$summary(c("beta0", "beta1", "sigma", "nu"))
# Use `knitr::kable()` for tabulation
knitr::kable(m1r_summ, digits = 2)
```

Table 8.2: Posterior summary of Student t regression model.

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
beta0	46.17	46.18	1.55	1.45	43.55	48.64	1	1628.35	1673.90
beta1	3.20	3.22	0.69	0.66	2.01	4.30	1	1598.75	1914.04
sigma	3.56	3.49	0.92	0.83	2.20	5.10	1	1044.24	586.21
nu	18.26	14.64	13.86	11.60	2.97	45.62	1	1234.64	638.30

```
m1_robust$draws("ytilde", format = "matrix") |>
    ppc_intervals(y = hibbs$vote, x = hibbs$growth) +
    labs(x = "Average recent growth in personal income",
         y = "Predicted incumbent party's vote share (%)") +
    ggrepel::geom_label_repel(
        aes(y = hibbs$vote, label = hibbs$year)
    )
```

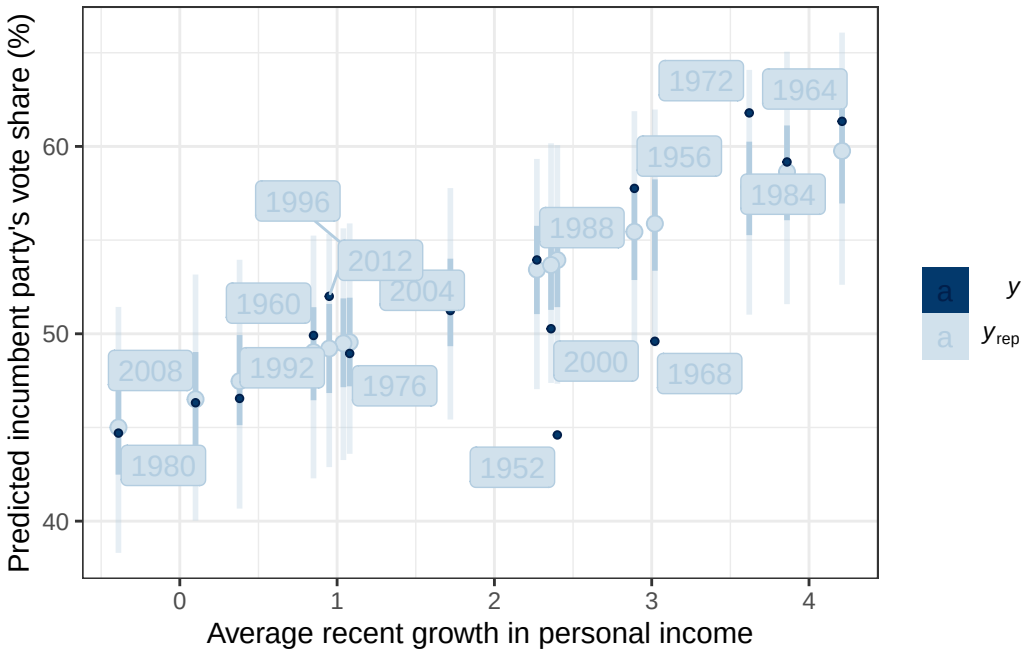


Figure 8.10: Posterior predictive intervals of vote share against personal income growth based on Student t regression.

9 Multiple Predictors

Here, we'll use an example from McElreath (2020), which contains some marriage and demographic statistics for the individual states in the United States. See https://rdrr.io/github/rmcelreath/rethinking/man/WaffleDivorce.html for more details.

```
if (!file.exists("data/WaffleDivorce.csv")) {
    download.file(
        "https://raw.githubusercontent.com/rmcelreath/rethinking/master/data/WaffleDivorce.cs
        "data/WaffleDivorce.csv"
    )
}
waffle_divorce <- read_delim(  # read delimited files
    "data/WaffleDivorce.csv",
    delim = ";"
)
# Rescale Marriage and Divorce by dividing by 10
waffle_divorce$Marriage <- waffle_divorce$Marriage / 10
waffle_divorce$Divorce <- waffle_divorce$Divorce / 10
waffle_divorce$MedianAgeMarriage <- waffle_divorce$MedianAgeMarriage / 10
# Recode `South` to a factor variable
waffle_divorce$South <- factor(waffle_divorce$South,
    levels = c(0, 1),
    labels = c("non-south", "south")
)
# See data description at https://rdrr.io/github/rmcelreath/rethinking/man/WaffleDivorce.html
```

9.1 Stratified Analysis

Let's consider whether the association between `MedianAgeMarriage` and `Divorce` differs between Southern and non-Southern states. Because (and **only because**) the groups are **independent**, we can fit a linear regression for each subset of states.

```
ggplot(waffle_divorce,
       aes(x = MedianAgeMarriage, y = Divorce, col = South)) +
    geom_point() +
    geom_smooth() +
    labs(x = "Median age marriage (10 years)",
         y = "Divorce rate (per 10 adults)") +
    ggrepel::geom_text_repel(aes(label = Loc), max.overlaps = 15)
```

```
`geom_smooth()` using method = 'loess' and formula = 'y ~ x'
```

```
Warning: ggrepel: 4 unlabeled data points (too many overlaps). Consider
increasing max.overlaps
```

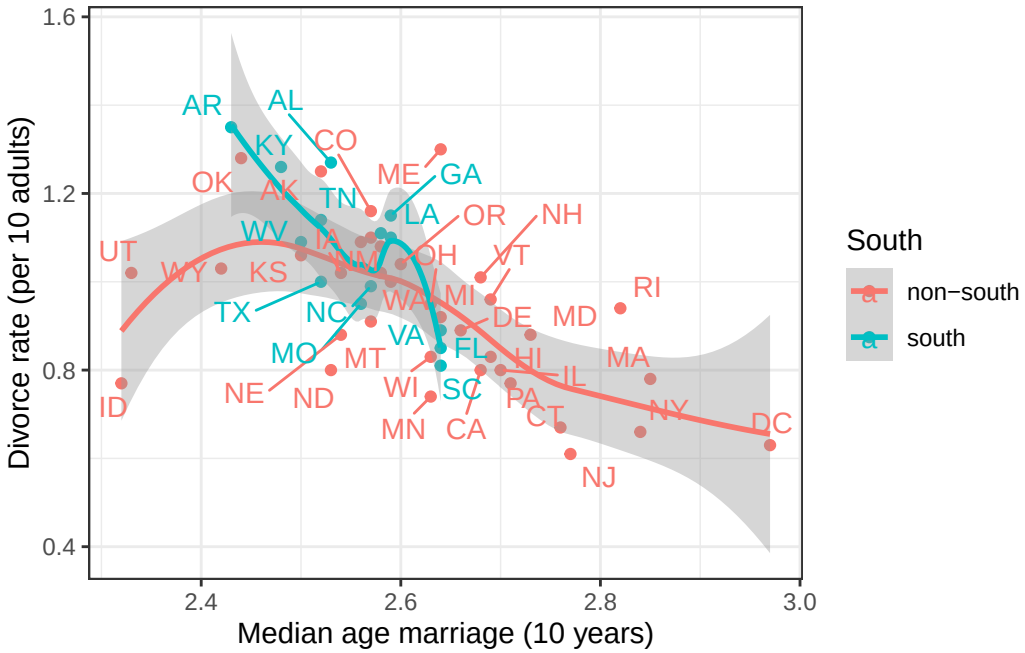


Figure 9.1: State-level association between median age of marriage and divorce rate.

9.2 Introducing the `brms` package

While Stan is very flexible, because the linear model and some related models are so widely used, some authors have created packages that would further simplify the fitting of such models. One of those packages is `brms`, which I believe stands for "Bayesian regression models with

Stan." It allows one to do MCMC sampling using Stan, but with syntax similar to that in R functions `lm()`, `glm()`, and `lme4::lmer()`. `brms` probably supports more models than any R packages that statisticians routinely used; there are models, like factor analysis, that are not directly supported. If you came across some fancy regression models, chances are you can do something similar in `brms`. You can find some resources for learning `brms` on this page: https://paul-buerkner.github.io/brms/.

Model formula

`brms` comes with some default prior options, but I recommend you always check what priors are used and think about whether they make sense for your data. You can use `get_priors()` to show the default priors used in `brms`.

To do MCMC sampling, we use the `brm()` function. The first argument is a formula in R. The variable before `~` is the outcome, whereas the ones after `~` are the predictors. For example,

```
vote ~ 1 + growth
```

means the model

$$E(\text{vote}_i) = \beta_0(1) + \beta_1(\text{growth}_i).$$

Usually, I write `vote ~ 1 + growth` as `vote ~ growth`, as the `1 +` part is automatically added.

Setting Priors

`brms` comes with some default prior options, but over the years, the package maintainers have changed those priors, so the default today may be different from the one next year. Therefore, you should always check what priors are used and think about whether they make sense for your data. You can use `get_priors()` to show the default priors used in `brms`. For example,

```
get_prior(Divorce ~ MedianAgeMarriage,
          data = waffle_divorce)
```

```
                prior     class              coef group resp dpar nlpar lb ub
               (flat)         b                                              
               (flat)         b MedianAgeMarriage                            
 student_t(3, 1, 2.5) Intercept                                              
 student_t(3, 0, 2.5)     sigma                                            0
```

```
       source
      default
 (vectorized)
      default
      default
```

```
m_nonsouth <-
    brm(Divorce ~ MedianAgeMarriage,
        # Filter `waffle_divorce` to only include non-southern states
        data = filter(waffle_divorce, South == "non-south"),
        # Use N(0, 2) and N(0, 10) as priors for beta1 and beta0,
        # and use t_4(0, 3) as a prior for sigma
        prior = prior(normal(0, 2), class = "b") +
            prior(normal(0, 10), class = "Intercept") +
            prior(student_t(4, 0, 3), class = "sigma"),
        seed = 941,
        iter = 4000,
        file = "m_nonsouth"
    )
```

```
m_south <-
    brm(Divorce ~ MedianAgeMarriage,
        data = filter(waffle_divorce, South == "south"),
        prior = prior(normal(0, 2), class = "b") +
            prior(normal(0, 10), class = "Intercept") +
            prior(student_t(4, 0, 3), class = "sigma"),
        seed = 2157,  # use a different seed
        iter = 4000,
        file = "m_south"
    )
```

We can make a table like Table 9.1 for `brms` results using the `modelsummary::msummary()` function.

```
msummary(list(South = m_south, `Non-South` = m_nonsouth),
         estimate = "{estimate} [{conf.low}, {conf.high}]",
         statistic = NULL, fmt = 2,
         gof_omit = "^(?!Num)"  # only include number of observations
)
```

```
Warning:
`modelsummary` uses the `performance` package to extract goodness-of-fit
```

Table 9.1: Intercepts and slopes for south and non-south states.

	South	Non-South
b_Intercept	6.09 [3.60, 8.45]	2.74 [1.75, 3.74]
b_MedianAgeMarriage	−1.96 [−2.89, −0.98]	−0.69 [−1.07, −0.31]
sigma	0.11 [0.07, 0.17]	0.15 [0.12, 0.20]
Num.Obs.	14	36

```
statistics from models of this class. You can specify the statistics you wish
to compute by supplying a `metrics` argument to `modelsummary`, which will then
push it forward to `performance`. Acceptable values are: "all", "common",
"none", or a character vector of metrics names. For example: `modelsummary(mod,
metrics = c("RMSE", "R2")` Note that some metrics are computationally
expensive. See `?performance::performance` for details.
 This warning appears once per session.
```

We can now ask two questions:

- Is the intercept different across southern and non-southern states?
- Is the slope different across southern and non-southern states?

The correct way to answer the above questions is to obtain the posterior distribution of the **difference** in the coefficients. Repeat: obtain the posterior distribution of the **difference**. The incorrect way is to compare whether the CIs overlap.

Here are the posteriors of the differences ($\beta_0^{\text{south}} - \beta_0^{\text{nonsouth}}$ and $\beta_1^{\text{south}} - \beta_1^{\text{nonsouth}}$):

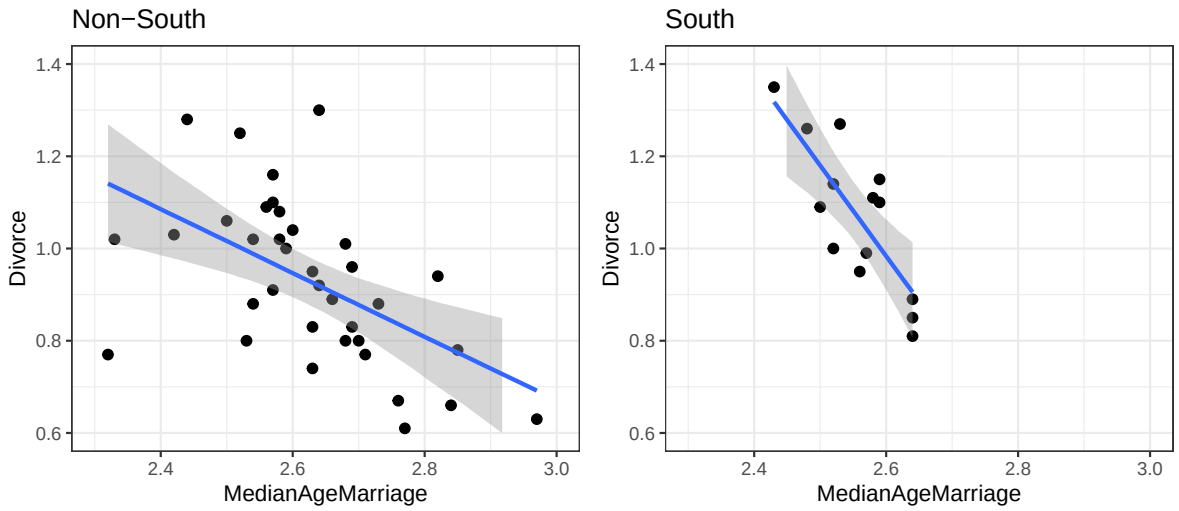
```
# Extract draws
draws_south <- as_draws_matrix(m_south,
    variable = c("b_Intercept", "b_MedianAgeMarriage")
)
draws_nonsouth <- as_draws_matrix(m_nonsouth,
    variable = c("b_Intercept", "b_MedianAgeMarriage")
)
# Difference in coefficients
draws_diff <- draws_south - draws_nonsouth
# Rename the columns
colnames(draws_diff) <- paste0("d", colnames(draws_diff))
# Summarize
summarize_draws(draws_diff) |>
    knitr::kable(digits = 2)
```

Table 9.2: Difference in intercept and slope for south and non-south states.

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
db_Intercept	3.32	3.34	1.34	1.29	1.14	5.45	1	6115.12	5017.01
db_MedianAgeMarriage	-1.26	-1.27	0.52	0.50	-2.09	-0.41	1	6112.20	5034.56

As you can see, the southern states have a higher intercept and a lower slope.

```
plot(
    conditional_effects(m_nonsouth),
    points = TRUE, plot = FALSE
)[[1]] + ggtitle("Non-South") + lims(x = c(2.3, 3), y = c(0.6, 1.4))
plot(
    conditional_effects(m_south),
    points = TRUE, plot = FALSE
)[[1]] + ggtitle("South") + lims(x = c(2.3, 3), y = c(0.6, 1.4))
```



(a) Non-southern states

(b) Southern states

Figure 9.2: Model-implied regression lines

9.3 Additive Model

An additive model assumes that the difference between predicted Y for two levels of X_1 is the same regardless of the level of X_2. In our example, we assume that the predicted difference

in divorce rate associated with the median age of marriage does not depend on whether the state is southern or not. Equivalently, we assume that the predicted difference in Southern and non-Southern states does not depend on the median age of marriage.

$$
\begin{aligned}
D_i &\sim N(\mu_i, \sigma) \\
\mu_i &= \beta_0 + \beta_1 S_i + \beta_2 A_i \\
\beta_0 &\sim N(0, 10) \\
\beta_1 &\sim N(0, 10) \\
\beta_2 &\sim N(0, 1) \\
\sigma &\sim t_4^+(0, 3)
\end{aligned}
$$

- β_1: Expected difference in divorce rate between southern and non-southern states with the same median age of marriage.
- β_2: Expected difference in divorce rate for one unit difference in median age of marriage, when both states are southern (or non-southern).

In the model, the variable S, southern state, is a dummy variable with 0 = non-southern and 1 = southern. Therefore,

Dummy Coding

- For non-southern states, $\mu = (\beta_0) + (\beta_2)A$;
- For southern states, $\mu = (\beta_0 + \beta_1) + \beta_2 A$

```
m_additive <- brm(
    Divorce ~ South + MedianAgeMarriage,
    data = waffle_divorce,
    prior = prior(normal(0, 2), class = "b") +
        prior(normal(0, 10), class = "b", coef = "Southsouth") +
        prior(normal(0, 10), class = "Intercept") +
        prior(student_t(4, 0, 3), class = "sigma"),
    seed = 941,
    iter = 4000,
    file = "m_additive"
)
```

```
m_additive
```

```
 Family: gaussian
  Links: mu = identity; sigma = identity
```

```
Formula: Divorce ~ South + MedianAgeMarriage
   Data: waffle_divorce (Number of observations: 50)
  Draws: 4 chains, each with iter = 4000; warmup = 2000; thin = 1;
         total post-warmup draws = 8000

Regression Coefficients:
                 Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Intercept            3.00      0.46     2.10     3.89 1.00     7435     5360
Southsouth           0.08      0.05    -0.01     0.18 1.00     7847     5519
MedianAgeMarriage   -0.79      0.18    -1.13    -0.45 1.00     7406     5423

Further Distributional Parameters:
      Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sigma     0.15      0.02     0.12     0.18 1.00     7217     5426

Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

9.4 Interaction Model: Different Slopes Across Two Groups

An alternative is to include an interaction term

$$
\begin{aligned}
D_i &\sim N(\mu_i, \sigma) \\
\mu_i &= \beta_0 + \beta_1 S_i + \beta_2 A_i + \beta_3 S_i \times A_i \\
\beta_0 &\sim N(0, 10) \\
\beta_1 &\sim N(0, 10) \\
\beta_2 &\sim N(0, 1) \\
\beta_3 &\sim N(0, 2) \\
\sigma &\sim t_4^+(0, 3)
\end{aligned}
$$

- β_1: Difference in intercept between southern and non-southern states.
- β_3: Difference in the coefficient for A $\rightarrow$ D between southern and non-southern states

Dummy Coding in Interaction Model

- For non-southern states, $\mu = (\beta_0) + (\beta_2)A$;
- For southern states, $\mu = (\beta_0 + \beta_1) + (\beta_2 + \beta_3)A$

```r
m_inter <- brm(
    Divorce ~ South * MedianAgeMarriage,
    data = waffle_divorce,
    prior = prior(normal(0, 2), class = "b") +
        prior(normal(0, 10), class = "b", coef = "Southsouth") +
        prior(normal(0, 10), class = "Intercept") +
        prior(student_t(4, 0, 3), class = "sigma"),
    seed = 941,
    iter = 4000,
    file = "m_inter"
)
```

The formula `Divorce ~ South * MedianAgeMarriage` is the same as

```r
Divorce ~ South + MedianAgeMarriage + South:MedianAgeMarriage
```

where `:` is the symbol in R for a product term.

```r
# Print summary of the model
m_inter
```

```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: Divorce ~ South * MedianAgeMarriage
   Data: waffle_divorce (Number of observations: 50)
  Draws: 4 chains, each with iter = 4000; warmup = 2000; thin = 1;
         total post-warmup draws = 8000

Regression Coefficients:
                           Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS
Intercept                      2.78      0.46     1.87     3.68 1.00     4716
Southsouth                     3.20      1.60     0.19     6.30 1.00     2863
MedianAgeMarriage             -0.70      0.18    -1.05    -0.35 1.00     4714
Southsouth:MedianAgeMarriage  -1.22      0.62    -2.42    -0.03 1.00     2876
                           Tail_ESS
Intercept                      4042
Southsouth                     3608
MedianAgeMarriage              4085
Southsouth:MedianAgeMarriage   3584

Further Distributional Parameters:
```

```
      Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sigma     0.14      0.02     0.12     0.18 1.00     4244     4998

Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

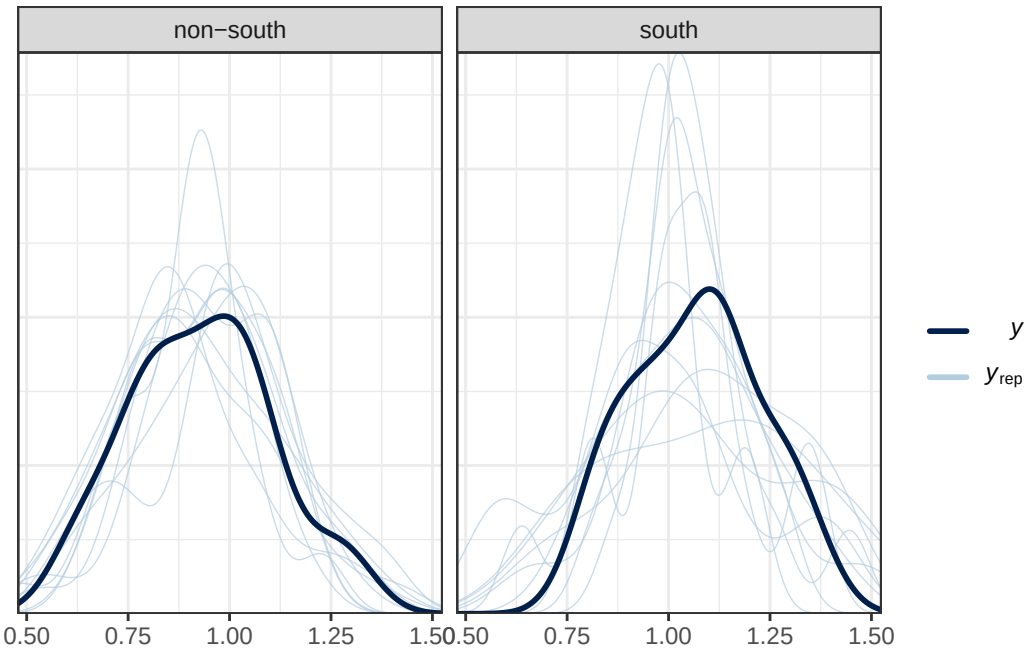
9.4.1 Posterior predictive checks

```
# Check density (normality)
pp_check(m_inter, type = "dens_overlay_grouped", group = "South")
```

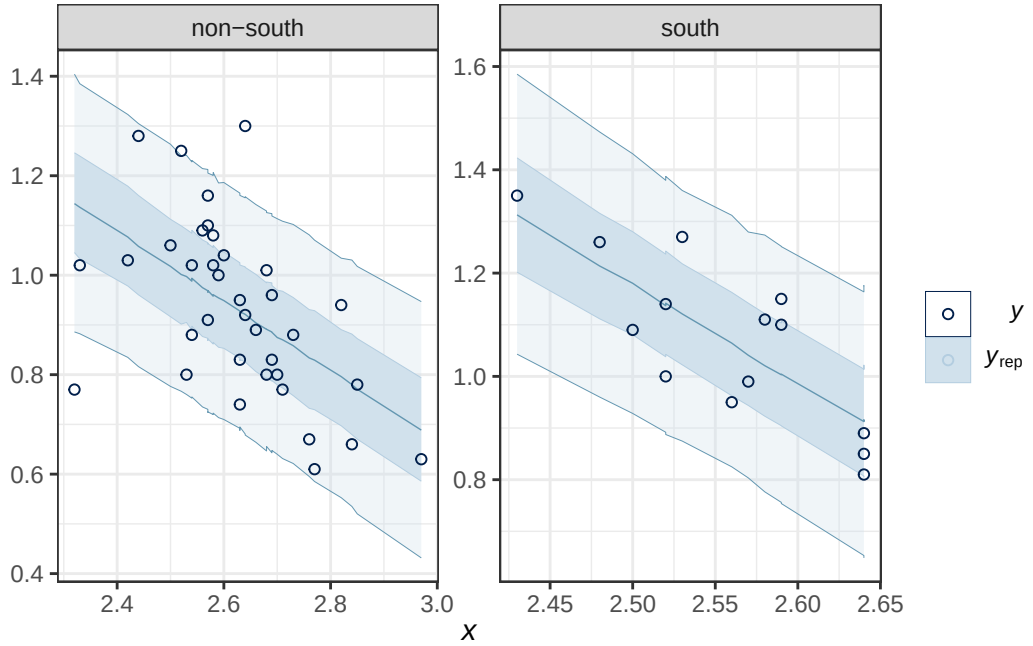
```
Using 10 posterior draws for ppc type 'dens_overlay_grouped' by default.
```

```
# Check prediction (a few outliers)
pp_check(m_inter,
    type = "ribbon_grouped", x = "MedianAgeMarriage",
    group = "South",
    y_draw = "points"
)
```

```
Using all posterior draws for ppc type 'ribbon_grouped' by default.
```



(a) Density overlayed plots



(b) Prediction intervals

Figure 9.3: Posterior predictive checks for the interaction model.

```
# Check errors (no clear pattern)
pp_check(m_inter,
    type = "error_scatter_avg_vs_x", x = "MedianAgeMarriage"
)
```

```
Using all posterior draws for ppc type 'error_scatter_avg_vs_x' by default.
```

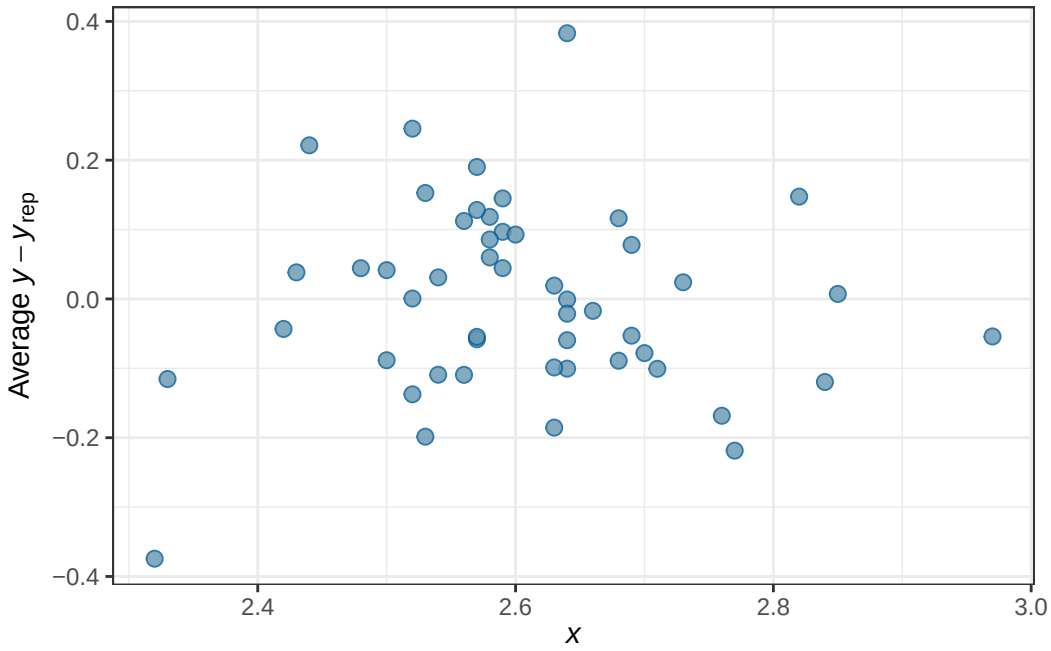


Figure 9.4: Average prediction error against the predictor. No clear pattern should be observed for a correctly specified model.

9.4.2 Conditional effects/simple slopes

Slope of `MedianAgeMarriage` when South = 0: β_1

Slope of `MedianAgeMarriage` when South = 1: $\beta_1 + \beta_3$

```
as_draws(m_inter) |>
    mutate_variables(
        b_nonsouth = b_MedianAgeMarriage,
        b_south = b_MedianAgeMarriage + `b_Southsouth:MedianAgeMarriage`
    ) |>
```

```
    posterior::subset_draws(
        variable = c("b_nonsouth", "b_south")
    ) |>
    summarize_draws() |>
    knitr::kable(digits = 2)
```

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
b_nonsouth	-0.70	-0.71	0.18	0.18	-1.00	-0.41	1	4713.61	4085.16
b_south	-1.92	-1.91	0.60	0.60	-2.91	-0.93	1	3168.15	3659.43

```
plot(
    conditional_effects(m_inter,
        effects = "MedianAgeMarriage",
        conditions = data.frame(South = c("south", "non-south"),
                                cond__ = c("South", "Non-South"))
    ),
    points = TRUE
)
```

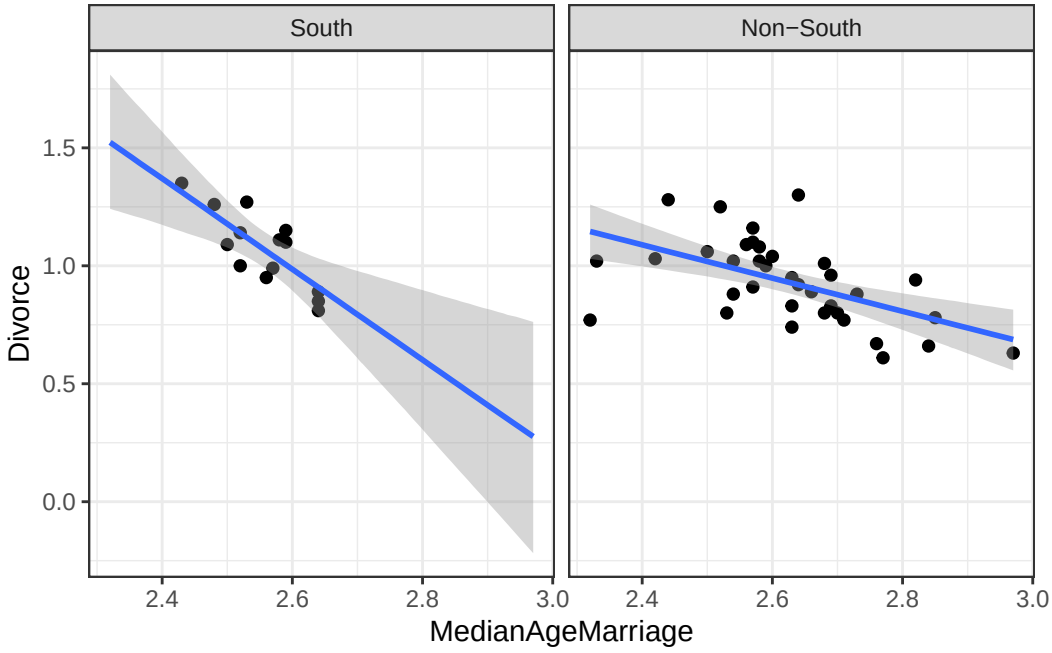


Figure 9.5: Model-implied simple slopes based on the interaction model.

9.5 Interaction of Continuous Predictors

```
int_fig <- plotly::plot_ly(waffle_divorce,
    x = ~Marriage,
    y = ~MedianAgeMarriage,
    z = ~Divorce
)
```

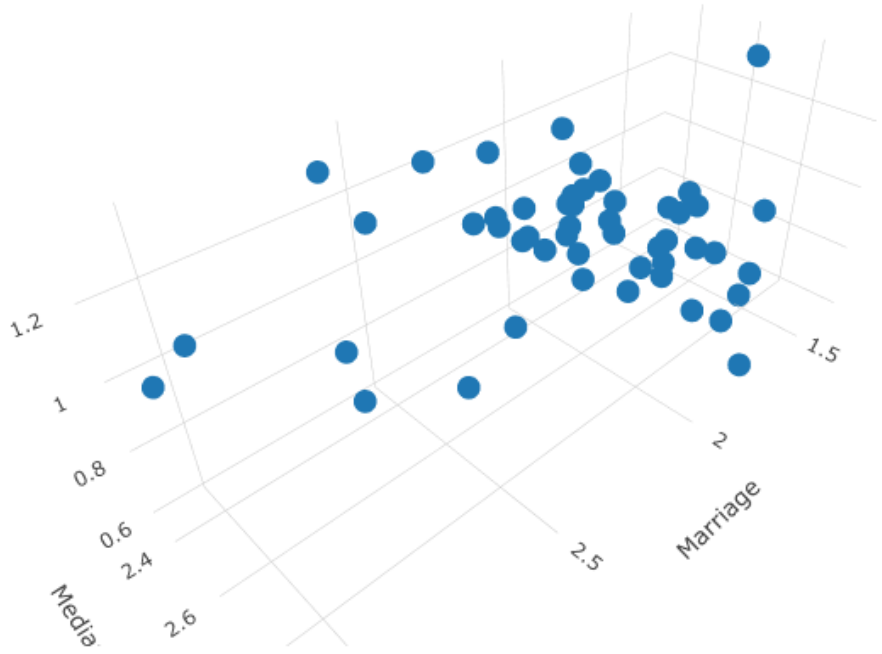


Figure 9.6: 3-D plot visualizing one outcome and two predictors.

$$D_i \sim N(\mu_i, \sigma)$$
$$\mu_i = \beta_0 + \beta_1 M_i + \beta_2 A_i + \beta_3 M_i \times A_i$$

```
# Use default priors (just for convenience here)
m_inter2 <- brm(Divorce ~ Marriage * MedianAgeMarriage,
    data = waffle_divorce,
```

```
    seed = 941,
    iter = 4000,
    file = "m_inter2"
)
```

9.6 Centering

In the previous model, β_1 is the slope of M $\rightarrow$ D when A is 0 (i.e., median marriage age = 0), and β_2 is the slope of A $\rightarrow$ D when M is 0 (i.e., marriage rate is 0). These two are not very meaningful. Therefore, it is common to make the zero values more meaningful by doing *centering*.

Here, I use M - 2 as the predictor, so the zero point means a marriage rate of 2 per 10 adults; I use A - 2.5 as the other predictor, so the zero point means a median marriage rate of 25 years old.

$$\mu_i = \beta_0 + \beta_1(M_i - 2) + \beta_2(A_i - 2.5) + \beta_3(M_i - 2) \times (A_i - 2.5)$$

```
# Use default priors (just for convenience here)
m_inter2c <- brm(Divorce ~ I(Marriage - 2) * I(MedianAgeMarriage - 2.5),
    data = waffle_divorce,
    seed = 941,
    iter = 4000,
    file = "m_inter2c"
)
```

```
msummary(list(`No centering` = m_inter2, `centered` = m_inter2c),
         estimate = "{estimate} [{conf.low}, {conf.high}]",
         statistic = NULL, fmt = 2)
```

As shown in the table above, while the two models are equivalent in fit and give the same posterior distribution for β_3, they differ in β_0, β_1, and β_2.

```
plot(
    conditional_effects(m_inter2c,
        effects = "Marriage:MedianAgeMarriage",
        int_conditions = list(MedianAgeMarriage = c(2.3, 2.5, 2.7)),
    ),
    points = TRUE
)
```

	No centering	centered
b_Intercept	7.38 [3.02, 11.58]	1.09 [1.02, 1.16]
b_Marriage	−1.93 [−4.00, 0.16]	
b_MedianAgeMarriage	−2.45 [−4.07, −0.78]	
b_Marriage × MedianAgeMarriage	0.74 [−0.07, 1.56]	
sigma	0.15 [0.12, 0.18]	0.15 [0.12, 0.18]
b_IMarriageM2		−0.08 [−0.24, 0.09]
b_IMedianAgeMarriageM2.5		−0.94 [−1.44, −0.44]
b_IMarriageM2 × IMedianAgeMarriageM2.5		0.75 [−0.08, 1.59]
Num.Obs.	50	50
R2	0.414	0.413
R2 Adj.	0.281	0.268
ELPD	21.5	21.2
ELPD s.e.	6.1	6.2
LOOIC	−42.9	−42.5
LOOIC s.e.	12.2	12.5
WAIC	−43.5	−43.1
RMSE	0.14	0.14

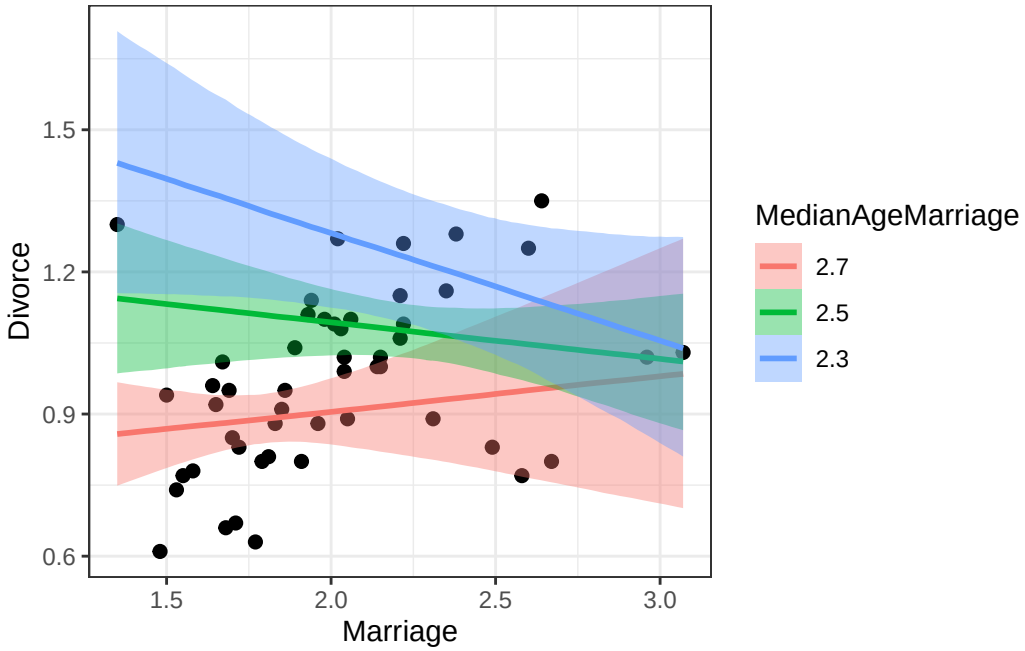


Figure 9.7: Model-implied simple slopes of marriage for different levels of median age of marriage.

10 Model Diagnostics

All statistical models are sets of assumptions about the data-generating process, and estimation will be meaningless or misleading if these assumptions do not hold for the data. As we have discussed, choosing a good model is generally more important than choosing a good prior. In this note, we will learn some tools to check the validity of linear models. Most of them are similar to what you have learned in frequentist regression.

10.1 Assumptions of Linear Models

The assumptions of the linear model is encoded in the model. The model is

$$
\begin{aligned}
Y_i &\sim N(\mu_i, \sigma) \\
\mu_i &= \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + ...
\end{aligned}
$$

From the model, we have the following assumptions, in the order of the most important one to the least important one:

1. *Correct specification of the model.* This means that all relevant predictors for Y have been included in the model. This is probably an assumption that is never satisfied in real data analysis, as one can never include all relevant factors that can have an impact on Y, be it small or large. However, it is important to be thoughtful to include major predictors that have been shown to relate to Y. Leaving out key predictors can bias the coefficients β.
2. *Linearity.* This is about the conditional mean, $\mu = E(Y|X_1, X_2, ...)$, being a linear function. If you have a function like $\mu = \exp[\beta_1 X_1 \sin(\beta_2 X_2)]$, the conditional mean is not a linear function. Note that linearity does not require μ to be a linear function of predictors; quadratic and exponential relationships, interaction, and polynomials can all be handled by linear models. (And technically, linearity requires μ to be a linear function of the coefficients.)
3. *Independent observations.* This assumption is not directly encoded in the model equation above, mainly because I omit that part when writing out the model. This assumption requires that the value of one observation is independent of the value of another observation after taking into account the conditional mean, μ. This will be discussed more in multilevel models.

4. *Equal variance of errors.* This means that σ^2 has to be constant for each observation. In general, Violating this assumption is generally a minor issue, although it can affect the posterior standard deviation (analogous to standard errors).
5. *Normality.* This requires that the conditional distribution of Y is normal. Violating of the normality assumption generally does not affect the estimation of the coefficients, and will be a minor issue when the sample size is large enough (> 30) and when the degree of nonnormality is small to moderate.

10.2 Diagnostic Tools

Now let's review some tools for regression diagnostics for Bayesian regression. There are hundreds of plots available that I will not cover here, and you can treat what is discussed in this note as a minimal requirement for regression diagnostics. The first one is about a correct specification of the model, which can be partly assessed with posterior predictive check.

10.2.1 Posterior Predictive Check

We've already seen a few examples of posterior predictive checks in the previous chapters. Continuing with the example of predicting the divorce rate, here are a few more plots.

Below is the posterior predictive graphical check for the interaction model we fit for the state-level divorce rate data:

Based on the graphical check, we do not see any major systematic discrepancies between the distribution of our data and what can be predicted from our model. The ribbon plot shows that some points are outside the 90% predictive intervals but not too far off.

We should do the posterior predictive check with test statistics too. The following functions show the mean, maximum value, and minimum value of the outcome.

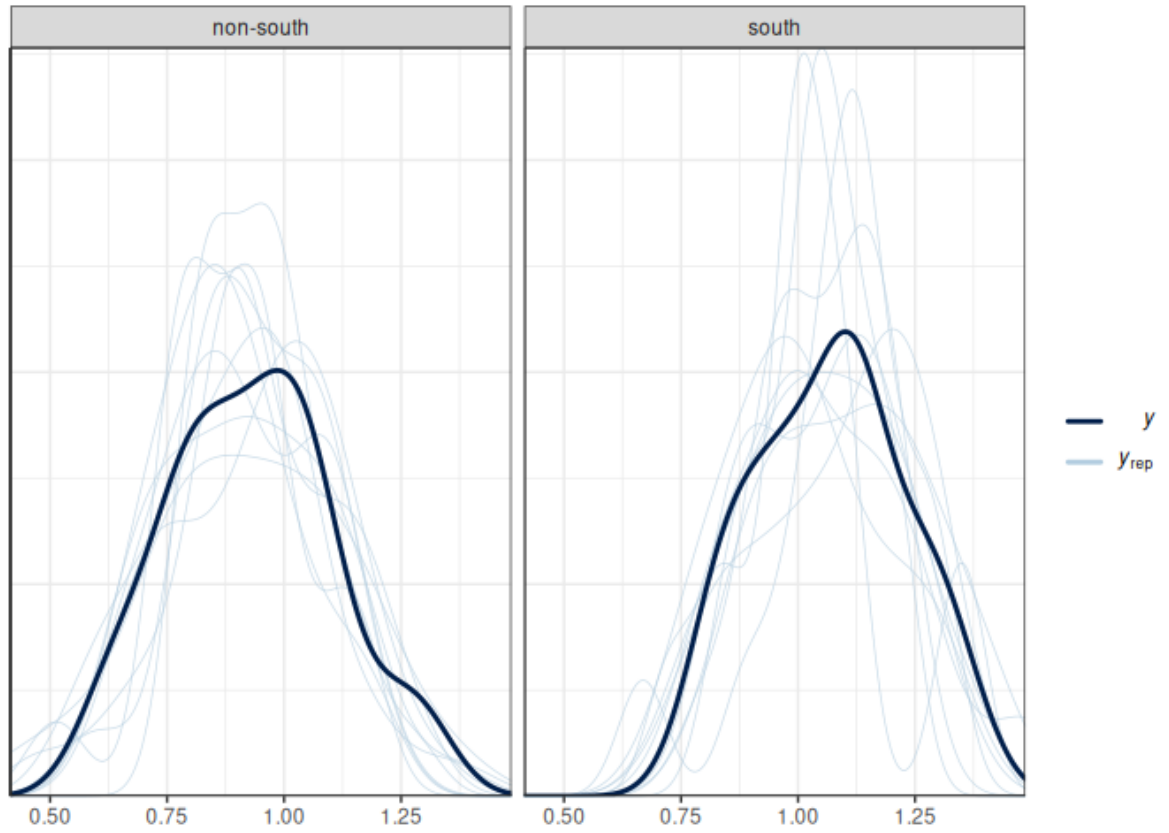
```
# PPC for the mean (it should always fit)
pp_check(m_inter, type = "stat_grouped", stat = "mean", group = "South")
```

```
Using all posterior draws for ppc type 'stat_grouped' by default.
```

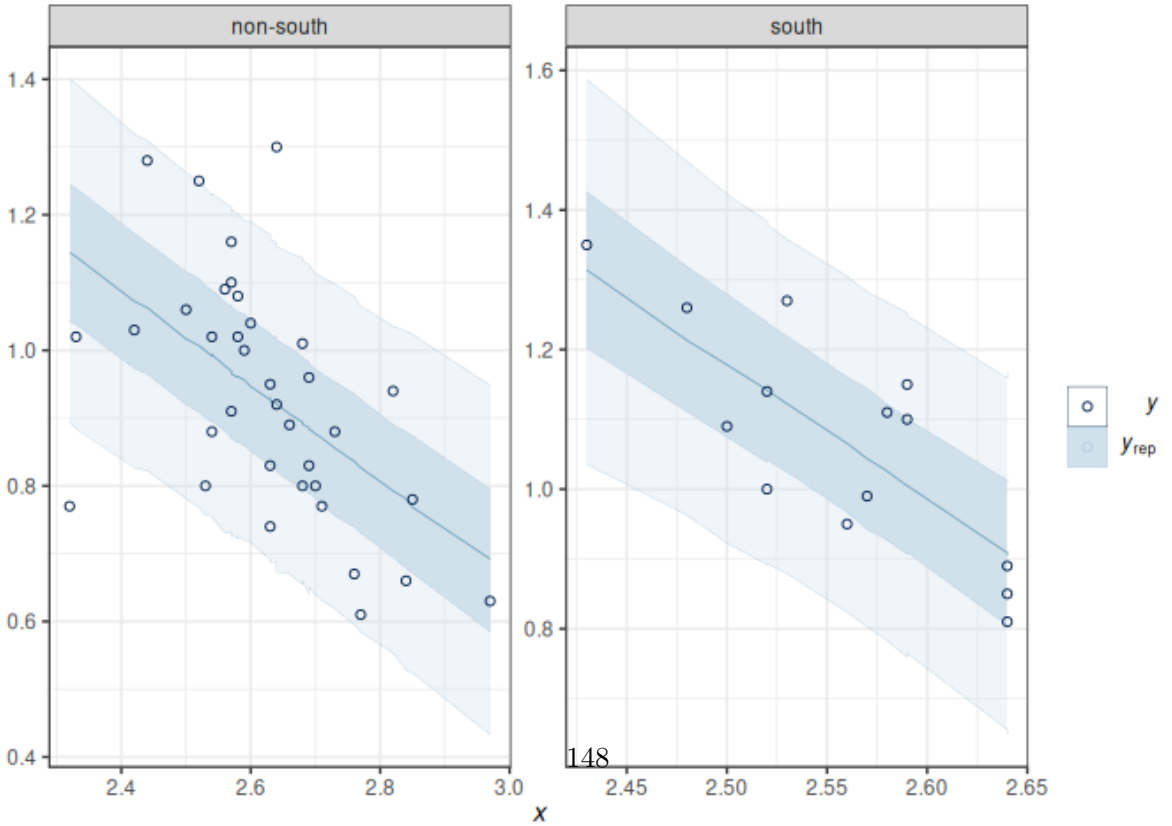
```
Loading required package: rstan
```

```
Loading required package: StanHeaders
```

```
rstan version 2.32.5 (Stan version 2.32.2)
```



(a) Density overlayed plots



(b) Prediction intervals

Figure 10.1: Posterior predictive checks for the interaction model.

```
For execution on a local, multicore CPU with excess RAM we recommend calling
options(mc.cores = parallel::detectCores()).
To avoid recompilation of unchanged Stan programs, we recommend calling
rstan_options(auto_write = TRUE)
For within-chain threading using `reduce_sum()` or `map_rect()` Stan functions,
change `threads_per_chain` option:
rstan_options(threads_per_chain = 1)


Attaching package: 'rstan'

The following object is masked from 'package:tidyr':

    extract

`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

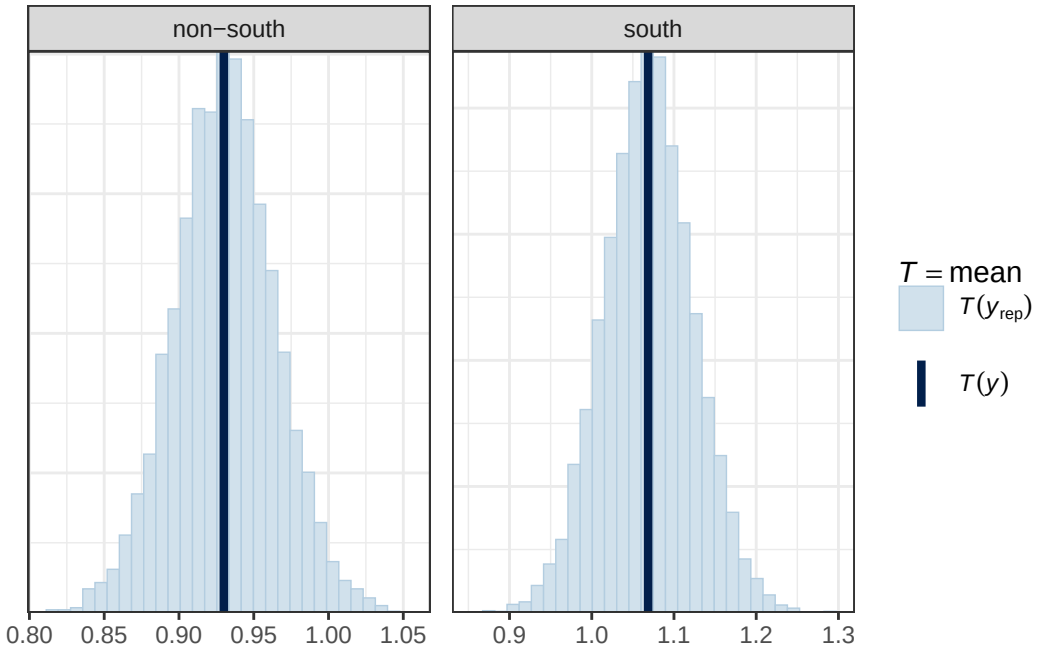


Figure 10.2: Posterior predictive check for the sample mean.

```r
# PPC for the mean (it should always fit)
# PPC for the maximum and minimum values
pp_check(m_inter, type = "stat_2d", stat = c("max", "min"))
```

```
Using all posterior draws for ppc type 'stat_2d' by default.
```

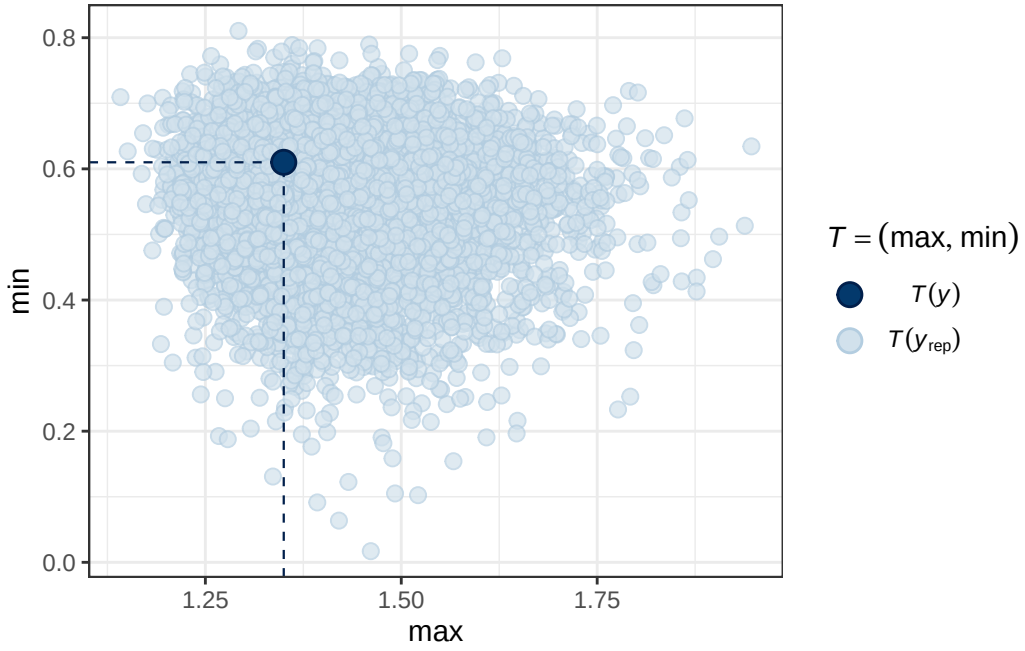


Figure 10.3: Posterior predictive check for the sample maximum and minimum.

10.2.2 Marginal model plots

To check the linearity assumption, we need to ensure that the conditional mean of Y fits according to the model. A marginal model plot compares the model predicted relationship between the outcome and each predictor, and the relationship obtained using nonparametric methods with smoothing.

```
pp_check(m_inter, type = "intervals_grouped",
         x = "MedianAgeMarriage", group = "South") +
    geom_smooth(se = FALSE, col = "blue") +
    geom_smooth(aes(y = y_obs), se = FALSE, col = "red", linetype = "dashed")
```

```
Using all posterior draws for ppc type 'intervals_grouped' by default.
```

```
`geom_smooth()` using method = 'loess' and formula = 'y ~ x'
```

```
Warning: The following aesthetics were dropped during statistical transformation: ymin,
ymax
i This can happen when ggplot fails to infer the correct grouping structure in
  the data.
i Did you forget to specify a `group` aesthetic or to convert a numerical
  variable into a factor?
The following aesthetics were dropped during statistical transformation: ymin,
ymax
i This can happen when ggplot fails to infer the correct grouping structure in
  the data.
i Did you forget to specify a `group` aesthetic or to convert a numerical
  variable into a factor?

`geom_smooth()` using method = 'loess' and formula = 'y ~ x'

Warning: The following aesthetics were dropped during statistical transformation: ymin,
ymax
i This can happen when ggplot fails to infer the correct grouping structure in
  the data.
i Did you forget to specify a `group` aesthetic or to convert a numerical
  variable into a factor?
The following aesthetics were dropped during statistical transformation: ymin,
ymax
i This can happen when ggplot fails to infer the correct grouping structure in
  the data.
i Did you forget to specify a `group` aesthetic or to convert a numerical
  variable into a factor?
```

```
# Alternative code
# plot(
#     conditional_effects(m_inter,
#         effects = "MedianAgeMarriage",
#         conditions = data.frame(South = c("south", "non-south"),
#                                 cond__ = c("South", "Non-South"))
#     ),
#     plot = FALSE
# )[[1]] +
#     # Add data points
#     geom_point(
#         data = m_inter$data,
#         aes(x = MedianAgeMarriage, y = Divorce),
#         inherit.aes = FALSE
```

```
#     ) +
#     # Add smoother
#     geom_smooth(
#         data = m_inter$data,
#         aes(x = MedianAgeMarriage, y = Divorce),
#         col = "red", linetype = "dashed",
#         inherit.aes = FALSE,
#         se = FALSE) +
#     facet_wrap(~ South)
```

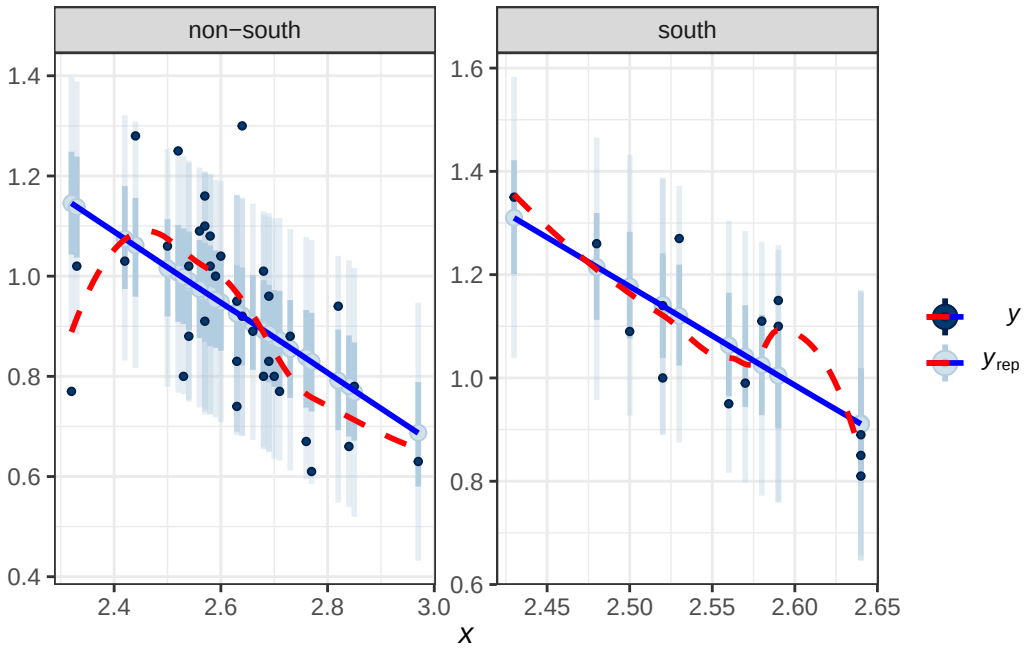


Figure 10.4: Marginal model plots with the model-implied (blue solid) and the nonparametric (red dashed) smoother.

Marginal model plots are more appropriate for ordinal or continuous predictors. As you can see above, the red line (for nonparametric fit) and the blue line (from the linear model) fit the data well, but not for the left tail area, where some of the non-Southern states have lower divorce rates than predicted. If the linearity assumption holds, these two lines should be very similar. Generally speaking, deviations in the middle indicate a strong misspecification that needs to be fixed.

Also, we want to check outliers that lie way outside the predictive interval. With a 95% predictive interval, we generally expect 5% to lie outside of the predictive interval band. In this example, we don't see a great problem with outliers.

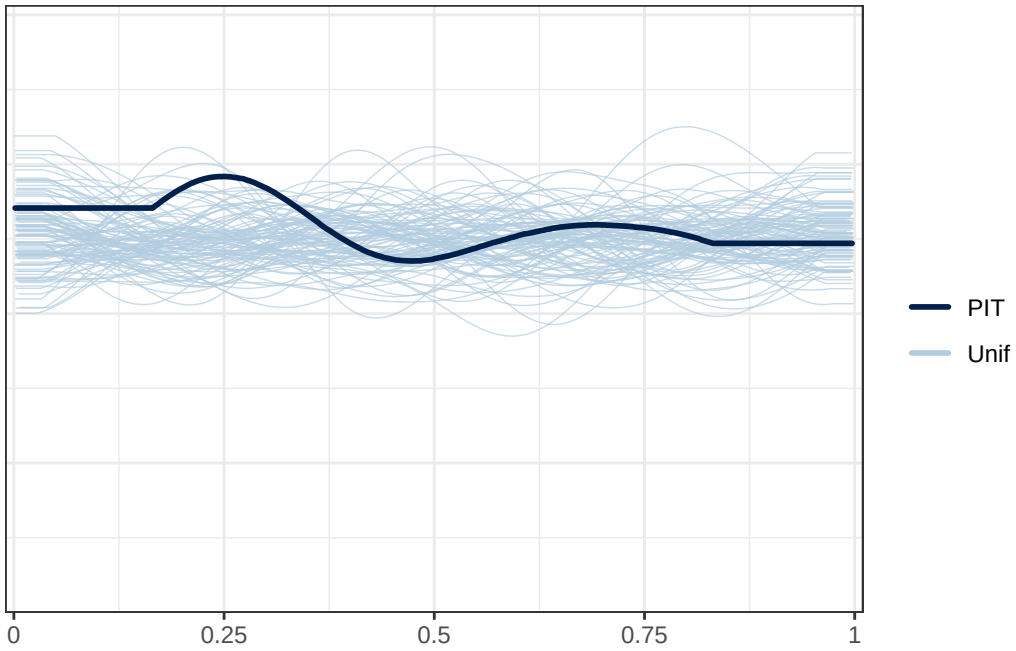
10.2.2.1 LOO PIT plots

Here's a check using probability integral transform. Roughly speaking, you can think of it as a flattened version of the marginal model plots, where you'd like to see the darkened line be relatively flat and within the range of the model prediction.

```
pp_check(m_inter, type = "loo_pit_overlay")
```

```
Using all posterior draws for ppc type 'loo_pit_overlay' by default.
```

```
NOTE: The kernel density estimate assumes continuous observations and is not optimal for dis
```



10.2.3 Residual plots

For regression analyses, one can learn a lot about model fit from the residuals, which is $y_i - \tilde{y}_i|\theta$, i.e., subtracting the observed y_i values by the posterior predictions. Because in Bayesian, there is not just one predicted value, but a whole predictive distribution, one also has an entire posterior distribution for each residual. Figure 10.5 is a check of the average residual Y (i.e., Y - $\hat{Y}$) and the true value of Y. If the model fit the data well, the points should be scattered with no specific pattern, like in Figure 10.5.

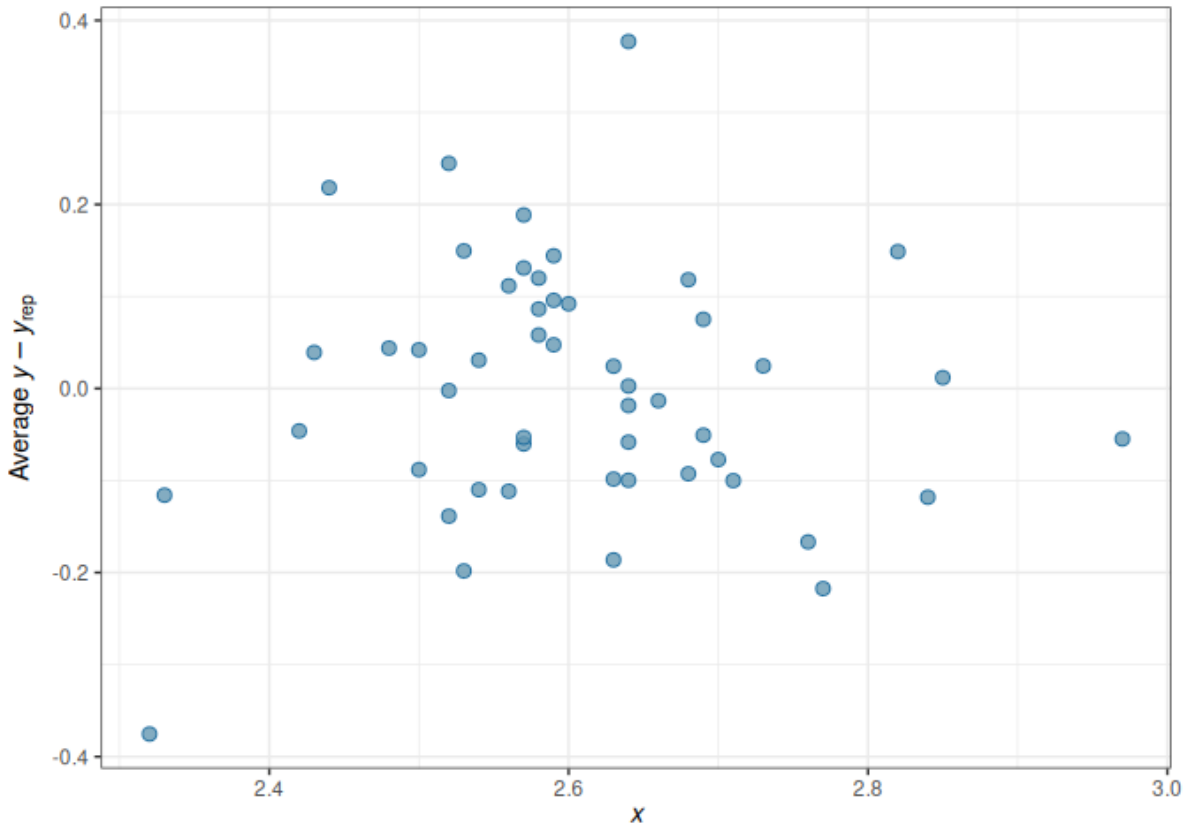


Figure 10.5: Average prediction error against the predictor. No clear pattern should be observed for a correctly specified model.

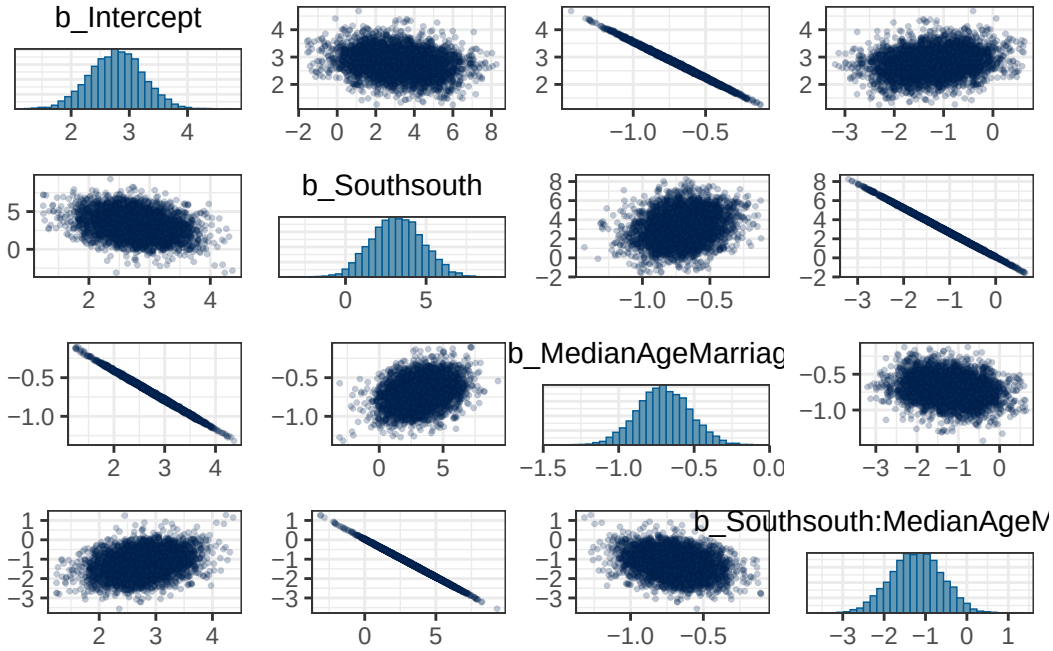
No big problem was found in the residuals. If you see that the *SD* of the residuals is not uniform, or the residuals have some non-linear relationships with the predictor, there can be some problems.

10.2.4 Multicollinearity

Strictly speaking, multicollinearity is not an assumption of regression. However, especially in frequentist analysis, having predictors that are strongly correlated can increase the uncertainty of the posterior distributions of the regression coefficients. On the other hand, the use of the prior distribution in Bayesian analyses can somewhat come to the rescue, as it makes it less likely for the posteriors to have extremely large posterior mean and standard deviation

You can look at the posterior density of the coefficients to see how correlated they are:

```
pairs(m_inter,
    variable = "^b",  # for all variables starting with b
    regex = TRUE,
    off_diag_args = # arguments of the scatterplots
        list(
            size = 0.5, # point size
            alpha = 0.25 # transparency
        )
)
```



If some coefficients are particularly strongly correlated, you may need to think about using a stronger prior or combining some predictors. In this case, the collinearity is a result of the interactions. Principal component and factor analysis are some approaches for that.

10.3 Other Topics

There are other topics we have yet to discuss here for diagnostics of multiple regression, but are just as important, including:

- Transformation (e.g., logarithm transformation with skewed outcomes and predictors, like income);
- Leverage points and influential observations (e.g., hat values, Cook's D)
- Measurement error of predictors

Part VI

Week 7

11 Model Comparison

11.1 Overfitting and Underfitting

In statistical modeling, a more complex model almost always results in a better fit to the data. Roughly speaking, a more complex model means a model with more parameters. However, as you will see later, determining the number of parameters in Bayesian analyses is not straightforward. On the extreme side, if one has 10 observations, a model with 10 parameters will perfectly predict every single data point (by just having a parameter to predict each data point). However, there are two problems with too complex a model. First, an increasingly complex model makes it increasingly hard to extract useful information from the data. Instead of describing the relationship between two variables, like `Marriage` and `Divorce`, by a straight line, one ends up with a crazy model that is difficult to make sense of. Second, as you will also see, the more complex a model, the more is the risk that it *overfits* the current data, such that it does not work for future observations.

For example, let's randomly sample 10 states in the `waffle_divorce` data set and build some models.

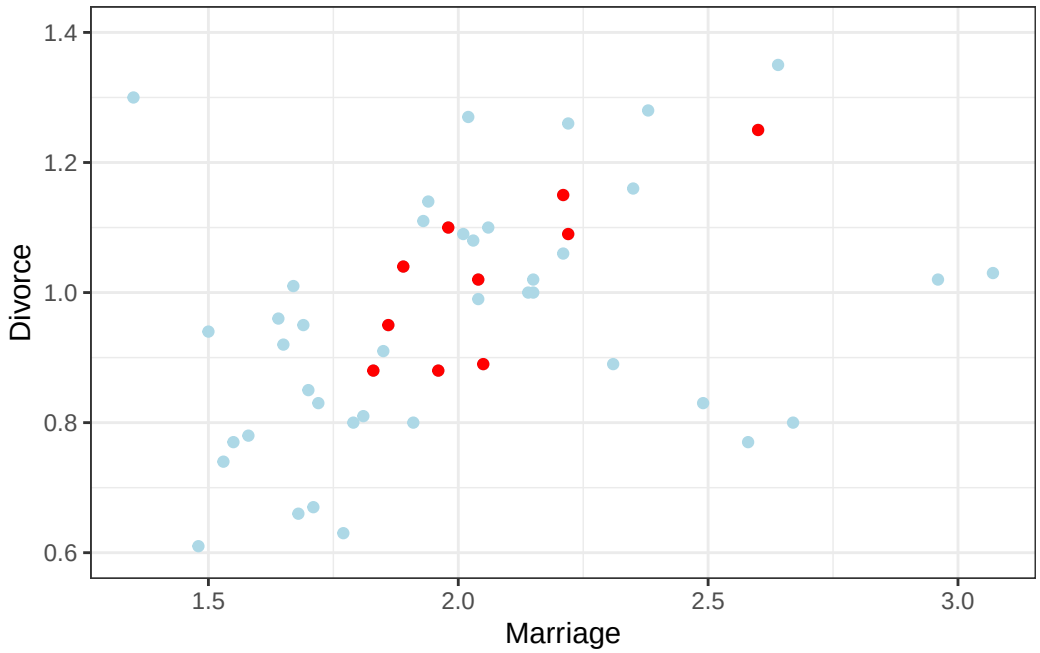
```
waffle_divorce <- read_delim(  # read delimited files
    "data/WaffleDivorce.csv",
    delim = ";"
)
```

```
Rows: 50 Columns: 13
-- Column specification --------------------------------------------------------
Delimiter: ";"
chr  (2): Location, Loc
dbl (11): Population, MedianAgeMarriage, Marriage, Marriage SE, Divorce, Div...

i Use `spec()` to retrieve the full column specification for this data.
i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
# Rescale Marriage and Divorce by dividing by 10
waffle_divorce$Marriage <- waffle_divorce$Marriage / 10
waffle_divorce$Divorce <- waffle_divorce$Divorce / 10
```

```
waffle_divorce$MedianAgeMarriage <- waffle_divorce$MedianAgeMarriage / 10
# Recode `South` to a factor variable
waffle_divorce$South <- factor(waffle_divorce$South,
    levels = c(0, 1),
    labels = c("non-south", "south")
)
```

```
set.seed(1547)  # set the seed for reproducibility
# Sample 10 observations
train <- sample.int(nrow(waffle_divorce), 10L)
wd_sub <- waffle_divorce[train, ]
base <- ggplot(aes(x = Marriage, y = Divorce),
               data = wd_sub) +
    geom_point() +
    coord_cartesian(ylim = c(0.6, 1.4)) +
    xlim(range(waffle_divorce$Marriage))
ggplot(waffle_divorce,
       aes(x = Marriage, y = Divorce)) +
    geom_point(col = "lightblue") +
    geom_point(size = 1.5, data = wd_sub, col = "red") +
    coord_cartesian(ylim = c(0.6, 1.4)) +
    xlim(range(waffle_divorce$Marriage))
```



When using `Marriage` to predict `Divorce`, we can use beyond a linear regression line by using higher-order *polynomials*. For example, a second-order polynomial represents a quadratic effect (with one turning point); it goes to cubic, quartic, and more. The figure below shows the fit from a linear effect of `Marriage`, a quadratic effect, and increasingly complex models up to a sixth-degree polynomial. As you can see, as the model gets more complex, the fitted line tries to capture all the 10 points really well, with an increasing R^2. However, the standard error around the fitted line also gets larger and bizarre, meaning more uncertainty in the model parameters.

```
r2 <- function(object, newresp, newdata) {
    # Function for computing R^2
    ypred <- predict(object, newdata = newdata)
    cor(ypred, newresp)^2
}
rmse <- function(object, newresp, newdata) {
    # Function for RMSE
    ypred <- predict(object, newdata = newdata)
    sqrt(mean((ypred - newresp)^2))
}
# Create six plots through a loop
p_list <- map(1:6, function(i) {
    # Use frequentist analyses for speed
    mod <- lm(Divorce ~ poly(Marriage, degree = i), data = wd_sub)
    base +
        geom_smooth(method = "lm", formula = y ~ poly(x, i), level = .80,
                    fullrange = TRUE) +
        annotate("text", x = 1.7, y = 1.4,
                 label = paste0("italic(R)^2 == ",
                                round(r2(mod, wd_sub$Divorce), 2)),
                 parse = TRUE) +
        annotate("text", x = 1.7, y = 1.2,
                 label = paste0("RMSE == ",
                                round(rmse(mod, wd_sub$Divorce), 2)),
                 parse = TRUE)
})
do.call(grid.arrange, c(p_list, nrow = 2))
```

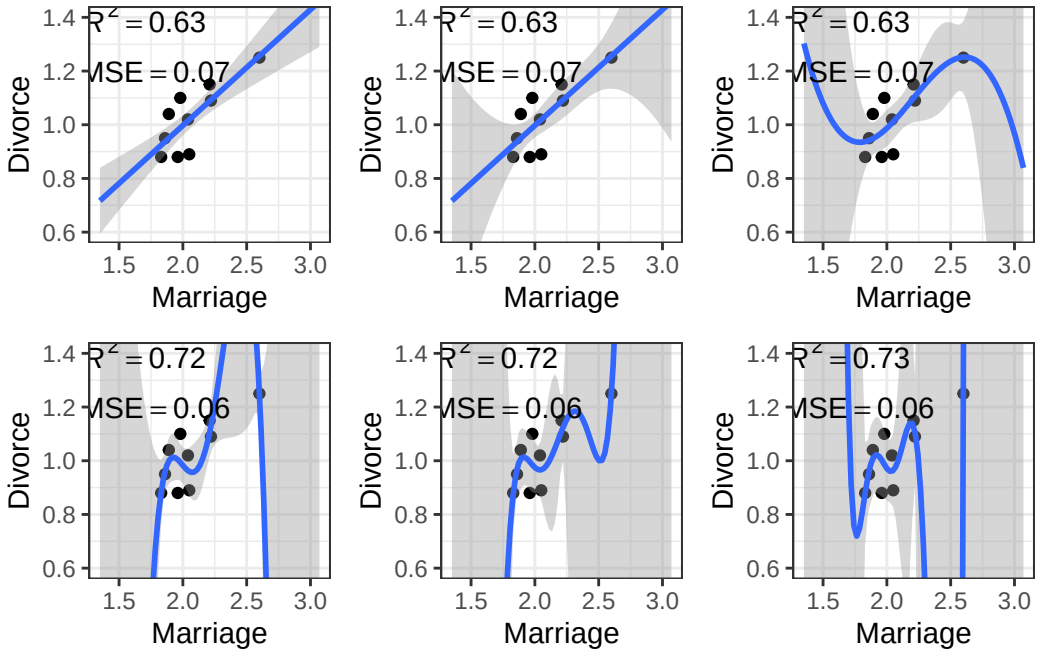


Figure 11.1: Fit of models on the 10 random cases. Top panel: linear, quadratic, and cubic; bottom panel: 4th, 5th, and 6th degree polynomials

Another way to look at model accuracy is the *Root Mean Squared Error* (RMSE), defined as the square root of the average squared prediction error. RMSE is a measure of prediction error. The smaller the RMSE, the better the prediction is. As you can see in the above figure, more complex models always reduce the RMSE in the data we use to fit the model (also called training data).

However, if I take the estimated regression line/curve based on the subsample of 10 observations, and predict the remaining cases in the data set, things will be different. As you can see in the figure below, whereas prediction error is comparable for the linear and the quadratic model, polynomials of higher degrees predict the data really badly. When you use a complex model in a data set, it tailors the coefficients to any sampling errors and noise in the data such that it will not generalize to new observations. Therefore, our goal in model comparison is to choose a model complex enough to capture the essence of the data generation process (and thus avoid *underfitting*), but not too complex such that it suffers from *overfitting*.

```
base2 <- ggplot(aes(x = Marriage, y = Divorce),
                data = waffle_divorce[-train, ]) +
    geom_point() +
    coord_cartesian(ylim = c(0.6, 1.4)) +
    xlim(range(waffle_divorce$Marriage))
```

```
# Create six plots through a loop
p_list2 <- map(1:6, function(i) {
    # Use frequentist analyses for speed
    mod <- lm(Divorce ~ poly(Marriage, degree = i), data = wd_sub)
    # New data and response
    test_dat <- waffle_divorce[-train, ]
    ynew <- test_dat$Divorce
    base2 +
        geom_smooth(data = wd_sub, method = "lm", formula = y ~ poly(x, i),
                    level = .80, fullrange = TRUE) +
        annotate("text", x = 1.7, y = 1.4,
                 label = paste0("italic(R)^2 == ",
                                round(r2(mod, ynew, test_dat), 2)),
                 parse = TRUE) +
        annotate("text", x = 1.7, y = 1.2,
                 label = paste0("RMSE == ",
                                round(rmse(mod, ynew, test_dat), 2)),
                 parse = TRUE)
})
do.call(grid.arrange, c(p_list2, nrow = 2))
```

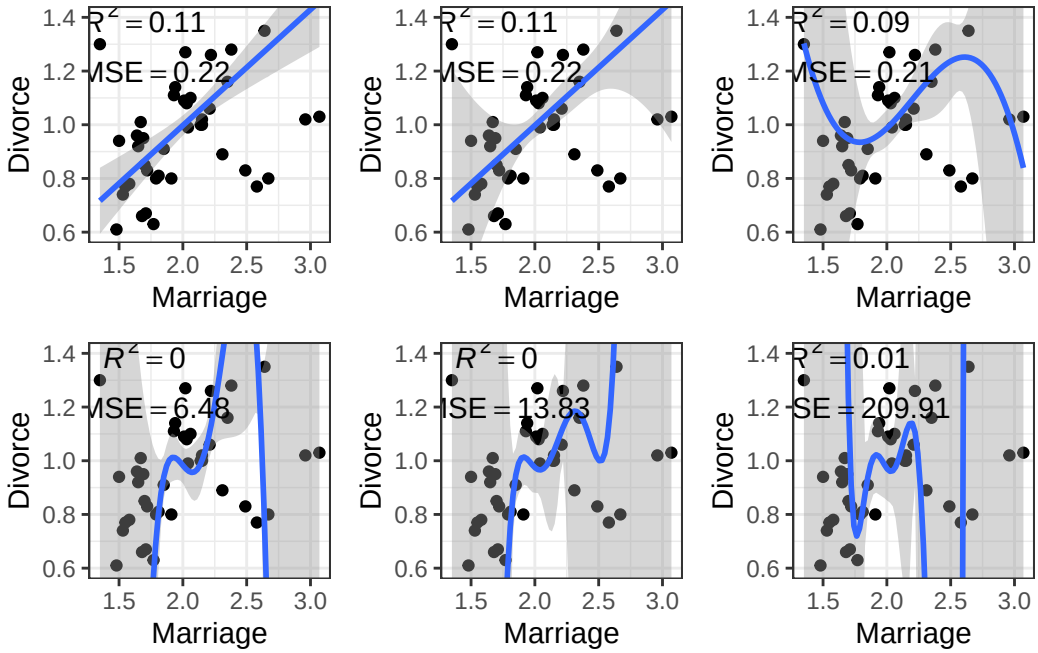


Figure 11.2: Using the regression lines based on 10 random cases to predict the remaining 40 cases. Top panel: linear, quadratic, and cubic; bottom panel: 4th, 5th, and 6th degree polynomials

The goal of statistical modeling is to choose an optimal model between the overfitting/underfitting dichotomy. In machine learning, this is also commonly referred to as the bias-variance trade-off, as a model that is too simple tends to produce biased predictions because it does not capture the essence of the data generating process. In contrast, a overly complex model is unbiased but results in a lot of uncertainty in the prediction because there are too many unnecessary components that can affect predictions, as indicated in the confidence bands around the 6th-degree polynomial line.

Polynomials of varying degrees are merely one example of comparing simple to complex models. You can think about:

- models with and without interactions,
- models with a few predictors versus hundreds of predictors,
- regression analyses versus multilevel models, etc.

Whereas one can always avoid underfitting by fitting a more and more complex model, we need tools to keep us from overfitting. This lecture is about finding an optimal model that avoids overfitting and avoids underfitting. You will learn to perform model comparisons with information criteria to find a model that has a better balance between overfitting and underfitting.

11.2 Kullback-Leibler Divergence

When comparing models (e.g., linear vs. quadratic), we prefer models closer to the "true" data-generating process. To do so, we need some ways to quantify the degree of "closeness" to the true model. In this context, models comprise both the distributional family *and* the parameter values. For example, the model $y_i \sim N(5, 2)$ is a different model than $y_i \sim N(3, 2)$, which is a different model than $y_i \sim \text{Gamma}(2, 2)$. The first two have the same family but different parameter values (different means, same *SD*). In contrast, the last two have different distributional families (Normal vs. Gamma).

To measure the degree of "closeness" between two models, M_0 and M_1, by far the most popular metric in statistics is the *Kullback-Liebler Divergence* (or Kullback-Liebler discrepancy; D_{KL}). By definition,

$$\begin{aligned} D_{\text{KL}}(M_0 \mid M_1) &= \int_{-\infty}^{\infty} p_{M_0}(\mathbf{y}) \log \frac{p_{M_0}(\mathbf{y})}{p_{M_1}(\mathbf{y})} \, \mathrm{d}\mathbf{y} \\ &= \int_{-\infty}^{\infty} p_{M_0}(\mathbf{y}) \log p_{M_0}(\mathbf{y}) \, \mathrm{d}\mathbf{y} - \int_{-\infty}^{\infty} p_{M_0}(\mathbf{y}) \log p_{M_1}(\mathbf{y}) \, \mathrm{d}\mathbf{y}. \end{aligned}$$

Note that strictly speaking, D_{KL} cannot be called a "distance" between two models because in general, $D_{\text{KL}}(M_0 \mid M_1) \neq D_{\text{KL}}(M_1 \mid M_0)$. As an example, assume that the data are generated by a true model M_0, and we have two candidate models M_1 and M_2, where

- $M_0 : y \sim N(3, 2)$
- $M_1 : y \sim N(3.5, 2.5)$
- $M_2 : y \sim \text{Cauchy}(3, 2)$

```
ggplot(data.frame(x = c(-3, 9)), aes(x = x)) +
    stat_function(fun = dnorm, args = list(mean = 3, sd = 2),
                  aes(col = "M0"), linewidth = 1) +
    stat_function(fun = dnorm, args = list(mean = 3.5, sd = 2.5),
                  aes(col = "M1"), linewidth = 2) +
    stat_function(fun = dcauchy, args = list(location = 3, scale = 2),
                  aes(col = "M2"), linewidth = 2) +
    scale_color_manual(values = c("black", "red", "blue"),
                       labels = c("M0", "M1", "M2")) +
    labs(x = "y", y = "density", col = NULL)
```

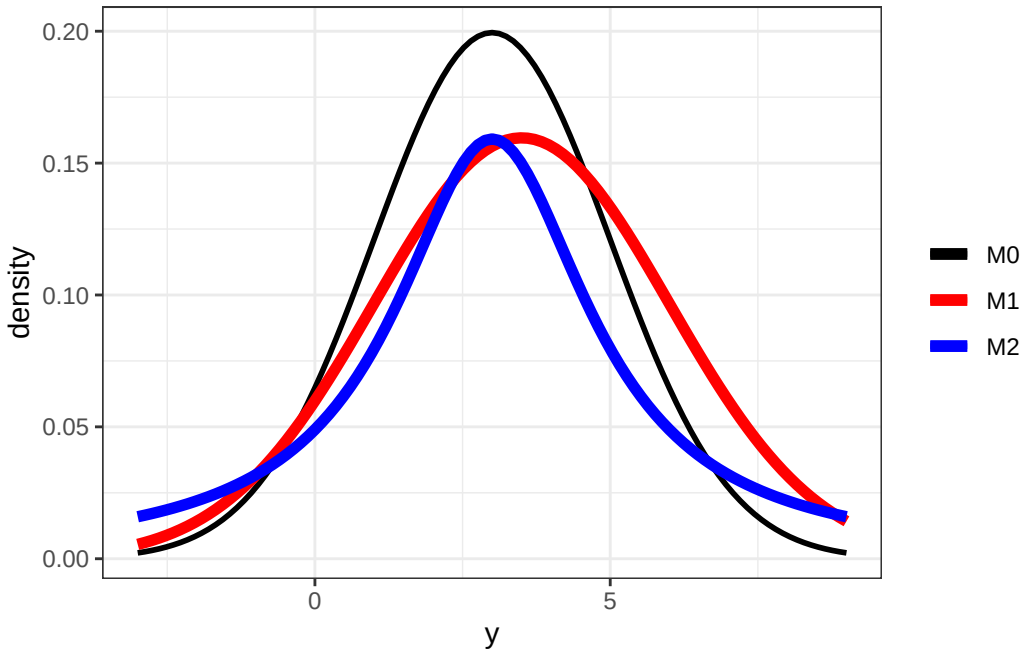


Figure 11.3: Density for M_0, M_1, and M_2

```
f1 <- function(x) {
    dnorm(x, 3, 2) * (dnorm(x, 3, 2, log = TRUE) -
        dnorm(x, 3.5, 2.5, log = TRUE))
}
f2 <- function(x) {
    dnorm(x, 3, 2) * (dnorm(x, 3, 2, log = TRUE) -
        dcauchy(x, 3, 2, log = TRUE))
}
```

One can compute that $D_{\mathrm{KL}}(M_0 \mid M_1) = 0.0631436$ and $D_{\mathrm{KL}}(M_0 \mid M_1) = 0.2592445$, and so M_1 is a better model than M_2.

Note that in the expression of D_{KL}, when talking about the same target model, the first term is always the same and describes the "true" model, M_0. Therefore, it is sufficient to compare models on the second term, $\int_{-\infty}^{\infty} p_{M_0}(\mathbf{y}) \log p_{M_1}(\mathbf{y})\, \mathrm{d}\mathbf{y}$, which can also be written as $\mathrm{E} = [\log p_{M_1}(\mathbf{y})]$, i.e., the *expected log predictive density* (*elpd*). In other words, a model with a larger elpd is preferred over a model with a smaller elpd.

However, we don't know what M_0 is in real data analysis. If we knew, then we would just need to choose M_0 as our model, and there will be no need for model comparisons. In addition, even if we know that the true model is, e.g., a normal model (which never happens in real data analysis), we still need to estimate the parameter values, and the estimates will not be exactly

the same as the true parameter values. However, elpd is defined as the expected value over the true predictive distribution, $p_{M_0}(y)$, which cannot be obtained without knowing what M_0 is.

So instead, we need to estimate the elpd. A naive way to estimate it is to use the data distribution in place of the true model, but that will lead to an overly optimistic estimate as the sample data are noisy. Computing elpd this way will always favor a more complex model. The ideal way is to collect data on a new, independent sample that share the same data generating process as the current sample, and estimate elpd on the new sample. This is called *out-of-sample validation*. The problem, of course, is that we usually do not have the resources to collect a new sample.

Therefore, statisticians have worked hard to find ways to estimate elpd from the current sample, and there are two broad approaches:

- Information criteria: AIC, DIC, and WAIC, which estimate the elpd in the current sample, minus a correction factor
- Cross-validation, which splits the current sample into K parts, estimates the parameters in $K - 1$ parts, and estimates the elpd in the remaining part. A special case is when $K = N$, each time one uses N - 1 data points to estimate the model parameters, and estimate the elpd for the observation that was left out. This is called *leave-one-out* cross-validation (LOO-CV).

11.3 Deviance

Without going too deep into the underlying math, it can be shown that a good estimate of elpd is

$$\sum_{i=1}^{n} \log p_{M_1}(y_i) - p,$$

where p is some measure of the number of parameters in M_1. The first term is the likelihood of the model in the current sample. The second term is an adjustment factor so that the quantity above represents the average likelihood of the model *in a new sample*. It is more common to work with *deviance* by multiplying the log-likelihood by -2, i.e.,

$$D = -2 \sum_{i=1}^{n} \log p_{M_1}(y_i).$$

11.3.1 Experiment on Deviance

Now, let's check the in-sample deviance and out-of-sample deviance of our `waffle_divorce` data with different polynomial functions. Here is a sample function for computing elpd (with frequentist, just for speed) for polynomials of different degrees:

```
# Function for computing deviance with different polynomial
deviance_divorce <- function(degree = 1,
                             train = 10,
                             y = waffle_divorce$Divorce,
                             x = waffle_divorce$Marriage) {
    N <- length(y)
    # get training sample
    if (length(train) == 1) {
        train <- sample.int(N, train)
    }
    ntrain <- length(train)
    # Obtain design matrix
    X <- cbind(1, poly(x, degree, simple = TRUE))
    # Get elpd for training sample
    Xtrain <- X[train, ]
    ytrain <- y[train]
    betahat <- qr.solve(Xtrain, ytrain)  # estimated betas
    res_train <- ytrain - Xtrain %*% betahat
    sigmahat <- sqrt(sum(res_train^2) /
        (ntrain - 1 - degree)) # estimated sigma
    deviance_train <- -2 * sum(dnorm(res_train, sd = sigmahat, log = TRUE))
    res_test <- y[-train] - X[-train, ] %*% betahat
    deviance_test <- -2 * sum(dnorm(res_test, sd = sigmahat, log = TRUE))
    data.frame(
        degree = degree,
        sample = c("in-sample", "out-of-sample"),
        deviance = c(deviance_train / ntrain,
                     deviance_test / (N - ntrain))
    )
}
```

Below shows the in-sample and out-of-sample elpd for the linear model:

```
deviance_divorce(degree = 1, train = train)
```

```
  degree        sample deviance
```

```
1      1     in-sample -2.37580
2      1 out-of-sample  3.78599
```

And for quadratic:

```
deviance_divorce(degree = 2, train = train)
```

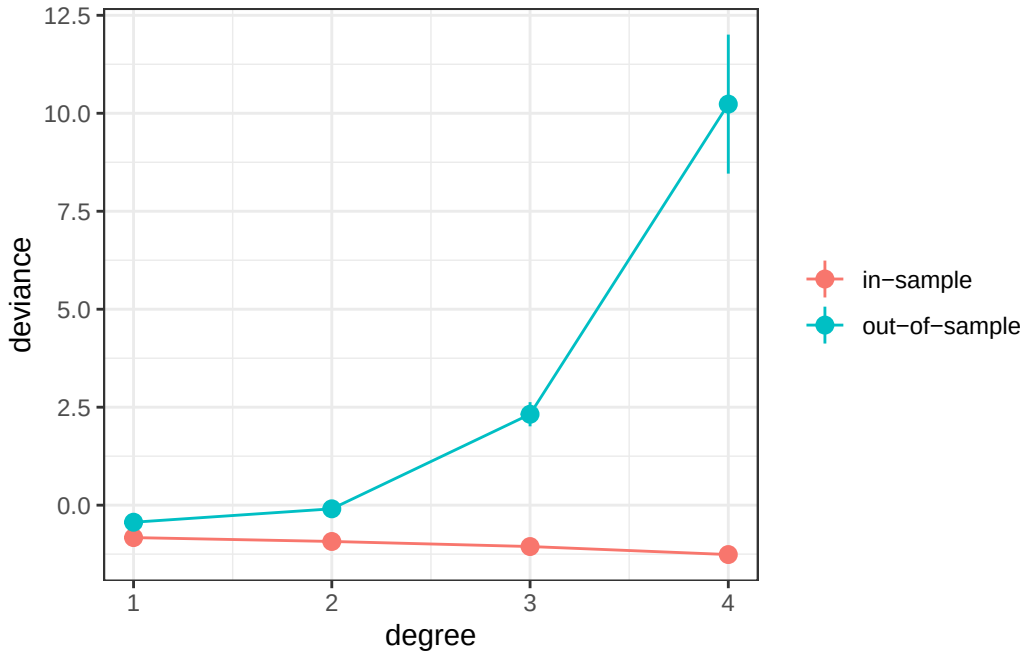
```
  degree        sample  deviance
1      2     in-sample -2.342268
2      2 out-of-sample  3.048412
```

In general, as you can see, the deviance is smaller for the current data than for the hold-out data. Note that because the training and testing data sets have different sizes, I divided the deviance by the sample size so that they can be compared.

Now let's run an experiment to check the elpd with different degrees polynomial, with a training sample size of 25:

```
set.seed(1733)
# Use the `map` function to run different polynomials, and use the `rerun`
# function run the deviance 100 times. The code below runs `deviance_divorce` by
# randomly sampling 25 training samples 100 times, and compute the in-sample
# and out-of-sample deviance for each.
# rerun(100, deviance_divorce(degree = 1, train = 25L)) |>
#     bind_rows()
# Now run 1 to 4 degree polynomial, each 1000 times:
dev_list <- lapply(1:4, FUN = function(p) {
    results <- replicate(1000, deviance_divorce(degree = p, train = 25L), simplify = FALSE)
    do.call(rbind, results)
})
dev_df <- do.call(rbind, dev_list)
# Plot the results
dev_df |>
    ggplot(aes(x = degree, y = deviance, col = sample)) +
    stat_summary() +
    stat_summary(geom = "line") +
    labs(col = NULL)
```

```
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
```



As you can see, the in-sample deviance (red line) keeps decreasing, indicating that a more complex model fits the data better, which is always the case. So if one were to use deviance to determine what model is optimal, one would always choose the most complex model, just like using R^2 (indeed, for linear models, deviance is basically the same as R^2).

Now, look at the blue line, which represents the deviance computed using the coefficients obtained from the training set but applied to the remaining data. As you can see, the deviance achieves its minimum around the linear and the quadratic model, and starts to increase, meaning that the more complex models do not fit the hold-out data.

A statistical model is used to learn something from a data set that can generalize to other observations. Therefore, we should care about the blue line, instead of the red one. The indices you will see in the remaining of this note are all attempts to approximate the blue line.

> More complex models always fit the current data better, but may not generalize to other data. In other words, models that are too complex are not generalizable.

11.4 Information Criteria

We will illustrate the computation of information criteria with `Marriage` predicting `Divorce`:

```
m1 <- brm(Divorce ~ Marriage, data = waffle_divorce,
          prior = c(prior(student_t(4, 0, 5), class = "Intercept"),
                    prior(normal(0, 2), class = "b"),
                    prior(student_t(4, 0, 1), class = "sigma")),
          iter = 4000,
          seed = 2302,
          file = "07_m1"
)
```

11.4.1 Akaike Information Criteria (AIC)

Multiplying the quantity of elpd - p by -2, or deviance + $2p$, with the deviance obtained using the maximum likelihood estimates (MLEs) for the parameters, gives you the formula for AIC:

$$\text{AIC} = D(\hat{\theta}) + 2p,$$

and p in AIC is just the number of parameters. As we have multiplied by a negative number, maximizing the estimate of elpd is equivalent to minimizing the AIC, so one would prefer a model with the smallest AIC.

The AIC is not Bayesian because it only uses point estimates (MLEs) of parameters rather than their posterior distributions. Also, it does not take into account any prior information.

```
# Frequentist model
m1_freq <- lm(m1$formula, data = m1$data)
AIC(m1_freq)
```

```
[1] -30.96869
```

11.4.2 Deviance Information Criteria (DIC)

The definition of AIC assumes that the parameter estimates are known or are maximum likelihood estimates. The DIC, instead, replaces those with the posterior distribution of the parameters. The general formula for DIC is

$$\text{DIC} = \text{E}(D \mid \mathbf{y}) + 2p_D,$$

where p_D is the effective number of parameters estimated in the Markov chain. Although DIC does take into account the prior distributions, it does not consider the full posterior distributions of the parameters.

```
# Function to compute DIC
dic_brmsfit <- function(object) {
    Dbar <- -2 * mean(rowSums(log_lik(object)))
    res <- residuals(object)[ , "Estimate"]
    sigma <- posterior_summary(object, variable = "sigma")[ , "Estimate"]
    Dhat <- -2 * sum(dnorm(res, sd = sigma, log = TRUE))
    p <- Dbar - Dhat
    elpd <- Dhat / -2 - p
    data.frame(elpd_dic = elpd, p_dic = p, dic = Dhat + 2 * p,
               row.names = "Estimate")
}
dic_brmsfit(m1)
```

```
Loading required package: rstan
```

```
Loading required package: StanHeaders
```

```


rstan version 2.32.5 (Stan version 2.32.2)
```

```
For execution on a local, multicore CPU with excess RAM we recommend calling
options(mc.cores = parallel::detectCores()).
To avoid recompilation of unchanged Stan programs, we recommend calling
rstan_options(auto_write = TRUE)
For within-chain threading using `reduce_sum()` or `map_rect()` Stan functions,
change `threads_per_chain` option:
rstan_options(threads_per_chain = 1)
```

```


Attaching package: 'rstan'
```

```
The following objects are masked from 'package:posterior':

    ess_bulk, ess_tail
```

```
The following object is masked from 'package:tidyr':

    extract
```

```
         elpd_dic    p_dic       dic
Estimate 15.36384 3.109187 -30.72769
```

11.4.3 Watanabe-Akaike Information Criteria (WAIC)

A further modification is to use the *log pointwise posterior predictive density*, with the effective number of parameters computed using the posterior variance of the likelihood.

$$\text{WAIC} = -2 \sum_{i=1}^{n} \log \text{E}[p(y_i \mid , \mathbf{y})] + 2p_{\text{WAIC}},$$

where $\text{E}[p(y_i \mid , \mathbf{y})]$ is the posterior mean of the likelihood of the ith observation. The WAIC incorporates prior information, and the use of pointwise likelihood makes it more robust when the posterior distributions deviate from normality. In general, WAIC is a better estimate of the out-of-sample deviance than AIC and DIC.

```
waic(m1)  # built-in function in brms
```

```
Computed from 8000 by 50 log-likelihood matrix.

          Estimate  SE
elpd_waic     15.2 4.9
p_waic         3.2 0.9
waic         -30.3 9.9

1 (2.0%) p_waic estimates greater than 0.4. We recommend trying loo instead.
```

11.4.4 Leave-One-Out Cross-Validation

The idea of cross-validation is to split the sample so that it imitates the scenario of estimating the parameters in part of the data and predicting the remaining part. The part used for estimation is called the *training set*, and the part used for prediction is called the *validation set*. Leave-one-out information criteria (LOO-IC) means that one uses $N - 1$ observations as the training set and 1 observation as the validation sample and repeat the process N times so that a different observation is being predicted each time. Adding up the prediction results

will give an estimate of elpd that closely approximates the results that would be obtained by collecting new data and doing the validation. To make it more concrete, we can go back to the `waffle_divorce` data with `Marriage` predicting `Divorce`. We can do this for case #1 (Alabama), as an example:

```
# Estimate the model without case #1
m1_no1 <- update(m1, newdata = waffle_divorce[-1, ])
```

```
# The log predictive density for case #1
mean(log_lik(m1_no1, newdata = waffle_divorce[1, ]))
```

```
[1] -0.7965575
```

Because LOO-IC requires fitting the model N times, it is generally very computationally intensive. There are, however, shortcuts for some models to make the computation faster. WAIC can also be treated as a fast approximation of LOO-IC, although LOO-IC is more robust and will be a better estimate of out-of-sample deviance. The `loo` package uses the so-called Pareto smoothed importance sampling (PSIS) to approximate LOO-IC without repeating the process N times.

Here is the LOO-IC for the model:

```
loo(m1)
```

```
Computed from 8000 by 50 log-likelihood matrix.

         Estimate  SE
elpd_loo     15.1 5.0
p_loo         3.3 1.0
looic       -30.2 9.9
------
MCSE of elpd_loo is 0.0.
MCSE and ESS estimates assume MCMC draws (r_eff in [0.7, 1.0]).

All Pareto k estimates are good (k < 0.7).
See help('pareto-k-diagnostic') for details.
```

You can save the WAIC and the LOO-IC information to the fitted result:

```
m1 <- add_criterion(m1, criterion = c("loo", "waic"))
```

See Vehtari et al. (2017) for more discussions on WAIC and LOO-IC.

11.4.5 Example

Consider four potential models in predicting `Divorce`:

$$\texttt{Divorce}_i \sim N(\mu_i, \sigma)$$

- M1: `Marriage`
- M2: `Marriage`, `South`, `Marriage` × `South`
- M3: `South`, smoothing spline of `Marriage` by `South`
- M4: `Marriage`, `South`, `MedianAgeMarriage`, `Marriage` × `South`, `Marriage` × `MedianAgeMarriage`, `South` × `MedianAgeMarriage`, `Marriage` × `South` × `MedianAgeMarriage`

```
# Note, m1 has been fit before; the `update()` function
# can be used to simply change the formula, and brms will
# determine whether it needs re-compiling.
# M2: Add South and interaction
m2 <- update(m1, formula = Divorce ~ Marriage * South,
             newdata = waffle_divorce)
m2 <- add_criterion(m2, c("loo", "waic"))
```

```
Warning:
1 (2.0%) p_waic estimates greater than 0.4. We recommend trying loo instead.
```

```
# M3: Spline function for Marriage
m3 <- update(m1, formula = Divorce ~ South + s(Marriage, by = South),
             newdata = waffle_divorce,
             control = list(adapt_delta = .999))
m3 <- add_criterion(m3, c("loo", "waic"))
```

```
Warning: Found 3 observations with a pareto_k > 0.7 in model 'm3'. We recommend
to set 'moment_match = TRUE' in order to perform moment matching for
problematic observations.
```

```
Warning:
4 (8.0%) p_waic estimates greater than 0.4. We recommend trying loo instead.
```

```
# M4: Three-way interactions
m4 <- update(m1, formula = Divorce ~ Marriage * MedianAgeMarriage * South,
             newdata = waffle_divorce,
             control = list(max_treedepth = 12))  # increase due to warning
m4 <- add_criterion(m4, c("loo", "waic"))
```

```
Warning: Found 1 observations with a pareto_k > 0.7 in model 'm4'. We recommend
to set 'moment_match = TRUE' in order to perform moment matching for
problematic observations.
```

```
Warning:
3 (6.0%) p_waic estimates greater than 0.4. We recommend trying loo instead.
```

The first model only has `Marriage` as a predictor, which means that the coefficients for `South` and `MedianAgeMarriage` are assumed to be zero. The second model added `South` and its interaction with `Marriage` as a predictor. The third model includes a smoothing spline term (a flexible non-linear function, within the class of linear models), whereas the fourth model also includes `MedianAgeMarriage` and all two-way and three-way interactions. Now, we can compare the four models:

```
loo_compare(m1, m2, m3, m4)
```

```
   elpd_diff se_diff
m4  0.0       0.0
m2 -5.5       4.0
m3 -6.1       4.0
m1 -8.6       4.2
```

```
# m4 is the best
```

```
msummary(list(M1 = m1, M2 = m2, M3 = m3, M4 = m4),
         estimate = "{estimate} [{conf.low}, {conf.high}]",
         statistic = NULL, fmt = 2)
```

```
Warning:
`modelsummary` uses the `performance` package to extract goodness-of-fit
statistics from models of this class. You can specify the statistics you wish
```

	M1	M2	M3
b_Intercept	0.61 [0.35, 0.87]	0.66 [0.41, 0.93]	0.94 [0.89, 0.99]
b_Marriage	0.18 [0.05, 0.31]	0.13 [0.01, 0.26]	
sigma	0.17 [0.14, 0.21]	0.16 [0.13, 0.20]	0.15 [0.12, 0.19]
b_Southsouth		−0.62 [−1.43, 0.21]	0.10 [−0.02, 0.22
b_Marriage × Southsouth		0.37 [−0.04, 0.76]	
bs_sMarriage × SouthnonMsouth_1			−0.45 [−3.32, 1.4
bs_sMarriage × Southsouth_1			1.27 [−2.09, 3.59
sds_sMarriageSouthnonMsouth_1			0.86 [0.05, 2.64]
sds_sMarriageSouthsouth_1			0.49 [0.02, 2.65]
b_MedianAgeMarriage			
b_Marriage × MedianAgeMarriage			
b_MedianAgeMarriage × Southsouth			
b_Marriage × MedianAgeMarriage × Southsouth			
Num.Obs.	50	50	50
R2	0.139	0.308	0.390
R2 Adj.	0.069	0.207	0.160
ELPD	15.1	18.2	17.6
ELPD s.e.	5.0	5.5	5.9
LOOIC	−30.2	−36.5	−35.2
LOOIC s.e.	9.9	11.1	11.7
WAIC	−30.3	−36.7	−36.7
RMSE	0.17	0.15	0.14

```
to compute by supplying a `metrics` argument to `modelsummary`, which will then
push it forward to `performance`. Acceptable values are: "all", "common",
"none", or a character vector of metrics names. For example: `modelsummary(mod,
metrics = c("RMSE", "R2")` Note that some metrics are computationally
expensive. See `?performance::performance` for details.
 This warning appears once per session.
```

Model 4 has the lowest LOO-IC, so one may conclude that Model 4 is the best model among the four, **for prediction purposes**.

---

12 Stacking, Regularization, and Variable Selection

12.1 Stacking/Model Averaging

Sometimes it may not be a good practice to only choose one model with low WAIC or LOO-IC, especially when several models have very imilar WAIC/LOO-IC, but they make somewhat different predictions. Instead, we can perform *stacking* or *model averaging* by weighting the *predictions* from multiple models, using weights that are based on their information criteria performance. Stacking approaches this by optimizing the leave-one-out mean squared error in the resulting prediction, whereas model averaging preserves the uncertainty and was not optimized for that task. The technical details can be found in Yao et al. (2018).

Note that the conventional Bayesian model averaging used the posterior model probability (Hoeting et al., 1999), which are approximated by the BIC. The discussion in this note is based on more recent discussion in, e.g., Yao et al. (2018).

We'll use a data set `kidiq` that is used in the textbook by Gelman et al. (2021), which can be downloaded and imported with the direct link:

```
kidiq <- haven::read_dta("http://www.stat.columbia.edu/~gelman/arm/examples/child.iq/kidiq.dt
head(kidiq)
```

```
# A tibble: 6 x 5
  kid_score mom_hs mom_iq mom_work mom_age
      <dbl>  <dbl>  <dbl>    <dbl>   <dbl>
1        65      1  121.         4      27
2        98      1   89.4        4      25
3        85      1  115.         4      27
4        83      1   99.4        3      25
5       115      1   92.7        4      27
6        98      0  108.         1      18
```

Let's run four models. First rescale some of the variables:

```
kidiq100 <- kidiq |>
  mutate(mom_iq = mom_iq / 100,  # divid mom_iq by 100
         kid_score = kid_score / 100,   # divide kid_score by 100
         mom_iq_c = mom_iq - 1,
         mom_hs = factor(mom_hs, labels = c("no", "yes")),
         mom_age_c = (mom_age - 18) / 10)
```

I will run four models, which is from the last note

$$\texttt{kidscore}_i \sim N(\mu_i, \sigma)$$

$$\begin{aligned}
\mu_i &= \beta_0 + \beta_1(\texttt{mom_iq}_i) \\
\mu_i &= \beta_0 + \beta_1(\texttt{mom_iq}_i) + \beta_2(\texttt{mom_hs}_i) \\
\mu_i &= \beta_0 + \beta_1(\texttt{mom_iq}_i) + \beta_2(\texttt{mom_hs}_i) + \beta_3(\texttt{mom_iq}_i \times \texttt{mom_hs}_i) \\
\mu_i &= \beta_0 + \beta_1(\texttt{mom_iq}_i) + \beta_2(\texttt{mom_hs}_i) + \beta_3(\texttt{mom_iq}_i \times \texttt{mom_hs}_i) + \beta_4(\texttt{mom_age}_i)
\end{aligned}$$

```
m1 <- brm(kid_score ~ mom_iq_c,
    data = kidiq100,
    prior = c(
        prior(normal(0, 1), class = "Intercept"),
        prior(normal(0, 1), class = "b"),
        prior(student_t(4, 0, 1), class = "sigma")
    ),
    seed = 2302,
    file = "07b_m1"
)
m1 <- add_criterion(m1, c("loo", "waic"))
# Use `update` will sometimes avoid recompiling
m2 <- update(m1, kid_score ~ mom_iq_c + mom_hs,
    newdata = kidiq100,
    file = "07b_m2"
)
```

```
The desired updates require recompiling the model
```

```
m2 <- add_criterion(m2, c("loo", "waic"))
m3 <- update(m2, kid_score ~ mom_iq_c * mom_hs,
    prior = c(prior(normal(0, 0.5),
        class = "b",
```

```
        coef = "mom_iq_c:mom_hsyes"
    )),
    file = "07b_m3"
)
```

```
The desired updates require recompiling the model
```

```
m3 <- add_criterion(m3, c("loo", "waic"))
m4 <- update(m3, kid_score ~ mom_iq_c * mom_hs + mom_age_c,
    newdata = kidiq100,
    file = "07b_m4"
)
```

```
The desired updates require recompiling the model
```

```
m4 <- add_criterion(m4, c("loo", "waic"))
```

12.1.1 Model Weights

We can see that `m3` and `m4` gave the best LOO-IC and WAIC:

```
loo_compare(m1, m2, m3, m4)
```

```
   elpd_diff se_diff
m3  0.0       0.0
m4 -0.6       1.1
m2 -3.5       2.5
m1 -6.0       3.9
```

So it makes sense that if we're to assign weights, `m4` should get most weights. Let's check the following:

```
# Weights based on WAIC
waic_wts <- model_weights(m1, m2, m3, m4, weights = "waic")
# Weights based on Stacking (based on the posterior predictive distribution)
stack_wts <- loo_model_weights(m1, m2, m3, m4)
```

```
Loading required package: rstan
```

```
Loading required package: StanHeaders


rstan version 2.32.5 (Stan version 2.32.2)

For execution on a local, multicore CPU with excess RAM we recommend calling
options(mc.cores = parallel::detectCores()).
To avoid recompilation of unchanged Stan programs, we recommend calling
rstan_options(auto_write = TRUE)
For within-chain threading using `reduce_sum()` or `map_rect()` Stan functions,
change `threads_per_chain` option:
rstan_options(threads_per_chain = 1)


Attaching package: 'rstan'

The following object is masked from 'package:tidyr':

    extract
```

```r
# Print out the weights
round(cbind(waic_wts, stack_wts), 3)
```

```
   waic_wts stack_wts
m1    0.002     0.100
m2    0.019     0.000
m3    0.635     0.882
m4    0.344     0.018
```

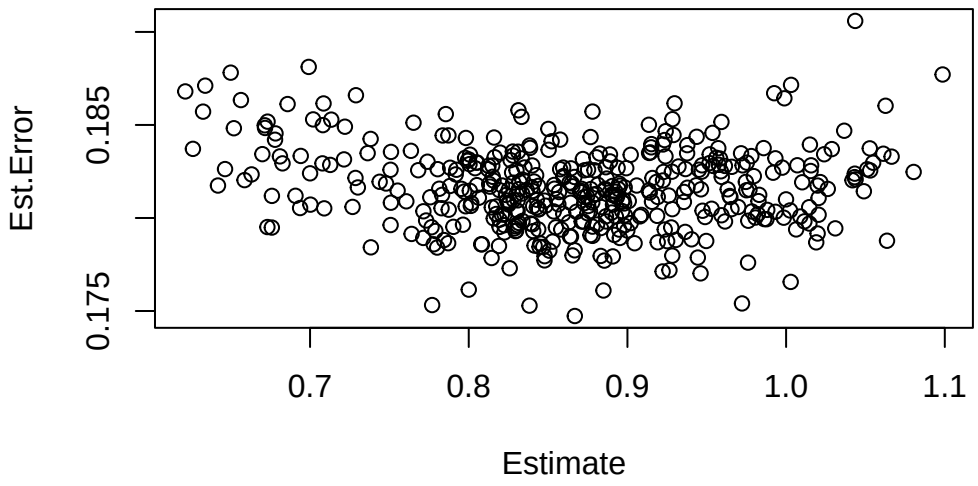
You can see `m3` would get the highest weight, but it's only 0.6352557 and thus less than half of the weights when all four models are considered together.

In Bayesian, we want to preserve all the uncertainty in our analyses. Therefore, if we're not certain which models to use and have tried multiple ones, it would make sense to use all of them to get the best information. So unlike what is commonly done in practice where a researcher would test multiple models and present the best model *as if* they intended only to test this model, Bayesian analysts should do the honest thing and use all models. The reward is usually better prediction!

12.1.2 Stacking

Stacking is one way to combine the predictions of different models. The technical details can be found in Yao et al. (2018), but you can obtain the predictions using the `pp_average` function:

```
# Prediction from stacking by Yao et al. (2018)
pred_stacking <- pp_average(m1, m2, m3, m4)
# Compare the weights
plot(pred_stacking)
```

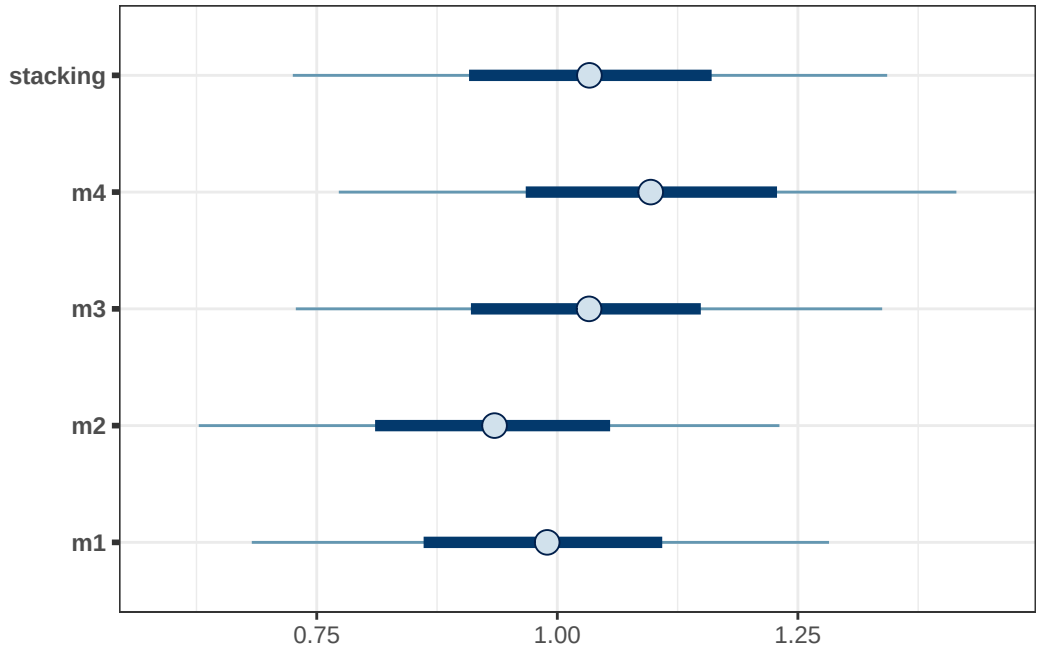


12.1.3 Prediction example

Consider a kid whose mother's IQ is 120 (`mom_iq` = .2), mother's age is 40, (`mom_age_c` = 2.2), mother does not have a high school degree, and mother did not work in first three years of child's life (`mom_work` = 1). Then the prediction based on the various models are:

```
newkid <- data.frame(mom_iq_c = .2,
                     mom_age_c = 2.2,
                     mom_work = 1,
                     mom_hs = "no")
# Visualize the prediction by different models
```

```
data.frame(stacking = pp_average(m1, m2, m3, m4, newdata = newkid,
                                 summary = FALSE),
           m4 = posterior_predict(m4, newdata = newkid),
           m3 = posterior_predict(m3, newdata = newkid),
           m2 = posterior_predict(m2, newdata = newkid),
           m1 = posterior_predict(m1, newdata = newkid)) |>
    mcmc_intervals()
```



Check out this blog post https://mc-stan.org/loo/articles/loo2-weights.html for more information on stacking and Averaging.

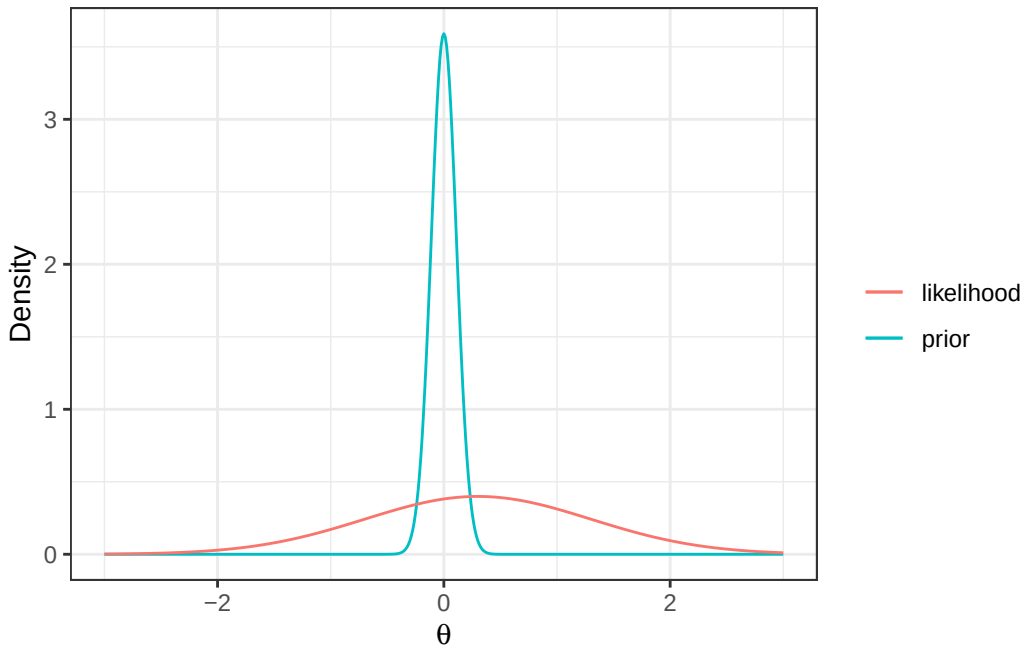
12.2 Shrinkage Priors

When the number of parameters to be estimated is large relative to the amount of data available, ordinary least square (in frequentist) and estimation using non-informative or weakly informative priors tend to overfit. For example, fitting a 6th degree polynomial (with 8 parameters) on a data set with only 10 observations will severely overfit the data, making the results not generalizable. One way to avoid overfitting is to perform *regularization*, that is, to shrink some of the parameters to closer to zero. This makes the model fit less well to the existing data, but will be much more generalizable to an independent data set.

12.2.1 Number of parameters

In Bayesian analyses, the concept of number of parameters is a little vague. This is because the posterior distribution is a function of both the prior and the data. For non-informative priors, it would make sense to simply count the number of parameters. However, say one put a very strong prior on one of the regression coefficients, which has about 9 times the weights of the information contributed by the data:

```
ggplot(data.frame(th = c(-3, 3)), aes(x = th)) +
    stat_function(
        fun = dnorm, args = list(mean = 0, sd = 1 / 9),
        aes(col = "prior"), n = 501
    ) +
    stat_function(
        fun = dnorm, args = list(mean = 0.3, sd = 1),
        aes(col = "likelihood"), n = 501
    ) +
    labs(y = "Density", x = expression(theta), col = "")
```



Then the posterior for the parameter only uses 1/10 of the information from the data! Therefore, it would make more sense to count this as 0.1 parameter, instead of 1 full parameter.

The concept of regularization is essentially to introduce a stronger prior so that the posterior is less likely to overfit the data, and the resulting model will have lower *effective number*

of parameters, which, when done appropriately, would find a model that is more likely to generalize to external data sets.

In Bayesian methods, regularization can be done by choosing a prior on the coefficient that has a sharp peak at 0, but also has a heavy tail. One such prior is what is called the *horseshoe* prior. The discussion here is based on the blog pot by Michael Betancourt: https://betanalpha.github.io/assets/case_studies/bayes_sparse_regression.html

It should first be pointed out that these priors were based on the assumption that the predictors and the outcome has been scaled to have a standard deviation of one. So we will do this here:

```
# For variable selection, scale the predictor and outcome to have unit variance
kidiq_std <- scale(kidiq)
head(kidiq_std)
```

```
      kid_score    mom_hs     mom_iq    mom_work    mom_age
[1,] -1.06793237  0.521631  1.4078352  0.93422435  1.5602285
[2,]  0.54886757  0.521631 -0.7092079  0.93422435  0.8197811
[3,] -0.08805362  0.521631  1.0295443  0.93422435  1.5602285
[4,] -0.18604150  0.521631 -0.0366907  0.08776638  0.8197811
[5,]  1.38176451  0.521631 -0.4836193  0.93422435  1.5602285
[6,]  0.54886757 -1.912647  0.5267892 -1.60514956 -1.7717849
```

12.2.2 Sparsity-Inducing Priors

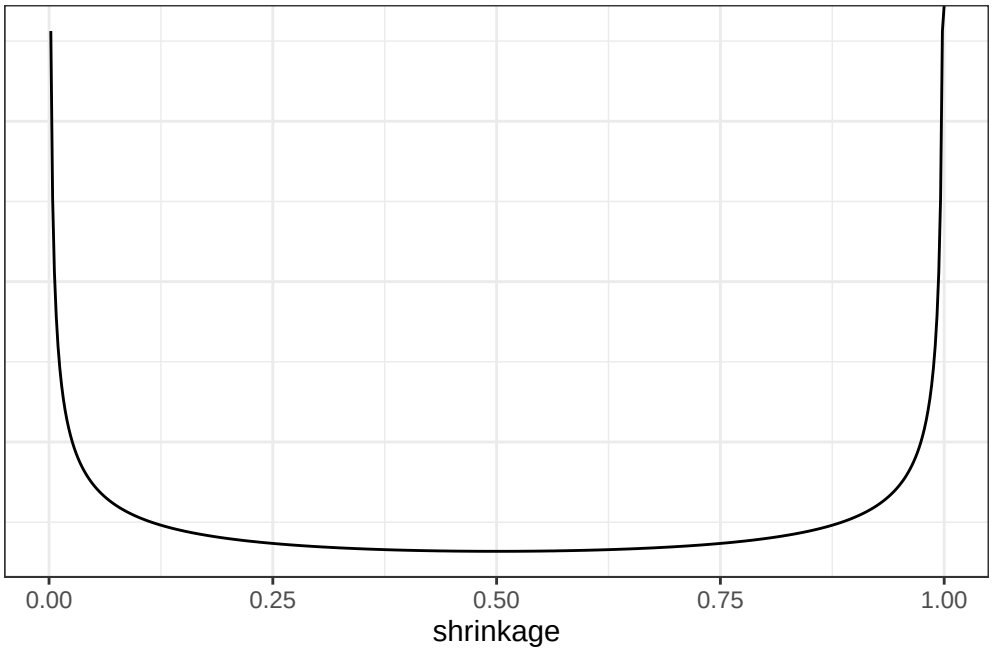
The *horseshoe* prior (Carvalho et al., 2010) is a type of hierarchical prior for regression models by introducing a global scale, τ, and local scale,λ_m, parameters on the priors for the regression coefficients (Piironen & Vehtari, 2017). Specifically, with p predictors,

$$
\begin{aligned}
Y_i &\sim N(\mu_i, \sigma^2) \\
\mu_i &= \beta_0 + \sum_{m=1}^{p} \beta_m X_m \\
\beta_0 &\sim N(0, 1) \\
\beta_m &\sim N(0, \tau\lambda_m) \\
\lambda_m &\sim \text{Cauchy}^+(0, 1) \\
\tau &\sim \text{Cauchy}^+(0, \tau_0)
\end{aligned}
$$

The local scale, λ_m, can flexibly shrink the coefficient to close to zero. Below is the implication of the prior on the shrinkage of β:

```
ggplot(data.frame(shrinkage = c(0, 1)), aes(x = shrinkage)) +
    stat_function(fun = function(x) {
        dcauchy(sqrt(1 / x - 1)) * 2 * (1 / x - 1)^(-1 / 2) * x^(-2) / 2
    }, n = 501) +
    theme(
        axis.text.y = element_blank(),
        axis.ticks.y = element_blank()
    ) +
    labs(y = "")
```

```
Warning: Removed 1 row containing missing values (`geom_function()`).
```



The U-shape here means that, for coefficients that are weakly supported by the data, the horseshoe will shrink it to very close to zero, whereas for coefficients that are more strongly supported by the data, the horseshoe will not shrink it much.

The red curve in the following is one example for the resulting prior distribution on β:

```
dhs <- Vectorize(
    function(y, df = 1) {
        ff <- function(lam) dnorm(y, 0, sd = lam) * dt(lam, df) * 2
        if (y != 0) {
```

```
            integrate(ff, lower = 0, upper = Inf)$value
        } else {
            Inf
        }
    }
)
ggplot(data.frame(x = c(-6, 6)), aes(x = x)) +
    stat_function(
        fun = dhs, args = list(df = 3), n = 501,
        aes(col = "HS"), linetype = 1
    ) +
    stat_function(
        fun = dnorm, n = 501,
        aes(col = "norm"), linetype = 2
    ) +
    scale_color_manual("",
        values = c("red", "black"),
        labels = c("horseshoe(3)", "N(0, 1)")
    ) +
    xlab("y") +
    ylab("density") +
    ylim(0, 0.75)
```

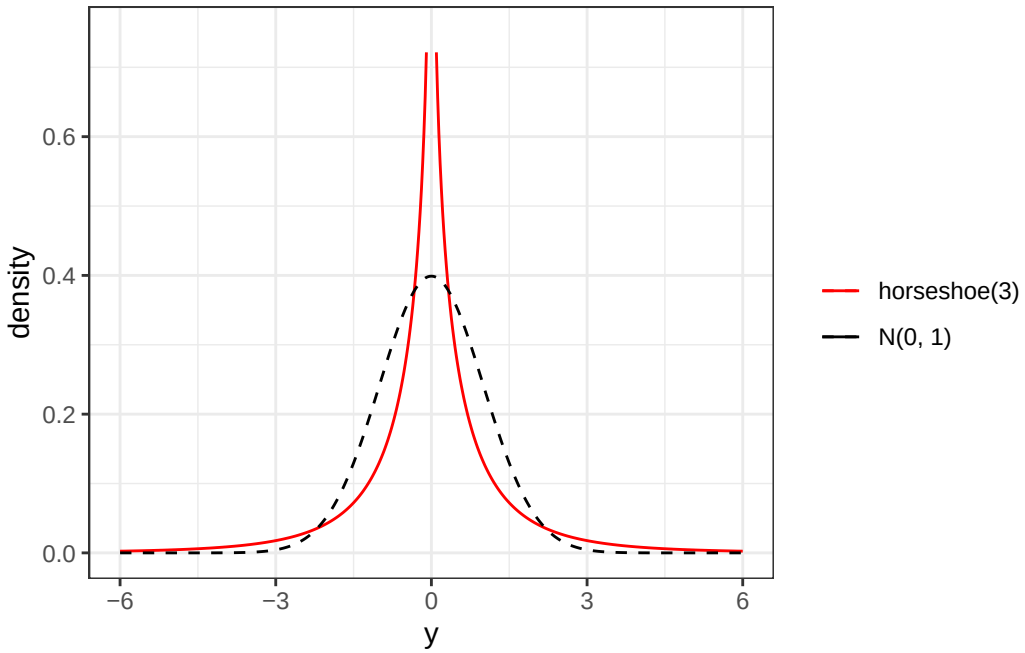


Figure 12.1: Density for the regularized horseshoe prior with 3 degrees of freedom

Such a prior has more density at 0, but also more density for extreme values, as compared to a normal distribution. Thus, for coefficients with very weak evidence, the regularizing prior will shrink it to zero, whereas for coefficients with strong evidence, the shrinkage will be very small. This is called a horseshoe prior. In `brms`, one can specify it with `horseshoe()`, which is a stabilized version of the original horseshoe prior (Carvalho et al., 2010).

12.2.3 Regularized Horseshoe/Hierarchical Shrinkage

The regularized horseshoe (https://projecteuclid.org/euclid.ejs/1513306866) prior is

$$
\begin{aligned}
\beta_m &\sim N(0, \tau\tilde{\lambda}_m) \\
\tilde{\lambda}_m &= \frac{c\lambda_m}{\sqrt{c^2 + \tau^2\lambda_m^2}} \\
\lambda_m &\sim \text{Cauchy}^+(0, 1) \\
c^2 &\sim \text{Inv-Gamma}(\nu/2, nu/2s^2) \\
\tau &\sim \text{Cauchy}^+(0, \tau_0)
\end{aligned}
$$

The additional parameters are chosen in the code below. First, fit a model without shrinkage:

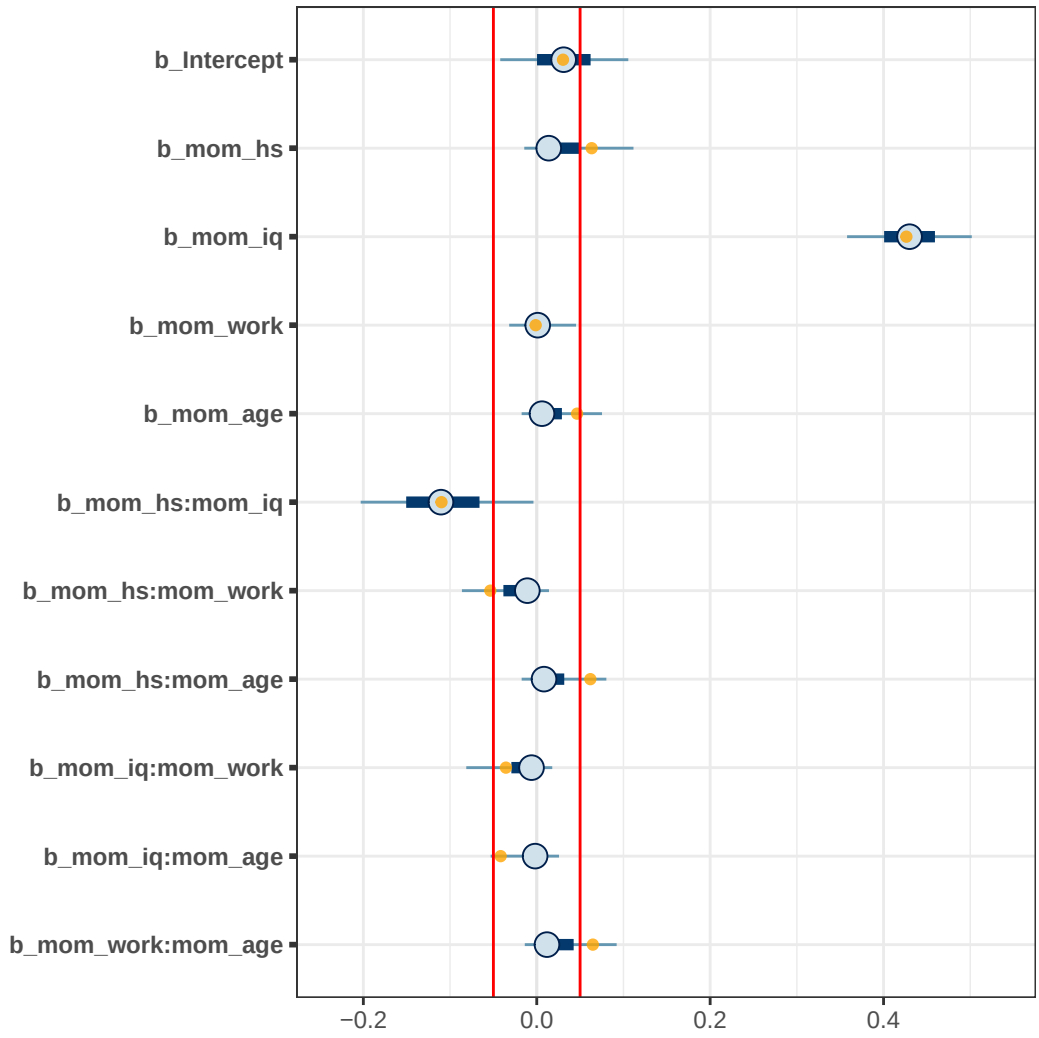
```
# A model with all main and interaction effects
m5 <- brm(kid_score ~ (.)^2,
    data = kidiq_std,
    prior = c(
        prior(normal(0, 1), class = "Intercept"),
        prior(normal(0, 1), class = "b"),
        prior(student_t(4, 0, 1), class = "sigma")
    ),
    seed = 2217,
    file = "07b_m5"
)
```

```
# A model with all main and interaction effects, and regularization
m_hs <- brm(kid_score ~ (.)^2,
    data = kidiq_std,
    prior = c(
        prior(normal(0, 1), class = "Intercept"),
        # Prior guess of 20% of the terms are non-zero
        prior(horseshoe(par_ratio = 2 / 8), class = "b"),
        prior(student_t(4, 0, 1), class = "sigma")
    ),
    # Need higher adapt_delta
    control = list(adapt_delta = .995, max_treedepth = 12),
    seed = 2217,
    file = "07b_m_hs"
)
```

We can plot the coefficients:

```
mcmc_plot(m_hs, variable = "^b_",
          regex = TRUE) +
    # Show the shrinkage as orange, transparent dots
    geom_point(
        data = posterior_summary(m5) |>
            as_tibble(rownames = "parameter") |>
            filter(parameter != "lp__"),
        aes(x = Estimate, y = parameter), alpha = 0.8,
        col = "orange"
    ) +
    geom_vline(xintercept = c(-.05, .05), col = "red")
```

```
Warning: Removed 3 rows containing missing values (`geom_point()`).
```



An arbitrary cutoff is to select only coefficients with posterior means larger than .05, in which case only `mom_iq` and `mom_hs` and their interaction were supported by the data.

You can also double check that the regularized version has better LOO-IC:

```
loo(m5, m_hs)
```

```
Output of model 'm5':

Computed from 4000 by 434 log-likelihood matrix.

         Estimate   SE
elpd_loo   -567.3 14.4
```

```
p_loo        12.8  1.4
looic      1134.6 28.8
------
MCSE of elpd_loo is 0.1.
MCSE and ESS estimates assume MCMC draws (r_eff in [0.6, 2.0]).

All Pareto k estimates are good (k < 0.7).
See help('pareto-k-diagnostic') for details.

Output of model 'm_hs':

Computed from 4000 by 434 log-likelihood matrix.

         Estimate   SE
elpd_loo   -565.2 14.4
p_loo         8.5  0.9
looic      1130.5 28.9
------
MCSE of elpd_loo is 0.1.
MCSE and ESS estimates assume MCMC draws (r_eff in [0.5, 1.3]).

All Pareto k estimates are good (k < 0.7).
See help('pareto-k-diagnostic') for details.

Model comparisons:
     elpd_diff se_diff
m_hs  0.0       0.0
m5   -2.1       2.3
```

And also that the effective number of parameters was smaller in `m_hs`.

12.3 Variable Selection

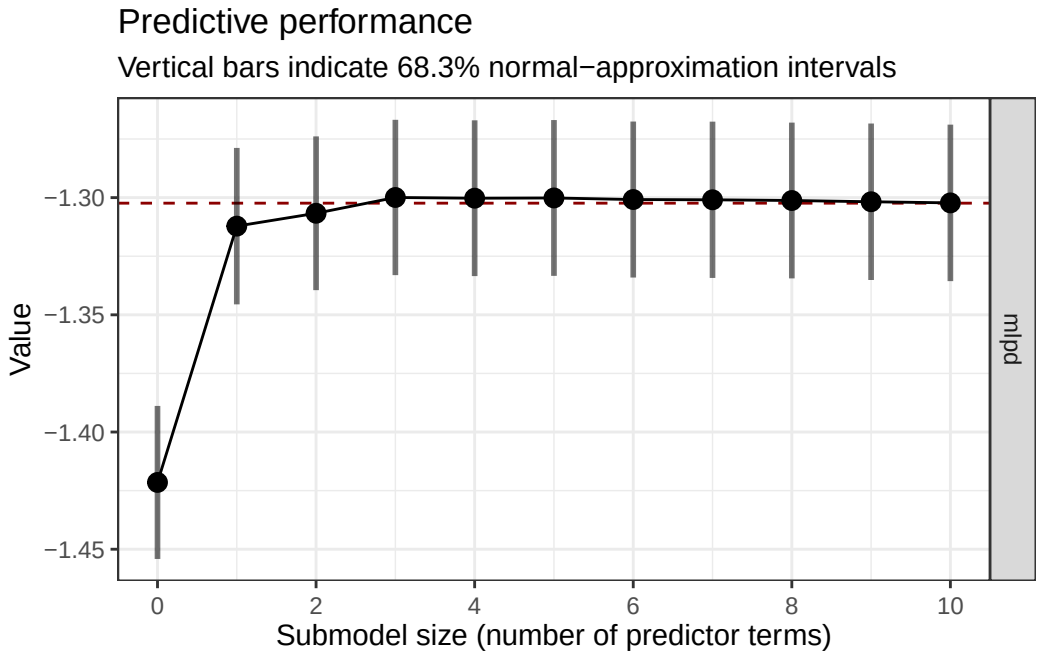
One way to identify variables that are relevant to predict a certain outcome is to use the projection-based method, as discussed in https://mc-stan.org/projpred/articles/projpred.html and in Piironen et al. (2020).

Building from the full model with shrinkage priors, we first do a trial run to identify the importance of various variables in terms of their importance for prediction:

```r
# Get reference model
refm_obj <- get_refmodel(m_hs)
# Preliminary run to find `nterms_max`
cvvs_fast <- cv_varsel(
    refm_obj,
    validate_search = FALSE
)
```

```
-----
Running the search ...
10% of terms selected
20% of terms selected
30% of terms selected
40% of terms selected
50% of terms selected
60% of terms selected
70% of terms selected
80% of terms selected
90% of terms selected
100% of terms selected
-----
-----
Running the performance evaluation with `refit_prj = TRUE` ...
-----
```

```r
# mlpd = mean log predictive density
plot(cvvs_fast, stats = "mlpd", ranking_nterms_max = NA)
```



From the plot, we find when the predictive performance starts to level off when we keep adding more terms to the model. In this case, it seems to be 4. Given that this is a trial run, we'll set `nterms_max` to 5, which is slightly higher.

We then set `validate_search = FALSE` for a final run. For computational feasibility, we'll use 10-fold validation.

```
# With 10-fold cross-validation
cvvs <- cv_varsel(
    refm_obj,
    validate_search = TRUE,
    cv_method = "kfold",
    K = 10,
    nterms_max = 5
)
```

```
-----
Running the search using the full dataset ...
20% of terms selected
40% of terms selected
60% of terms selected
80% of terms selected
100% of terms selected
```

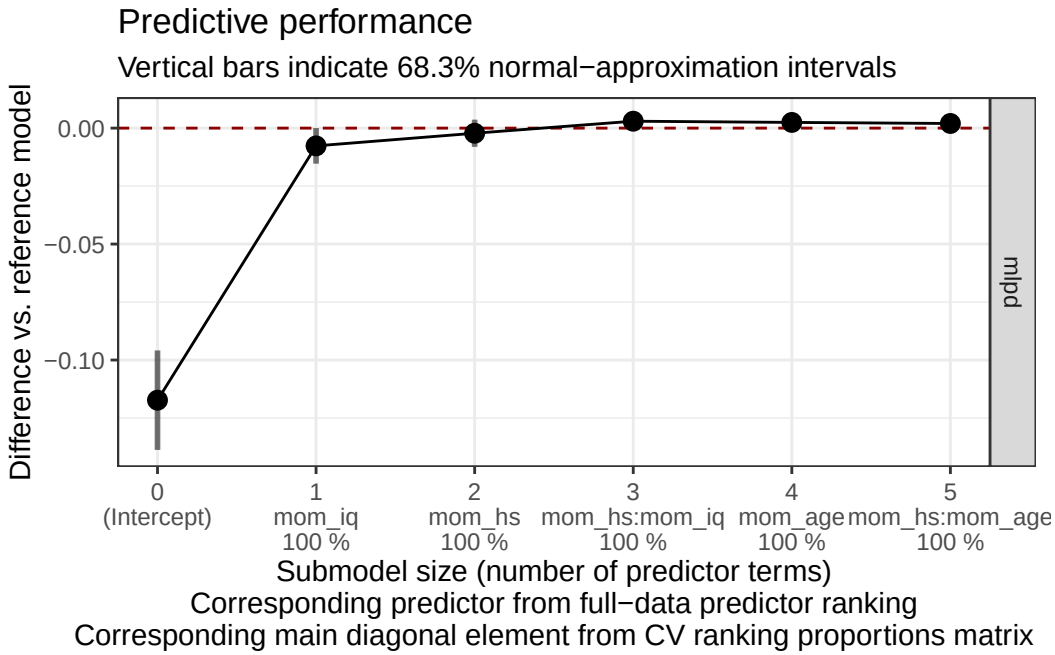
```
-----
-----
Refitting the reference model K = 10 times (using the fold-wise training data) ...
Running MCMC with 4 sequential chains...

Chain 1 finished in 2.7 seconds.
Chain 2 finished in 2.0 seconds.
Chain 3 finished in 2.8 seconds.
Chain 4 finished in 2.5 seconds.

All 4 chains finished successfully.
Mean chain execution time: 2.5 seconds.
Total execution time: 10.3 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 2.6 seconds.
Chain 2 finished in 2.1 seconds.
Chain 3 finished in 2.5 seconds.
Chain 4 finished in 2.1 seconds.

All 4 chains finished successfully.
Mean chain execution time: 2.3 seconds.
Total execution time: 9.5 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 2.4 seconds.
Chain 2 finished in 2.1 seconds.
Chain 3 finished in 2.1 seconds.
Chain 4 finished in 2.1 seconds.

All 4 chains finished successfully.
Mean chain execution time: 2.2 seconds.
Total execution time: 8.9 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 2.5 seconds.
Chain 2 finished in 2.0 seconds.
Chain 3 finished in 2.2 seconds.
Chain 4 finished in 2.2 seconds.
```

```
All 4 chains finished successfully.
Mean chain execution time: 2.2 seconds.
Total execution time: 9.2 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 2.2 seconds.
Chain 2 finished in 1.8 seconds.
Chain 3 finished in 1.9 seconds.
Chain 4 finished in 1.8 seconds.

All 4 chains finished successfully.
Mean chain execution time: 1.9 seconds.
Total execution time: 8.1 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 1.5 seconds.
Chain 2 finished in 2.2 seconds.
Chain 3 finished in 1.6 seconds.
Chain 4 finished in 1.7 seconds.

All 4 chains finished successfully.
Mean chain execution time: 1.8 seconds.
Total execution time: 7.5 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 1.8 seconds.
Chain 2 finished in 1.9 seconds.
Chain 3 finished in 1.4 seconds.
Chain 4 finished in 2.5 seconds.

All 4 chains finished successfully.
Mean chain execution time: 1.9 seconds.
Total execution time: 8.1 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 2.0 seconds.
Chain 2 finished in 1.9 seconds.
Chain 3 finished in 2.1 seconds.
Chain 4 finished in 1.8 seconds.
```

```
All 4 chains finished successfully.
Mean chain execution time: 1.9 seconds.
Total execution time: 8.0 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 2.2 seconds.
Chain 2 finished in 2.0 seconds.
Chain 3 finished in 2.3 seconds.
Chain 4 finished in 1.8 seconds.

All 4 chains finished successfully.
Mean chain execution time: 2.1 seconds.
Total execution time: 8.8 seconds.

Running MCMC with 4 sequential chains...

Chain 1 finished in 1.6 seconds.
Chain 2 finished in 1.9 seconds.
Chain 3 finished in 1.6 seconds.
Chain 4 finished in 1.8 seconds.

All 4 chains finished successfully.
Mean chain execution time: 1.7 seconds.
Total execution time: 7.3 seconds.

-----
-----
Running the search and the performance evaluation with `refit_prj = TRUE` for each of the K +

  |
  |                                                                      |   0%
  |
  |=======                                                               |  10%
  |
  |==============                                                        |  20%
  |
  |======================                                                |  30%
  |
  |=============================                                         |  40%
  |
  |====================================                                  |  50%
```

```
  |
  |=======================================                               |  60%
  |
  |=============================================                         |  70%
  |
  |=================================================                     |  80%
  |
  |=======================================================               |  90%
  |
  |=============================================================================| 100%
-----
```

```
plot(cvvs, stats = "mlpd", deltas = TRUE)
```




```
# model size suggested by the program
suggest_size(cvvs, stat = "mlpd")
```

```
[1] 1
```

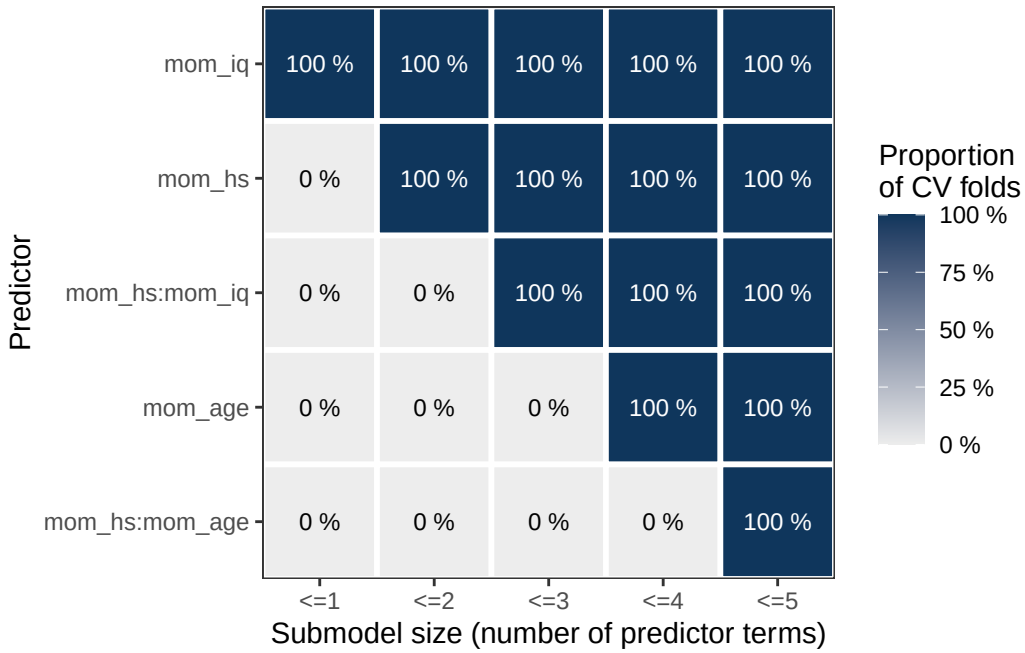
```
# Same with RMSE
suggest_size(cvvs, stat = "rmse")
```

```
[1] 1
```

```
# Summary of the variable selection results
summary(cvvs,
    stats = "mlpd", type = c("mean", "lower", "upper"),
    deltas = TRUE
)
```

```
Family: gaussian
Link function: identity

Formula: kid_score ~ mom_hs + mom_iq + mom_work + mom_age + mom_hs:mom_iq +
    mom_hs:mom_work + mom_hs:mom_age + mom_iq:mom_work + mom_iq:mom_age +
    mom_work:mom_age
Observations: 434
Projection method: traditional
CV method: K-fold CV with K = 10 and search included (i.e., fold-wise searches)
Search method: forward
Maximum submodel size for the search: 5
Number of projected draws in the search: 20 (from clustered projection)
Number of projected draws in the performance evaluation: 400
Argument `refit_prj`: TRUE

Submodel performance evaluation summary with `deltas = TRUE` and `cumulate = FALSE`:
 size ranking_fulldata cv_proportions_diag    mlpd mlpd.lower mlpd.upper
    0      (Intercept)                  NA -0.1173   -1.4e-01   -9.6e-02
    1           mom_iq                   1 -0.0077   -1.5e-02    1.7e-05
    2           mom_hs                   1 -0.0022   -8.1e-03    3.6e-03
    3    mom_hs:mom_iq                   1  0.0030    6.4e-05    5.9e-03
    4          mom_age                   1  0.0025   -3.8e-04    5.3e-03
    5   mom_hs:mom_age                   1  0.0020   -4.0e-04    4.4e-03

Reference model performance evaluation summary with `deltas = TRUE`:
      mlpd mlpd.lower mlpd.upper
         0          0          0
```

```
# Predictor ranking(s)
rk <- ranking(cvvs)
plot(cv_proportions(rk, cumulate = TRUE))
```



Here it suggests to either include only `mom_iq` and `mom_hs`, or to also include their interactions.

12.3.1 Projection-Based Method

The projection-based method will obtain the posterior distributions based on a projection from the full model on the simplified model. In other words, we're asking the question:

> If we want a model with only `mom_iq` and `mom_hs`, what coefficients should be obtained so that the resulting prediction accuracy is as closed to the full model as possible?

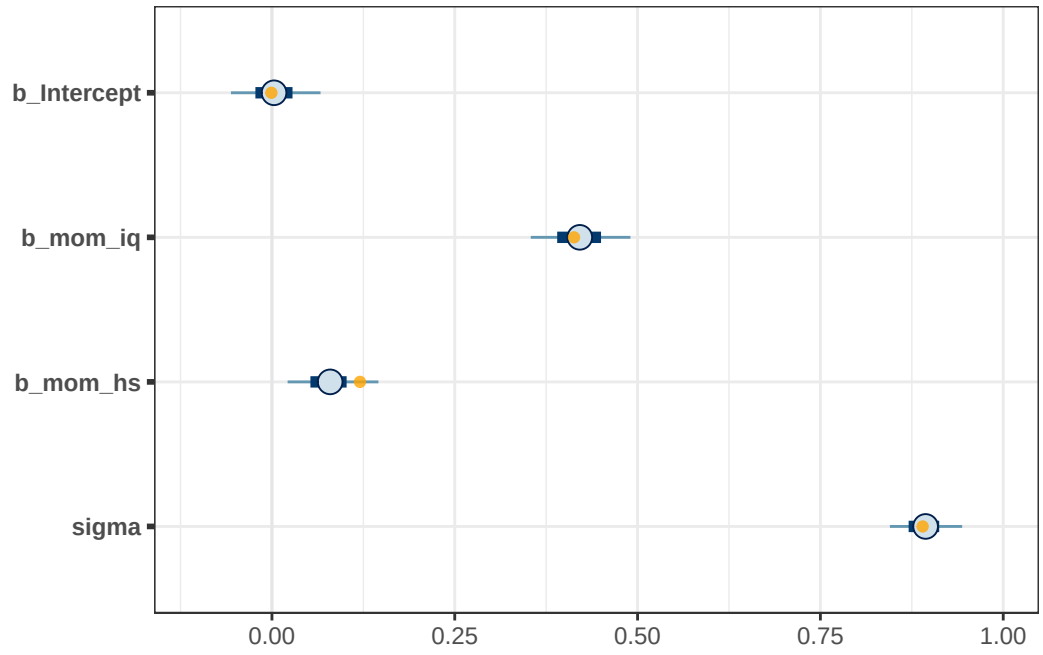
Note that the coefficients will be different from if you were to directly estimate the model using the two predictors (i.e., `m2`). In this case, simulation results showed that the projection-based method will yield a model with better predictive performance.

```
# Fit m2 with the standardized data
m2_std <- brm(kid_score ~ mom_hs + mom_iq,
    data = kidiq_std,
    prior = c(
        prior(normal(0, 1), class = "Intercept"),
        prior(normal(0, 1), class = "b"),
        prior(student_t(4, 0, 1), class = "sigma")
```

```
    ),
    seed = 2302,
    file = "07b_m2_std"
)
```

```
# Visualise the projected three most relevant variables
prj <- project(refm_obj,
    predictor_terms = c("mom_iq", "mom_hs"),
    verbose = FALSE
)
mcmc_intervals(as.matrix(prj)) +
    # Show the non-projection version as black, transparent dots
    geom_point(
        data =
            posterior_summary(m2_std) |>
                as_tibble(rownames = "parameter"),
        aes(x = Estimate, y = parameter), alpha = 0.8,
        col = "orange"
    )
```

```
Warning: Removed 3 rows containing missing values (`geom_point()`).
```



Part VII

Week 9

13 Causal Inference

Causal inference is an important topic in statistics, but it also has a complicated history with statistics. Early-day statisticians saw causality as a taboo such that researchers were discouraged from drawing any causal conclusions in nonexperimental research. In the past few decades, much progress has been made on causal inference in epidemiology, computer science, and statistics, with several frameworks proposed and many tools developed for experimental and nonexperimental data.[1] This note will introduce the causal diagram framework for encoding causal assumptions, which can be used to guide analysis for drawing causal conclusions. The goal is to give you some basic ideas so that you can learn more from other sources, such as the book *Causality* by Pearl and the book *Causal Inference for Statistics, Social, and Biomedical Sciences: An Introduction* by Imbens and Rubin.

Two prominent frameworks for causal inference are

1. Structural causal model, which uses tools such as DAGs and d-separation, is thoroughly described in the book *Causality* by Pearl, and
2. Potential outcome model, which is thoroughly described in the book *Causal Inference for Statistics, Social, and Biomedical Sciences: An Introduction* by Imbens and Rubin.

In this note, we will draw on both frameworks.

What is Causal Inference?

Causal inference is the process of determining the causal effect of one variable on another, based on data and causal assumptions. Two common ways of interpreting a causal effect are (a) *intervention*: how Y will change if X is manipulated to be x; (b) *counterfactual*: what would Y be if X were set to x.

[1] See this paper: https://doi.org/10.1177/1745691620921521 for an argument of how the taboo against causal inference has impeded the progress of psychology research.

13.1 Potential Outcomes

Consider a binary treatment variable. For each individual, there are two *potential outcomes*: one if they receive the treatment (T = 1) and one if they do not (T = 0). Here is a hypothetical data set of a new drug for improving statistics knowledge, with the treatment condition receiving the drug and the control condition receiving a placebo:

```
po_dat <- data.frame(
    person = c(1, 2, 3, 4, 5, 6, 7, 8),
    attitude = c(4, 7, 3, 9, 5, 6, 8, 2),
    treat = c(75, 80, 70, 90, 85, 82, 95, 78),
    control = c(70, 88, 75, 92, 82, 85, 90, 78)
)
knitr::kable(po_dat,
    col.names = c("Person", "Math Attitude", "Y (if T = 1)", "Y (if T = 0)"))
```

Person	Math Attitude	Y (if T = 1)	Y (if T = 0)
1	4	75	70
2	7	80	88
3	3	70	75
4	9	90	92
5	5	85	82
6	6	82	85
7	8	95	90
8	2	78	78

If one could observe the two potential outcomes for each person (which is impossible in the real world), one could compute the treatment effect for each person:

```
(te <- po_dat$treat - po_dat$control)
```

```
[1]  5 -8 -5 -2  3 -3  5  0
```

and the **average treatment effect (ATE)** (here we just compute it on the sample, so the sample ATE):

```
(ate <- mean(te))
```

```
[1] -0.625
```

However, in practice, we can only observe one of the two potential outcomes. For example, if persons 2, 4, 6, 7 are in the treatment condition, we have

```
po_dat$t <- ifelse(po_dat$person %in% c(2, 4, 6, 7), 1, 0)
po_dat$y <- ifelse(po_dat$t, po_dat$treat, po_dat$control)
po_dat[c("t", "y")] |>
    knitr::kable(col.names = c("Treatment", "Observed Y"))
```

Treatment	Observed Y
0	70
1	80
0	75
1	90
0	82
1	82
1	95
0	78

and the naive comparison of those in the treatment condition and those in the control condition will have a mean difference of

```
mean(po_dat$y[po_dat$t == 1]) - mean(po_dat$y[po_dat$t == 0])
```

```
[1] 10.5
```

which gives a misleading estimate of the ATE.

13.2 Directed Acyclic Graph (DAG)

DAG is a tool for encoding causal assumptions. It contains nodes and paths. A node is usually a variable that can be measured in the data or unmeasured. Generally, paths in a DAG are directional (as implied by *directed*), which indicates the directions of causal relations. Acyclic means the causal chain does not close in a loop.

We will use an example described in McElreath (2020), chapter 5, about data from 50 U.S. states from the 2009 American Community Survey (ACS), which we have already seen in Chapter 9 and Figure 9.1.

```
waffle_divorce <- read_delim(  # read delimited files
    "https://raw.githubusercontent.com/rmcelreath/rethinking/master/data/WaffleDivorce.csv",
    delim = ";"
)
```

```
Rows: 50 Columns: 13
-- Column specification --------------------------------------------------------
Delimiter: ";"
chr  (2): Location, Loc
dbl (11): Population, MedianAgeMarriage, Marriage, Marriage SE, Divorce, Div...

i Use `spec()` to retrieve the full column specification for this data.
i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```
# Rescale Marriage and Divorce by dividing by 10
waffle_divorce$Marriage <- waffle_divorce$Marriage / 10
waffle_divorce$Divorce <- waffle_divorce$Divorce / 10
waffle_divorce$MedianAgeMarriage <- waffle_divorce$MedianAgeMarriage / 10
# See data description at https://rdrr.io/github/rmcelreath/rethinking/man/WaffleDivorce.html
```

The outcome of interest is the divorce rate. Remember the plot shows how marriage rate is related to divorce rate at the state level. It looks like marriage rate can predict divorce rate. A causal interpretation would be a stronger assertion, such that we expect a higher divorce rate if policymakers encourage more people to get married. In order to make a causal claim, we need to remove potential confounders.

A potential confounder is when people get married. Suppose people are forced to get married later in life. In that case, fewer people in the population will be married, and people may have less time, opportunity, and motivation to get divorced (as it may be harder to find a new partner). Therefore, we can use the following DAG:

```
dag1 <- dagitty("dag{ A -> D; A -> M; M -> D }")
coordinates(dag1) <- list(x = c(M = 0, A = 1, D = 2),
                          y = c(M = 0, A = 1, D = 0))
# Plot
ggdag(dag1) + theme_dag()
```

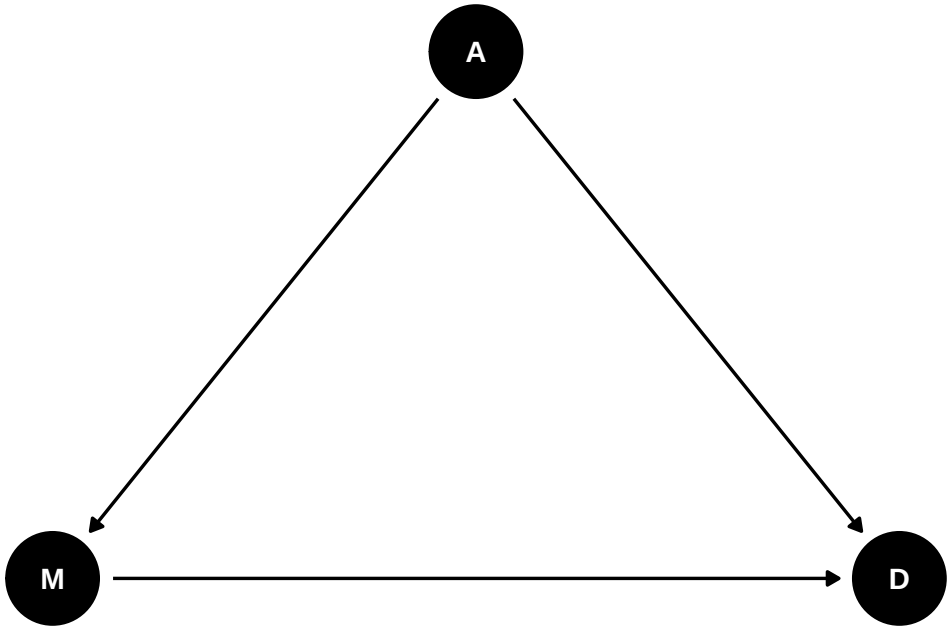


Figure 13.1: DAG for the relationship between marriage rate (M) and divorce rate (D) example, with median age of marriage (A) as a potential confounder.

We can look at how the median age people get married in different states relates to the divorce rate:

```
ggplot(waffle_divorce,
       aes(x = MedianAgeMarriage, y = Divorce)) +
    geom_point() +
    geom_smooth() +
    labs(x = "Median age marriage (10 years)",
         y = "Divorce rate (per 10 adults)") +
    ggrepel::geom_text_repel(aes(label = Loc))
```

```
`geom_smooth()` using method = 'loess' and formula = 'y ~ x'
```

```
Warning: ggrepel: 9 unlabeled data points (too many overlaps). Consider
increasing max.overlaps
```

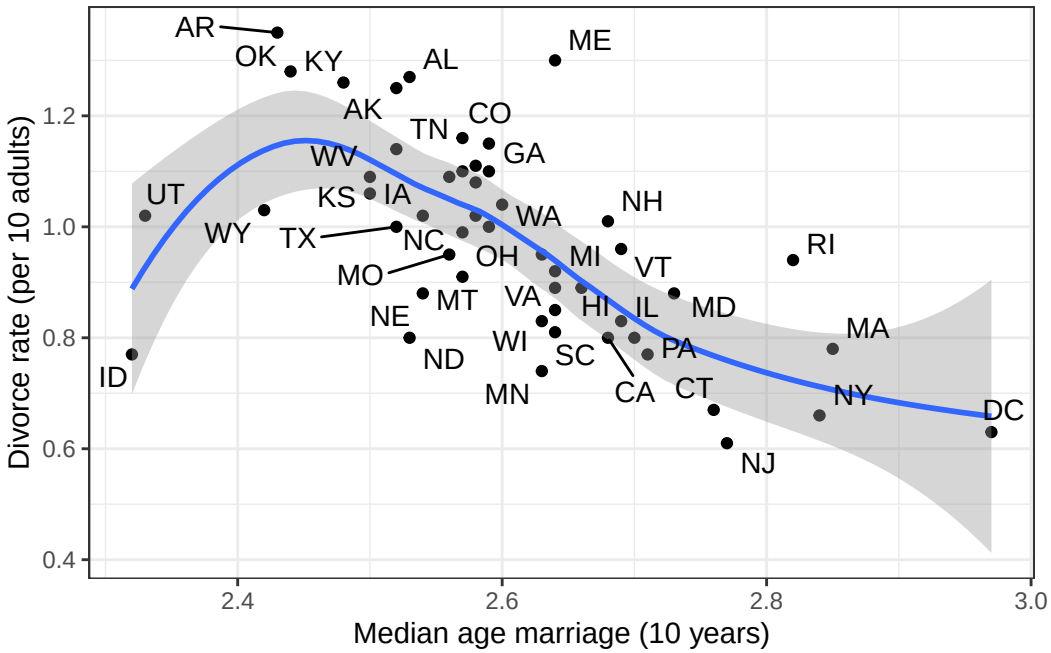


Figure 13.2: Scatter plot of divorce rate (y) vs median age of marriage (x).

13.2.1 Assumptions in a DAG

In a graphical model, there are usually two kinds of assumptions conveyed. Perhaps counterintuitively, the weaker assumptions are the ones you can see, whereas the stronger assumptions are ones you **do not see**.

For example, a weak assumption is:

- Marriage age *may* directly influence the number of people who are married

On the other hand, examples of a strong assumption are:

- Marriage rate does not directly influence the age people get married
- there is no other variable in the causal pathway M $\rightarrow$ D

The last assumption will not hold if there is a common cause of M and D other than A.

13.2.2 Basic Types of Junctions

- Fork: A $\leftarrow$ B $\rightarrow$ C
  - A and C are correlated due to a common cause B

- Chain/Pipe: A → B → C
  - B is on the causal pathway of A to C
- Collider: A → B ← C
  - B is a *descendant* of both A and C

Going back to our example, there is a fork relation: M → A → D. In this case, A is a confounder when estimating the causal relation between M and D. In this case, the causal effect of M to D can be obtained by adjusting for A, which means looking at the subsets of data where A is constant. In regression, adjustment is obtained by including both M and A as predictors of D.

13.3 The Back-Door Criterion: Estimating Causal Effect in Nonexperimental Data

Randomization is one—but not the only—way to rule out confounding variables. Much progress has been made in clarifying that causal effects **can** be estimated in nonexperimental data. After all, researchers have not randomly assigned individuals to smoke x cigarettes per day, but we are confident that smoking causes cancer; we never manipulated the moon's gravitational force, but we are pretty sure that the moon is a cause of high and low tides.

In a DAG, the back-door criterion can be used to identify variables that we should adjust for to obtain a causal effect. The set of variables to be adjusted should (a) blocks every path between X and Y that contains an arrow entering X and (b) does not contain variables that are descendant of X.

```
dag4 <- dagitty(
    "dag{
      X -> Y; W1 -> X; U -> W2; W2 -> X; W1 -> Y; U -> Y
    }"
)
latents(dag4) <- "U"
coordinates(dag4) <- list(x = c(X = 0, W1 = 0.66, U = 1.32, W2 = 0.66, Y = 2),
                          y = c(X = 0, W1 = 1, U = 1, W2 = 0.5, Y = 0))
ggdag(dag4) + theme_dag()
```

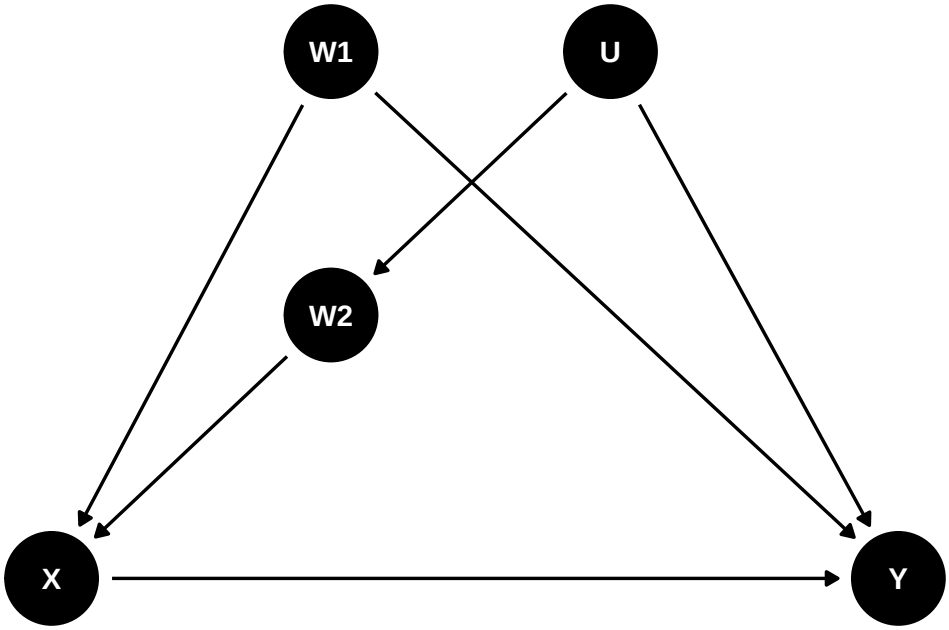


Figure 13.3: DAG for a hypothetical model with two measured and one unobserved confounder.

We can use a function in the `daggity` package to identify the set of variables that satisfy the back-door criterion. In this case, we say that X and Y are *d*-separated by this set of adjusted variables:

```
adjustmentSets(dag4, exposure = "X", outcome = "Y",
               effect = "direct")
```

```
{ W1, W2 }
```

13.4 Using Multiple Regression Model

$$
\begin{aligned}
D_i &\sim N(\mu_i, \sigma) \\
\mu_i &= \beta_0 + \beta_1 A_i + \beta_2 M_i \\
\beta_0 &\sim N(0, 1) \\
\beta_1 &\sim N(0, 1) \\
\beta_2 &\sim N(0, 1)
\end{aligned}
$$

Assuming a correctly specified DAG, all all assumptions of a linear model are met, β_2 is the causal effect of M on D. Here is the `brms` code:

```
m1 <- brm(Divorce ~ MedianAgeMarriage + Marriage,
          data = waffle_divorce,
          prior = prior(std_normal(), class = "b") +
              prior(normal(0, 5), class = "Intercept") +
              prior(student_t(4, 0, 3), class = "sigma"),
          seed = 941,
          iter = 4000,
          file = "08_m1"
)
```

13.4.1 Table

```
msummary(m1,
         estimate = "{estimate} [{conf.low}, {conf.high}]",
         statistic = NULL, fmt = 2
)
```

```
Warning:
`modelsummary` uses the `performance` package to extract goodness-of-fit
statistics from models of this class. You can specify the statistics you wish
to compute by supplying a `metrics` argument to `modelsummary`, which will then
push it forward to `performance`. Acceptable values are: "all", "common",
"none", or a character vector of metrics names. For example: `modelsummary(mod,
metrics = c("RMSE", "R2")` Note that some metrics are computationally
expensive. See `?performance::performance` for details.
 This warning appears once per session.
```

As shown in the table, when holding constant the median marriage age of states, marriage rate has only a small effect on divorce rate.

13.4.2 Posterior predictive checks

```
pp_check(m1, ndraws = 100) # density
pp_check(m1, type = "intervals", x = "Marriage") +
    labs(x = "Marriage", y = "Divorce")
```

```
Using all posterior draws for ppc type 'intervals' by default.
```

Table 13.3: Model results for the divorce rate example.

	(1)
b_Intercept	3.49 [1.98, 5.02]
b_MedianAgeMarriage	−0.93 [−1.43, −0.45]
b_Marriage	−0.04 [−0.20, 0.12]
sigma	0.15 [0.12, 0.19]
Num.Obs.	50
R2	0.349
R2 Adj.	0.282
ELPD	21.0
ELPD s.e.	6.4
LOOIC	−42.0
LOOIC s.e.	12.9
WAIC	−42.2
RMSE	0.14

```
pp_check(m1, type = "intervals", x = "MedianAgeMarriage") +
    labs(x = "MedianAgeMarriage", y = "Divorce")
```

```
Using all posterior draws for ppc type 'intervals' by default.
```

The model does not fit every state (e.g., UT, ME, ID).

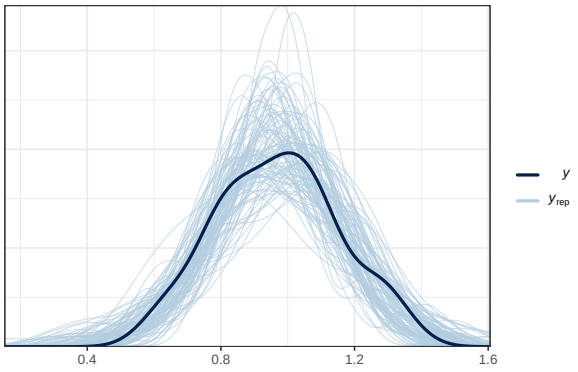
13.5 Predicting an Intervention

If the causal assumption in our DAG is reasonable, we have obtained an estimate of the causal effect of marriage rate on divorce rate at the state level. This allows us to answer questions like

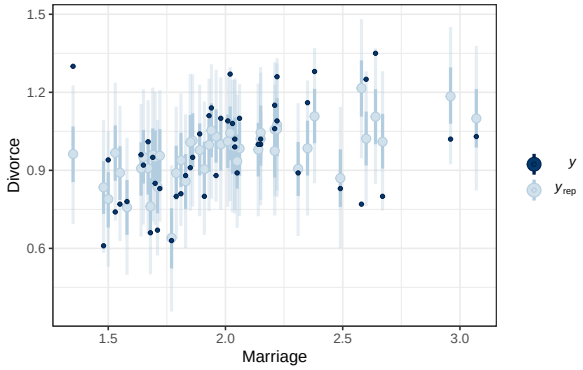
> What would happen to the divorce rate if we encouraged more people to get married (so the marriage rate would increase by 10 percentage points)?

We can use the Bayesian model, which is generative, to make such predictions. Consider a state with a marriage rate of 2 (per 10 adults). The predicted divorce rate is

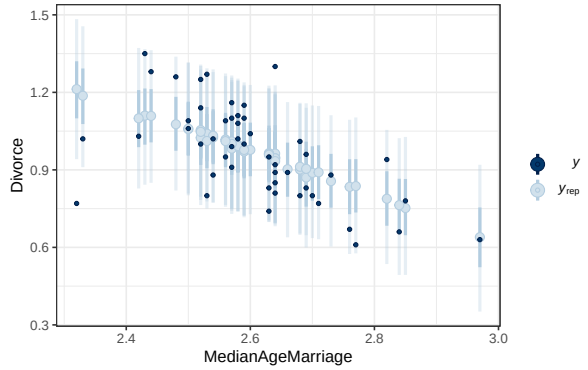
$$\beta_0 + \beta_1 A + \beta_2(2)$$



(a) Posterior predictive density of divorce rate.



(b) Posterior predictive intervals of marriage rate predicting divorce rate.



(c) Posterior predictive intervals of median marriage age predicting marriage rate.

Figure 13.4: Posterior predictive checks for the multiple regression model.

Consider an intervention that increases the marriage rate from 2 to 3. The predicted divorce rate will be

$$\beta_0 + \beta_1 A + \beta_2(3)$$

The change in divorce rate is

$$\beta_0 + \beta_1 A + \beta_2(3) - \beta_0 + \beta_1 A + \beta_2(2) = \beta_2$$

Here is what the model would predict in terms of the change in the divorce rate (holding median marriage age to 25 years old), using R:

```
pred_df <- data.frame(
    Marriage = c(2, 3),
    MedianAgeMarriage = c(2.5, 2.5)
)
cbind(pred_df, fitted(m1, newdata = pred_df)) %>%
    knitr::kable(digits = 3)
```

Marriage	MedianAgeMarriage	Estimate	Est.Error	Q2.5	Q97.5
2	2.5	1.068	0.035	1.002	1.138
3	2.5	1.026	0.067	0.894	1.160

The difference should be just the estimate of β_2, which has the following posterior distribution:

```
mcmc_dens(m1, pars = "b_Marriage")
```

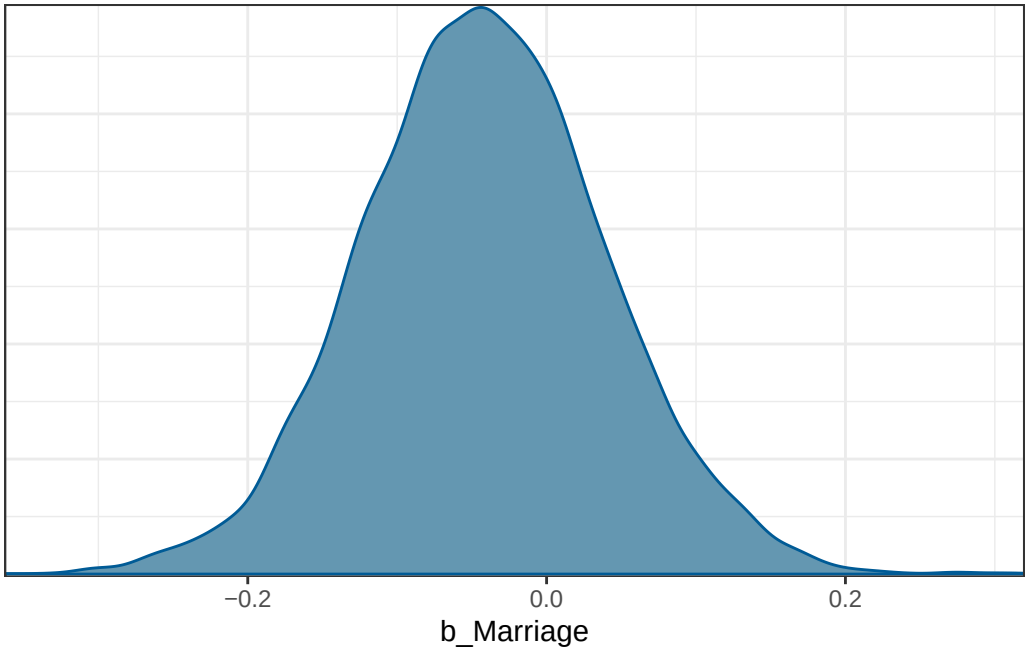


Figure 13.5: Estimated "causal" effect of marriage rate on divorce rate, based on the specified DAG and a linear model.

13.6 Collider

A collider is a descendant of two parent nodes. When one holds the collider constant, it induces a spurious association between the parents. This leads to many unexpected results in data analysis and daily life. For example, consider people who are nice and who are good-looking. Is there an association between a person being nice and a person being good-looking? Maybe. But this association can be induced when we condition on a collider. Let's say a friend of yours only dates people who are either nice or good-looking. So we have this colliding relation:

Nice → Dating ← Good looking

Suppose you look at just the people that your friend dated. In that case, they are either nice or good-looking, but the fact that you select to look at (condition on) only the people that your friend dated would automatically eliminate people who are neither nice nor good-looking. This induces a spurious negative association between nice and good-looking, so your friend may believe that nice people would be less likely to have appearances that fit their taste, and vice versa.

As another example, is research that is newsworthy less trustworthy? There could be a negative association due to collider bias, because people who select research to be reported, funded, or

published, consider both newsworthiness and trustworthiness. Assume that trustworthiness has no causal relation with newsworthiness, below shows what happens when we only focus on papers that are either high on newsworthiness or trustworthiness:

```
set.seed(2221) # different seed from the text
num_proposals <- 200 # number of grant proposals
prop_selected <- 0.1 # proportion to select
# Simulate independent newsworthiness and trustworthiness
plot_dat <- data.frame(
    nw = rnorm(num_proposals),
    tw = rnorm(num_proposals)
)
plot_dat <- plot_dat |>
    mutate(total = nw + tw)
sel_dat <- plot_dat |>
    # select top 10% of combined scores
    slice_max(order_by = total, prop = prop_selected)
plot_dat |>
    ggplot(aes(x = nw, y = tw)) +
    geom_point() +
    geom_point(data = sel_dat, shape = 1, size = 3,
               color = "red") +
    geom_smooth(method = "lm", se = FALSE) +
    geom_smooth(data = sel_dat, method = "lm", se = FALSE,
                col = "purple") +
    labs(x = "newsworthiness", y = "trustworthiness")
```

```
`geom_smooth()` using formula = 'y ~ x'
`geom_smooth()` using formula = 'y ~ x'
```

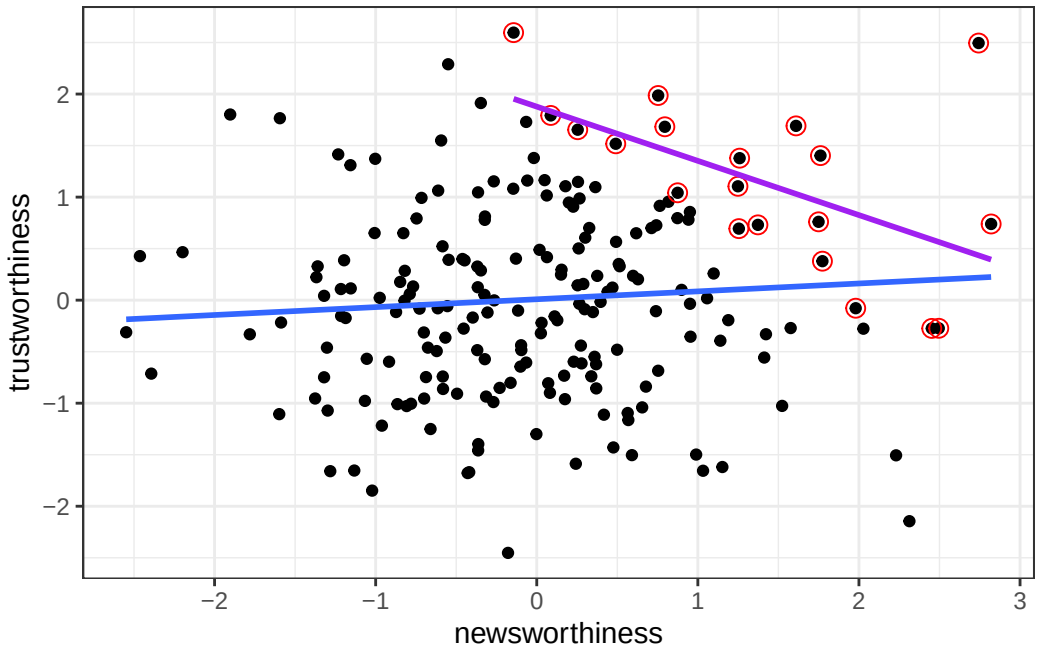


Figure 13.6: Simulation of newsworthiness and trustworthiness.

As you can see, a negative correlation happens. This is collider bias: spurious correlation due to conditioning on the common descendant. This also goes by the name Berkson's Paradox.

In the DAG below, X and Y have no causal association. Conditioning on S, however, induces a negative correlation between X and Y. With the DAG below,

> Generally speaking, do not condition on a collider, unless you're going to de-confound the spurious association using other variables.

```
dag7 <- dagitty(
    "dag{
      X -> Y; X -> S; Y -> S
    }"
)
coordinates(dag7) <- list(x = c(X = 0, S = 1, Y = 2),
                          y = c(X = 0, S = -1, Y = 0))
ggdag(dag7) + theme_dag()
```

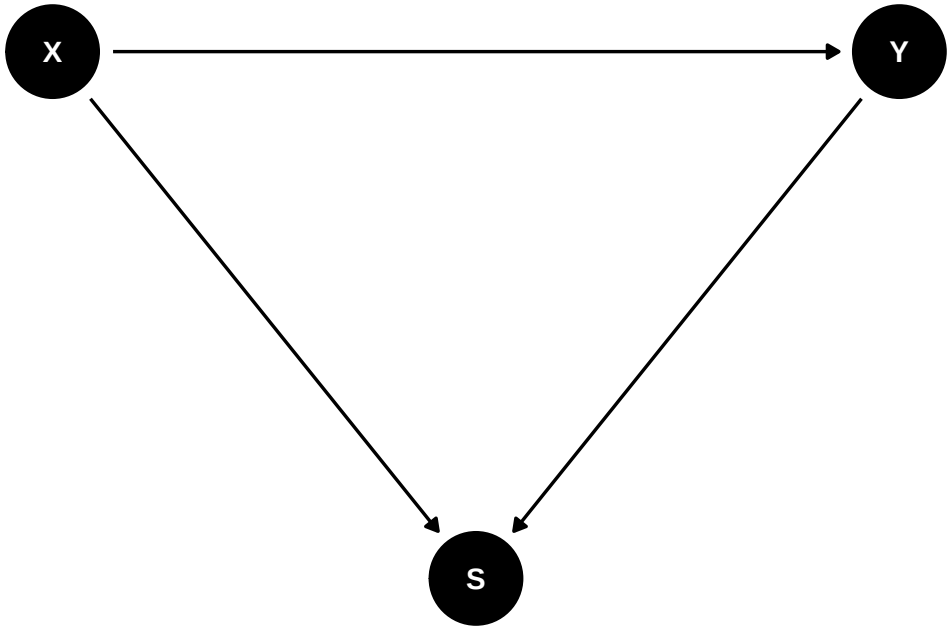


Figure 13.7: DAG with collider bias.

Age and Happiness, conditioned on Marital Status (Example from text)

In this example, we assume that age and happiness are not related, but as people age, they are more likely to get married.

```r
# Code adapted from the rethinking package (https://github.com/rmcelreath/rethinking/blob/m
sim_happiness <- function(seed = 1977, N_years = 100,
                          max_age = 65, N_births = 50,
                          aom = 18) {
    set.seed(seed)
    H <- M <- A <- c()
    for (t in seq_len(N_years)) {
        A <- A + 1 # age existing individuals
        A <- c(A, rep(1, N_births)) # newborns
        H <- c(H, seq(from = 1, to = 5, length.out = N_births)) # sim happiness trait - new
        M <- c(M, rep(0, N_births)) # not yet married
        # for each person over 17, chance get married
        M[A >= aom & M == 0] <-
            rbinom(A[A >= aom & M == 0], size = 1,
                   prob = plogis(H[A >= aom & M == 0] - 7.9))
        # mortality
        deaths <- which(A > max_age)
        if (length(deaths) > 0) {
            A <- A[-deaths]
            H <- H[-deaths]
            M <- M[-deaths]
        }
    }
    d <- data.frame(age = A, married = M, happiness = H)
    return(d)
}
dd <- sim_happiness(2024, N_years = 100)
```

```r
ggplot(dd, aes(x = age, y = happiness)) +
    geom_point(alpha = .1, size = .5)
```

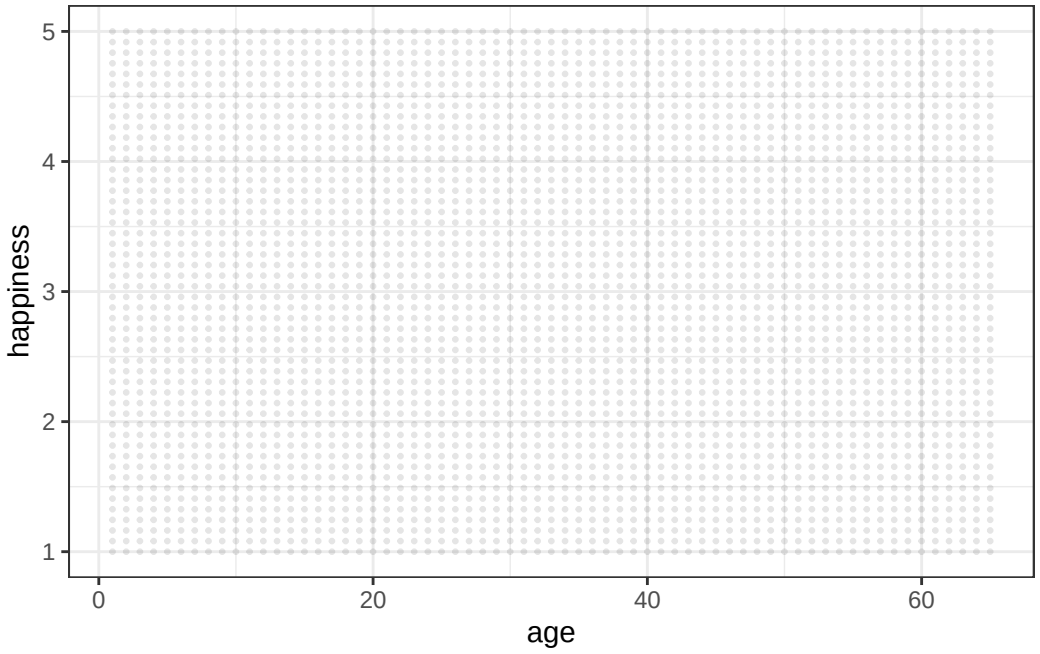


Figure 13.8: Age and happiness.

```
ggplot(dd[dd$married == 1, ], aes(x = age, y = happiness)) +
    geom_point(alpha = .5, size = .5)
```

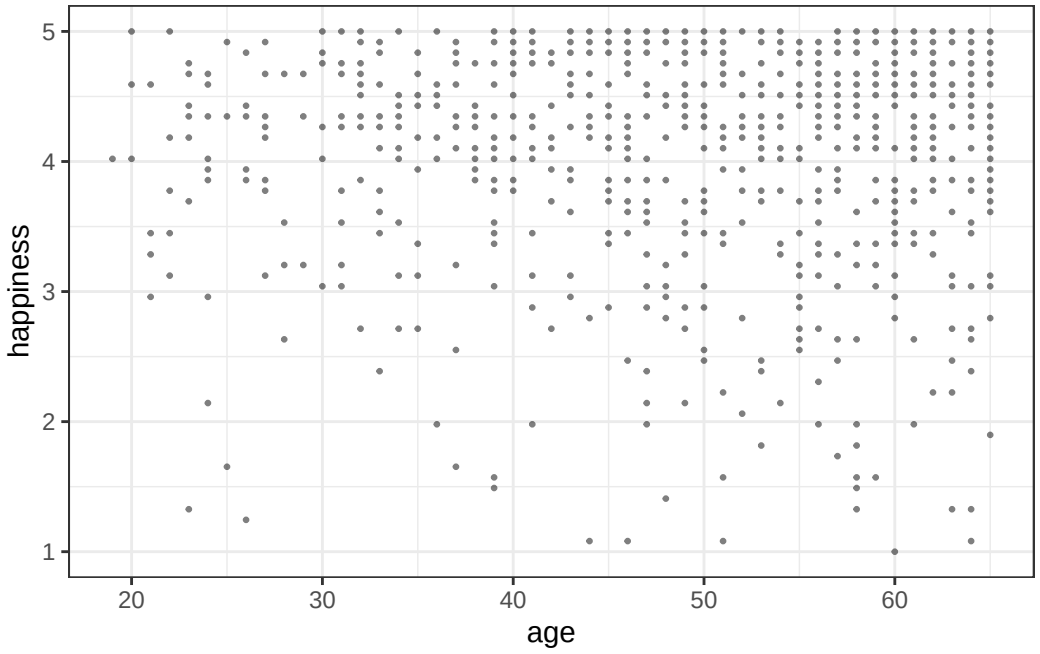


Figure 13.9: Age and happiness, conditioned on married couples.

Some other collider examples:

- impulsivity → high-risk youth ← delinquency
- healthcare worker → COVID-19 testing ← COVID-19 severity
- standardized test → admission ← research skills
- maternal smoking → birth weight → birth defect ← mortality

13.7 Some Additional References

- https://doi.org/10.1177/25152459221095823
- https://doi.org/10.1038/s41562-024-01939-z

14 Mediation

We'll use the `framing` data set from the `mediation` package, so you'll need to have the package installed first. The data were analyzed in a report in the American Journal of Political Science. The study examined whether "news about the costs of immigration boosts white opposition" (p. 959).

14.1 Summary Statistics Tables

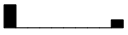
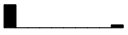
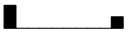
I'll take a quick detour to introduce you to some useful functions for tabulating your data. The functions will be from the `modelsummary` package.

```
data(framing, package = "mediation")
# Subtract the `emo` variable by 3 so that it starts from 0-9
framing$emo <- framing$emo - 3
# Quick summary of selected variables
datasummary_skim(framing)
```

```
# Summary by treatment condition (`tone`)
datasummary_balance(~ tone, data = framing)
```

```
# More tailor-made table with selected variables by treatment condition
datasummary(emo + p_harm + cong_mesg ~ Factor(tone) * (Mean + SD + Histogram),
            data = framing)
```

```
# Correlation table
framing |>
    select(tone, emo, cong_mesg) |>
    datasummary_correlation(method = "pearson")
```

	Unique (#)	Missing (%)	Mean	SD	Min	Median	Max	
age	63	0	47.8	16.0	18.0	47.0	85.0	
income	19	0	10.8	3.9	1.0	11.0	19.0	
emo	10	0	4.0	2.8	0.0	4.0	9.0	
p_harm	7	0	5.9	1.8	2.0	6.0	8.0	
tone	2	0	0.5	0.5	0.0	1.0	1.0	
eth	2	0	0.5	0.5	0.0	1.0	1.0	
treat	2	0	0.3	0.4	0.0	0.0	1.0	
immigr	4	0	3.0	1.0	1.0	3.0	4.0	
anti_info	2	0	0.1	0.3	0.0	0.0	1.0	
cong_mesg	2	0	0.3	0.5	0.0	0.0	1.0	

14.2 Randomization Removes Incoming Paths for Treatment

Let's consider a DAG without randomization, for the following two variables:

- X: Exposure to a negatively framed news story about immigrants
- Y: Anti-immigration political action

There are many possible confounders when we observe these two variables in data (e.g., an individual's political affiliation and the state in which a person resides). We can represent these unobserved confounders as U, so the DAG will be something like

```
dag2 <- dagitty(
    "dag{
      X -> Y; U -> X; U -> Y
      U [unobserved]
    }"
)
coordinates(dag2) <- list(x = c(X = 0, U = 1, Y = 2),
                          y = c(X = 0, U = 1, Y = 0))
# Plot
ggdag(dag2) + theme_dag()
```

		0		1			
		Mean	Std. Dev.	Mean	Std. Dev.	Diff. in Means	Std. Erro
age		48.4	16.0	47.1	16.0	-1.3	2.
income		11.0	3.9	10.6	3.9	-0.4	0.
emo		3.4	2.6	4.5	2.8	1.1	0.
p_harm		5.5	1.8	6.2	1.7	0.7	0.
eth		0.5	0.5	0.5	0.5	0.0	0.
treat		0.0	0.0	0.5	0.5	0.5	0.
immigr		2.8	1.0	3.2	0.9	0.4	0.
anti_info		0.1	0.3	0.1	0.3	0.0	0.
cong_mesg		0.3	0.5	0.4	0.5	0.0	0.
		N	Pct.	N	Pct.		
cond	not asked	0	0.0	0	0.0		
	refused	0	0.0	0	0.0		
	control	0	0.0	0	0.0		
	1	0	0.0	68	50.4		
	2	0	0.0	67	49.6		
	3	67	51.5	0	0.0		
	4	63	48.5	0	0.0		
anx	not asked	0	0.0	0	0.0		
	refused	0	0.0	0	0.0		
	very anxious	34	26.2	26	19.3		
	somewhat anxious	48	36.9	38	28.1		
	a little anxious	31	23.8	43	31.9		
	not anxious at all	17	13.1	28	20.7		
educ	not asked	0	0.0	0	0.0		
	refused	0	0.0	0	0.0		
	less than high school	6	4.6	14	10.4		
	high school	48	36.9	44	32.6		
	some college	31	23.8	39	28.9		
	bachelor's degree or higher	45	34.6	38	28.1		
gender	not asked	0	0.0	0	0.0		
	refused	0	0.0	0	0.0		
	male	64	49.2	62	45.9		
	female	66	50.8	73	54.1		
english	Strongly Favor	1	0.8	6	4.4		
	Favor	15	11.5	10	7.4		
	Oppose	44	33.8	38	28.1		
	Strongly Oppose	70	53.8	81	60.0		

	0			1		
	Mean	SD	Histogram	Mean	SD	Histogram
emo	3.39	2.63		4.53	2.81	
p_harm	5.53	1.77		6.23	1.69	
cong_mesg	0.31	0.46		0.36	0.48	

	tone	emo	cong_mesg
tone	1	.	.
emo	0.21	1	.
cong_mesg	0.05	0.37	1

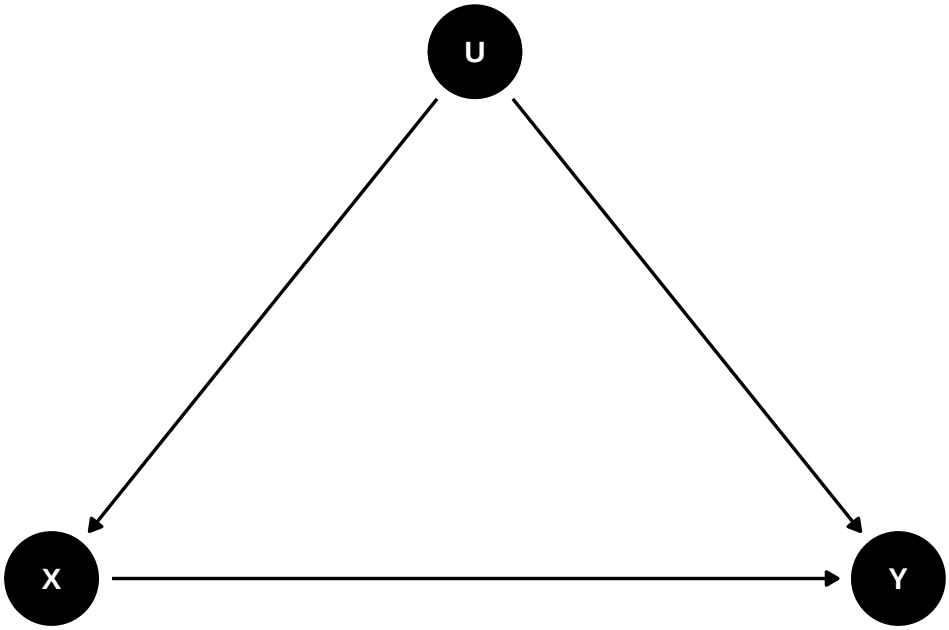


Figure 14.1: DAG with an unobserved confounder

The magic of randomization—randomly assigning individuals to a manipulated level of X—is that it blocks the path U → X. Therefore, with randomization, the reason a person sees a negatively-framed news story about immigrants is not related to reasons that the person may have intentions for anti-immigration actions. The DAG becomes

```
dag3 <- dagitty(
    "dag{
```

```
      X -> Y; U -> Y
      U [unobserved]
    }"
)
coordinates(dag3) <- list(x = c(X = 0, U = 1, Y = 2),
                          y = c(X = 0, U = 1, Y = 0))
# Plot
ggdag(dag3) + theme_dag()
```

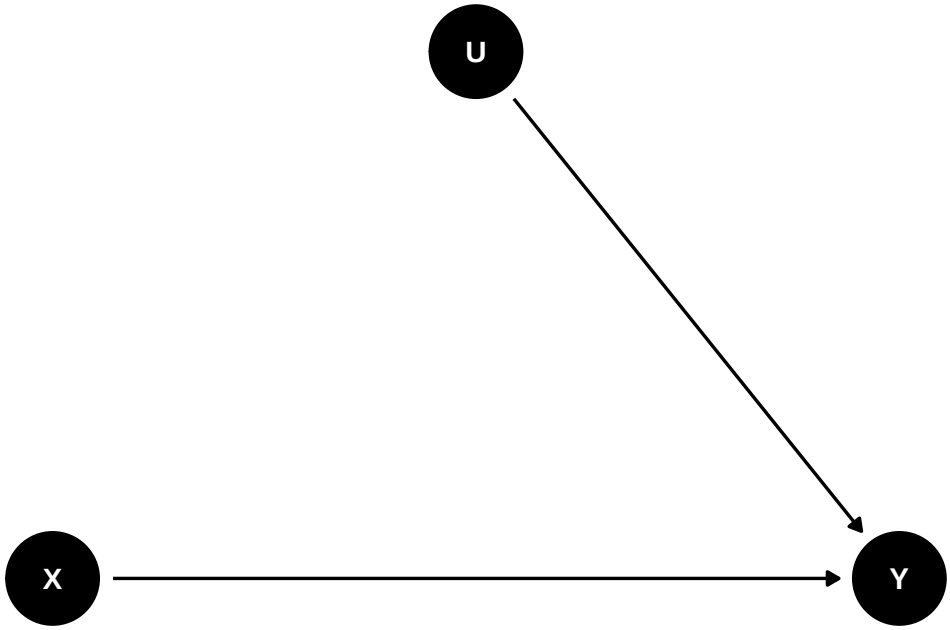


Figure 14.2: DAG with randomization

Therefore, when randomization is successful, the path coefficient of X → Y is the causal effect of X on Y. However, randomized experiments do not always rule out all confounding. For example, suppose participants are randomly assigned to different experimental conditions, but those who disagree with the presented news story drop out. In that case, such attrition can induce a non-zero correlation between X and Y in the remaining sample.

14.3 Causal Chains

14.3.1 Post-Treatment Bias

Here are some key variables from the `framing` data set:

- `cong_mesg`: binary variable indicating whether or not the participant agreed to send a letter about immigration policy to his or her member of Congress
- `emo`: posttest anxiety about increased immigration (0-9)
- `tone`: framing of news story (0 = positive, 1 = negative)

We can compare the results of two models:

1. `tone` → `cong_mesg`
2. `tone` → `cong_mesg`, adjusting for `emo`

Which model gives us the causal effect estimate for `tone`? Let's run the two models.

```
m_no_adjust <- brm(cong_mesg ~ tone,
                   data = framing,
                   family = bernoulli(link = "logit"),
                   file = "08b_m_no_adjust")
m_adjust <- brm(cong_mesg ~ tone + emo,
                data = framing,
                family = bernoulli(link = "logit"),
                file = "08b_m_adjust")
```

We can combine the results in a table:

```
msummary(list(`No adjustment` = m_no_adjust,
              `Adjusting for feeling` = m_adjust),
         estimate = "{estimate} [{conf.low}, {conf.high}]",
         statistic = NULL, fmt = 2
)
```

```
Warning:
`modelsummary` uses the `performance` package to extract goodness-of-fit
statistics from models of this class. You can specify the statistics you wish
to compute by supplying a `metrics` argument to `modelsummary`, which will then
push it forward to `performance`. Acceptable values are: "all", "common",
"none", or a character vector of metrics names. For example: `modelsummary(mod,
metrics = c("RMSE", "R2")` Note that some metrics are computationally
expensive. See `?performance::performance` for details.
 This warning appears once per session.
```

	No adjustment	Adjusting for feeling
b_Intercept	−0.81 [−1.19, −0.46]	−2.00 [−2.63, −1.44]
b_tone	0.21 [−0.28, 0.71]	−0.13 [−0.71, 0.43]
b_emo		0.32 [0.21, 0.43]
Num.Obs.	265	265
R2	0.003	0.142
ELPD	−170.1	−152.6
ELPD s.e.	5.5	7.4
LOOIC	340.2	305.2
LOOIC s.e.	11.0	14.8
WAIC	340.2	305.2
RMSE	0.47	0.44

We can see that the Bayes estimate of the coefficient for `tone` was positive without `emo`, but was negative with `emo`. Which one should we believe? The information criteria (LOOIC and WAIC) suggested that the model with `emo` was better for prediction, but just because something helps predict the outcome does not make it a causal variable. To repeat,

> Coefficients in a predictive model are not causal effects.

And to emphasize again,

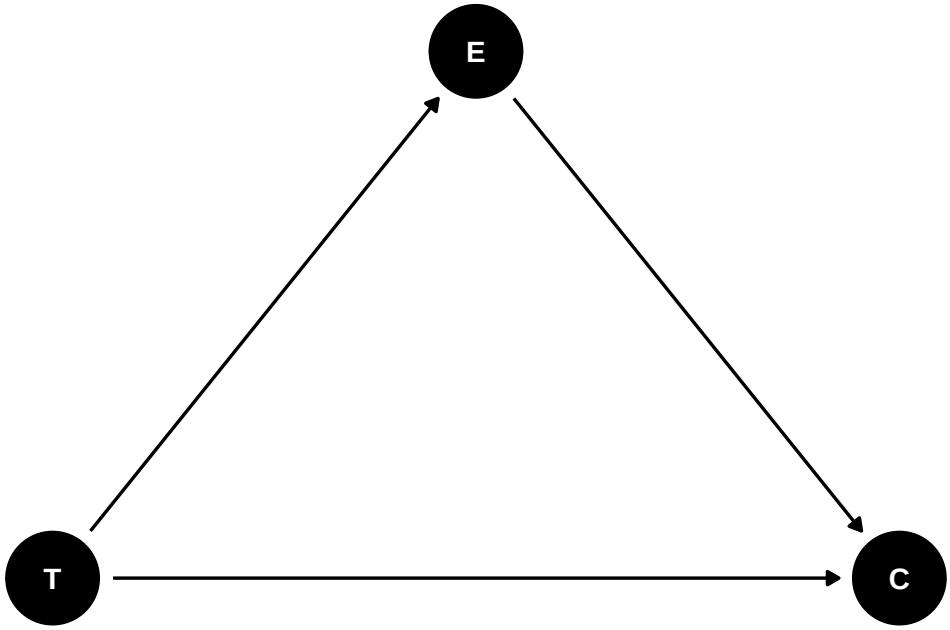
> Causal inference requires causal assumptions, and these assumptions are not in the data.

So instead, we need a DAG. Given that we know `emo` is measured **after** the intervention, it seems reasonable to think that a negatively framed story about immigrants would elicit some negative emotions about increased immigration, and that emotion may prompt people to take anti-immigrant actions. Therefore, we have the following DAG:

```
dag5 <- dagitty(
    "dag{
      T -> C; T -> E; E -> C
    }"
)
coordinates(dag5) <- list(x = c(T = 0, E = 1, C = 2),
                          y = c(T = 0, E = 1, C = 0))
# Plot
ggdag(dag5) + theme_dag()
```

This is an example of a pipe/chain. It is a causal chain going from T(one) → E(motion) → C(ongress message). If we are interested in the causal effect of T, we should not condition

Table 14.1: DAG for a mediation model with emotion as a mediator.



on E; conditioning on E would mean comparing those who saw the negatively-framed story and *those who saw the positively-framed story but had the same negative emotion towards immigrants.* In other words, adjusting for E would mean taking out part of the effect of T on C through E.

As another example, think about a drug that is supposed to lower the risk of a heart attack. Imagine someone conducting a study comparing drug/no drug conditions on their probability of getting heart attacks. Should we adjust for participants' blood pressure after the intervention? If we want to know the drug's effect, and that the drug works by lowering blood pressure, we should not adjust for posttest blood pressure. Otherwise, we would be asking the question: Does the drug help prevent heart attacks through something other than lowering one's blood pressure?

The latter question can be answered in mediation analysis.

14.4 Causal Mediation

In the DAG above, E is a post-treatment variable potentially influenced by T, which we call a **mediator**. Mediator is an important topic in causal inference, as it informs the mechanism of how a variable has a causal effect on an outcome.

One thing to be careful of is that, statistically speaking, a mediator behaves very much like a confounder, and their difference is based on causal assumptions.

Let's analyze the mediation model in Figure X. There are two variables that are on the receiving end of some causal effects: `emo` and `cong_mesg`. Whereas the generalized linear model handles one outcome, with `brms`, we can have a system of equations—one for each outcome—estimated simultaneously, as shown in the code below.

14.4.1 Using `brms`

```
m_med <- brm(
    # Two equations for two outcomes
    bf(cong_mesg ~ tone + emo) +
        bf(emo ~ tone) +
        set_rescor(FALSE),
    # A list of two family arguments for two outcomes
    family = list(bernoulli("logit"), gaussian("identity")),
    data = framing,
    prior = prior(normal(0, 2), class = "b", resp = "emo") +
        prior(student_t(4, 0, 5), class = "sigma", resp = "emo") +
        prior(student_t(4, 0, 2.5), class = "b", resp = "congmesg"),
    seed = 1338,
    file = "08b_m_med"
)
```

14.4.2 Using Stan

Here's some Stan code for running the same mediation model

```
data {
    int<lower=0> N0;  // number of observations (control)
    int<lower=0> N1;  // number of observations (treatment)
    array[N0] int y0; // outcome (control);
    array[N1] int y1; // outcome (treatment);
    vector[N0] m0;    // mediator (control);
    vector[N1] m1;    // mediator (treatment);
}
parameters {
    real alpham;  // regression intercept for M
    real alphay;  // regression intercept for M
```

```
    real beta1;   // X -> M
    real beta2;   // X -> Y
    real beta3;   // M -> Y
    real<lower=0> sigmam;  // SD of prediction error for M
}
model {
    // model
    m0 ~ normal(alpham, sigmam);
    m1 ~ normal(alpham + beta1, sigmam);
    y0 ~ bernoulli_logit(alphay + beta3 * m0);
    y1 ~ bernoulli_logit(alphay + beta2 + beta3 * m1);
    // prior
    alpham ~ normal(4.5, 4.5);
    alphay ~ normal(0, 5);
    beta1 ~ std_normal();
    beta2 ~ std_normal();
    beta3 ~ std_normal();
    sigmam ~ student_t(4, 0, 5);
}
```

```
med_mod <- cmdstan_model("stan_code/mediation_logit_normal.stan")
```

```
# 1. Form the data list for Stan
stan_dat <- with(
    framing,
    list(
        N0 = sum(tone == 0),
        N1 = sum(tone == 1),
        m0 = emo[which(tone == 0)],
        m1 = emo[which(tone == 1)],
        y0 = cong_mesg[which(tone == 0)],
        y1 = cong_mesg[which(tone == 1)]
    )
)
# 2. Run Stan
m_med_stan <- med_mod$sample(
    data = stan_dat,
    seed = 1338,
    refresh = 1000
)
```

14.4.3 Direct and Indirect Effects

In a mediation model, the effect of X on Y has two mechanisms: - Indirect effect: X causes Y because X causes M, and M causes Y - Direct effect: X causes Y without involving M

More specifically, the direct effect is the change in Y for one unit change in X, *holding M constant*. In our example, it means comparing subsets of the treatment and the control groups, under the condition that both subsets have the same level of negative emotion about increased immigration. The indirect effect takes more effort to understand: it is the change in Y for the control group (or the treatment group) if their mediator value is set to the same level as the treatment group. In our example, it would mean comparing the control group and the *counterfactual* where the control group had their negative emotion changed to the same level as the treatment group.

The *causal mediation* literature has more distinctions on the different types of direct and indirect effects. Below, I give codes for obtaining these effects without going into detail.[1]

14.4.4 Controlled direct effect (CDE)

CDE is the direct effect when the mediator is set to a specific level. Below is the CDE for `emo` = 0 and `emo` = 9, respectively.

```
cond_df <- data.frame(tone = c(0, 1, 0, 1),
                      emo = c(0, 0, 9, 9))
cond_df |>
    bind_cols(
        fitted(m_med, newdata = cond_df)[ , , "congmesg"]
    ) |>
    knitr::kable()
```

Table 14.2: Estimated direct effect of `tone` on `cong_mesg` at two different levels of `emo`.

tone	emo	Estimate	Est.Error	Q2.5	Q97.5
0	0	0.1212844	0.0320367	0.0662354	0.1907005
1	0	0.1084567	0.0330696	0.0538386	0.1830547
0	9	0.6982051	0.0698306	0.5559154	0.8234034
1	9	0.6702609	0.0631406	0.5418592	0.7855347

[1]You can find more information about causal mediation in this paper: https://ftp.cs.ucla.edu/pub/stat_ser/r389.pdf

14.4.5 Natural direct effect (NDE)

The "natural" effects are quantities for some kind of population averages. NDE is the direct effect when the mediator is held constant at the level of the control group. As a first step, we need to obtain the potential outcome of `emo` when `tone` $= 0$. We call this potential outcome variable M_0 (potential outcome of M if $X = 0$). This has already been observed for the control group but will be a counterfactual for the treatment group.

We will use a general approach by Imai et al. (2010) to simulate potential outcomes for each observation, before computing NDE (and NIE). For each observation, we will first simulate the potential outcome of `emo` when `tone` $= 0$ (M_0), and then simulate the potential outcome of `emo` when `tone` $= 1$ (M_1).

```
# Simulate potential outcomes for mediator when T = 0
dat0 <- m_med$data
dat0$tone <- 0
# Predicted emo when T = 0
po_m0 <- posterior_predict(m_med, newdata = dat0, resp = "emo")
# Simulate potential outcomes for mediator when T = 1
dat1 <- m_med$data
dat1$tone <- 1
# Predicted emo when T = 1
po_m1 <- posterior_predict(m_med, newdata = dat1, resp = "emo")
```

Next, we will simulate four potential outcomes for `cong_mesg` (Y):

- Y(T $= 0$, M $= M_0$)
- Y(T $= 1$, M $= M_0$)
- Y(T $= 0$, M $= M_1$)
- Y(T $= 1$, M $= M_1$)

```
m_med_draws <- as_draws_df(m_med)
# Predicted logit of congmesg when T = 0 and emo = po_m0
po_y0_m0 <- m_med_draws$b_congmesg_Intercept + m_med_draws$b_congmesg_emo * po_m0
# Predicted logit of congmesg when T = 1 and emo = po_m0
po_y1_m0 <- m_med_draws$b_congmesg_Intercept +
    m_med_draws$b_congmesg_tone +
    m_med_draws$b_congmesg_emo * po_m0
# Predicted logit of congmesg when T = 0 and emo = po_m1
po_y0_m1 <- m_med_draws$b_congmesg_Intercept + m_med_draws$b_congmesg_emo * po_m1
# Predicted logit of congmesg when T = 1 and emo = po_m1
po_y1_m1 <- m_med_draws$b_congmesg_Intercept +
```

Table 14.3: Estimated natural direct and indirect effects for the control group.

```
draws_nde_nie <- as_draws(list(NDE = nde, NIE = nie))
posterior::summarise_draws(draws_nde_nie)
```

```
# A tibble: 2 x 10
  variable    mean  median     sd    mad      q5    q95  rhat ess_bulk ess_tail
  <chr>      <dbl>   <dbl>  <dbl>  <dbl>   <dbl>  <dbl> <dbl>    <dbl>    <dbl>
1 NDE      -0.0246 -0.0249 0.0518 0.0523 -0.110  0.0615  1.00    5171.    3113.
2 NIE       0.0681  0.0668 0.0276 0.0267  0.0246 0.116   1.00    3916.    2977.
```

```
    m_med_draws$b_congmesg_tone +
    m_med_draws$b_congmesg_emo * po_m1
```

The NDE is defined as Y(T = 1, M = M_0) - Y(T = 0, M = M_0).

```
# NDE = Y(1, M(0)) - Y(0, M(0))
nde <- rowMeans(plogis(po_y1_m0)) - rowMeans(plogis(po_y0_m0))
```

14.4.5.1 Natural indirect effect (NIE)

NIE is the difference in the outcome between the actual control group and a counterfactual control group. The counterfactual here is a control group that did not receive the treatment, but had their `emo` value set to be equal to the treatment group. The NIE is defined as Y(T = 0, M = M_1) - Y(T = 0, M = M_0).

```
# NIE = Y(0, M(1)) - Y(0, M(0))
nie <- rowMeans(plogis(po_y0_m1)) - rowMeans(plogis(po_y0_m0))
```

```
mcmc_areas(draws_nde_nie, bw = "SJ")
```

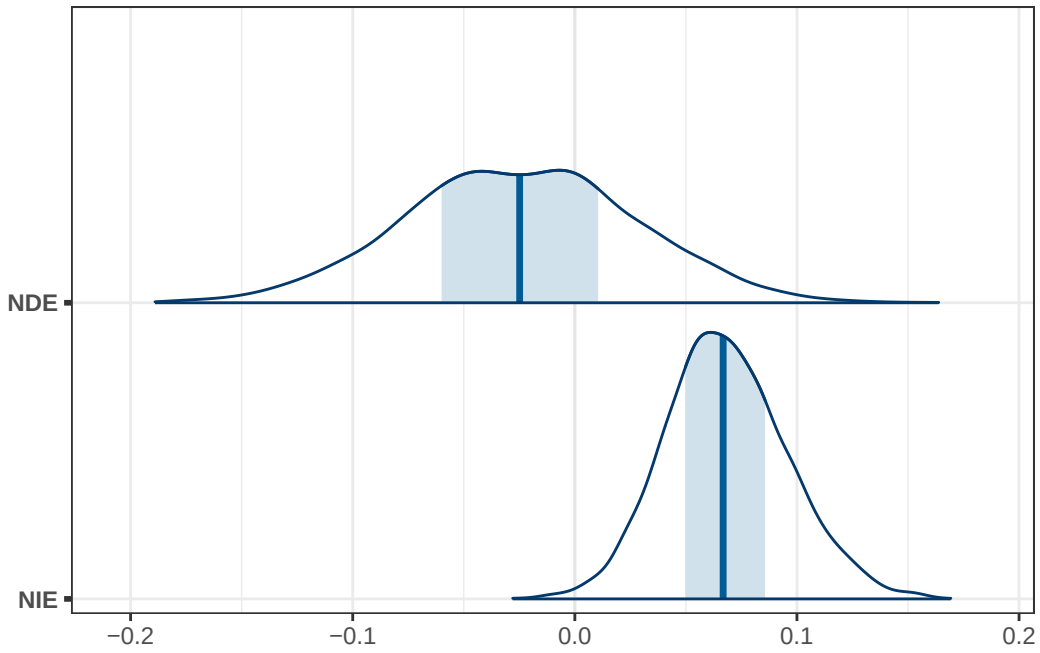


Figure 14.3: Estimated natural direct and indirect effects for the control group.

14.4.6 Sensitivity analysis

```
dag6 <- dagitty(
    "dag{
      T -> C; T -> E; E -> C; U -> E; U -> C
    }"
)
coordinates(dag6) <- list(x = c(T = 0, E = 1, C = 2, U = 2),
                          y = c(T = 0, E = 1, C = 0, U = 1))
ggdag(dag6) + theme_dag()
```

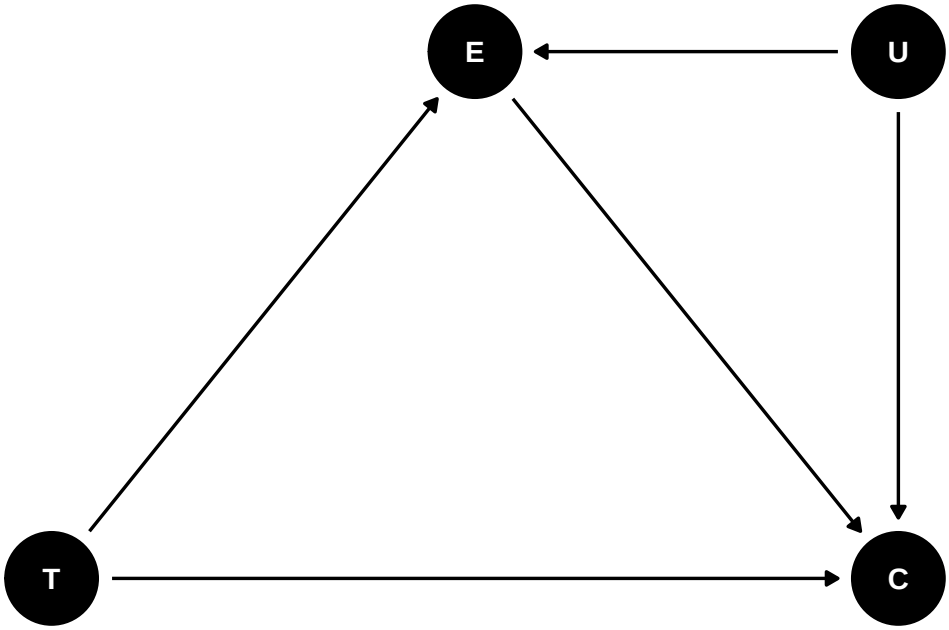


Figure 14.4: DAG for a mediation model with an unobserved mediator-outcome confounder.

Assumptions of Causal Mediation

Mediation effects can be estimated properly when the causal diagram and the corresponding model are specified correctly. In our model, we assume

- No unmeasured treatment-outcome confounding
- No unmeasured mediator-outcome confounding
- No unmeasured treatment-mediator confounding
- The mediator-outcome path is not moderated by the treatment

Note that randomization of the treatment does not rule out confounding for the mediator-outcome path.

One important assumption in mediation is that there is no unobserved confounding variable between the mediator and the outcome. This assumption requires researchers' input, as usually we don't have studies that randomly assign both the treatment variable and the mediator. An additional technique is to ask: what would the effect be if there were unobserved confounding variables of a certain magnitude? With Bayesian, we can represent the strength of the confounding effect by a prior distribution (see McCandless & Somers, 2019, p. 10.1177/0962280217729844). The following shows the mediation estimates assuming the effect of the confounding variable to the mediator is 1, and to the outcome has a prior of N(0.5,

0.2).

```
data {
    int<lower=0> N0;  // number of observations (control)
    int<lower=0> N1;  // number of observations (treatment)
    array[N0] int y0; // outcome (control);
    array[N1] int y1; // outcome (treatment);
    vector[N0] m0;    // mediator (control);
    vector[N1] m1;    // mediator (treatment);
}
parameters {
    real alpham;  // regression intercept for M
    real alphay;  // regression intercept for M
    real beta1;   // X -> M
    real beta2;   // X -> Y
    real beta3;   // M -> Y
    vector[N0] u0;  // confounding variable
    vector[N1] u1;  // confounding variable
    real beta4;   // U -> Y
    real<lower=0> sigmam;  // SD of prediction error for M
}
model {
    // model
    u0 ~ std_normal();
    u1 ~ std_normal();
    m0 ~ normal(alpham + u0, sigmam);
    m1 ~ normal(alpham + beta1 + u1, sigmam);
    y0 ~ bernoulli_logit(alphay + beta3 * m0 + beta4 * u0);
    y1 ~ bernoulli_logit(alphay + beta2 + beta3 * m1 + beta4 * u1);
    // prior
    alpham ~ normal(4.5, 4.5);
    alphay ~ normal(0, 5);
    beta1 ~ std_normal();
    beta2 ~ std_normal();
    beta3 ~ std_normal();
    beta4 ~ normal(0.5, 0.2);
    sigmam ~ student_t(4, 0, 5);
}
```

```
med_mod_sens <- cmdstan_model("stan_code/mediation_logit_normal_sensitivity.stan")
```

```r
# 1. form the data list for Stan
stan_dat <- with(
    framing,
    list(
        N0 = sum(tone == 0),
        N1 = sum(tone == 1),
        m0 = emo[which(tone == 0)],
        m1 = emo[which(tone == 1)],
        y0 = cong_mesg[which(tone == 0)],
        y1 = cong_mesg[which(tone == 1)]
    )
)
# 2. Run Stan
m_med_sens <- med_mod_sens$sample(
    data = stan_dat,
    seed = 1338,
    refresh = 1000
)
```

```
Running MCMC with 4 sequential chains...

Chain 1 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 1 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 1 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 1 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 1 finished in 1.4 seconds.
Chain 2 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 2 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 2 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 2 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 2 finished in 1.1 seconds.
Chain 3 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 3 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 3 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 3 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 3 finished in 1.0 seconds.
Chain 4 Iteration:    1 / 2000 [  0%]  (Warmup)
Chain 4 Iteration: 1000 / 2000 [ 50%]  (Warmup)
Chain 4 Iteration: 1001 / 2000 [ 50%]  (Sampling)
Chain 4 Iteration: 2000 / 2000 [100%]  (Sampling)
Chain 4 finished in 1.0 seconds.
```

```
All 4 chains finished successfully.
Mean chain execution time: 1.1 seconds.
Total execution time: 4.9 seconds.
```

beta1 = tone -> emo; beta2 = tone -> cong_mesg; beta3 = emo -> cong_mesg

```
m_med_sens$draws(
    c("alpham", "alphay",
      "beta1", "beta2", "beta3")
) |>
    mcmc_intervals()
```

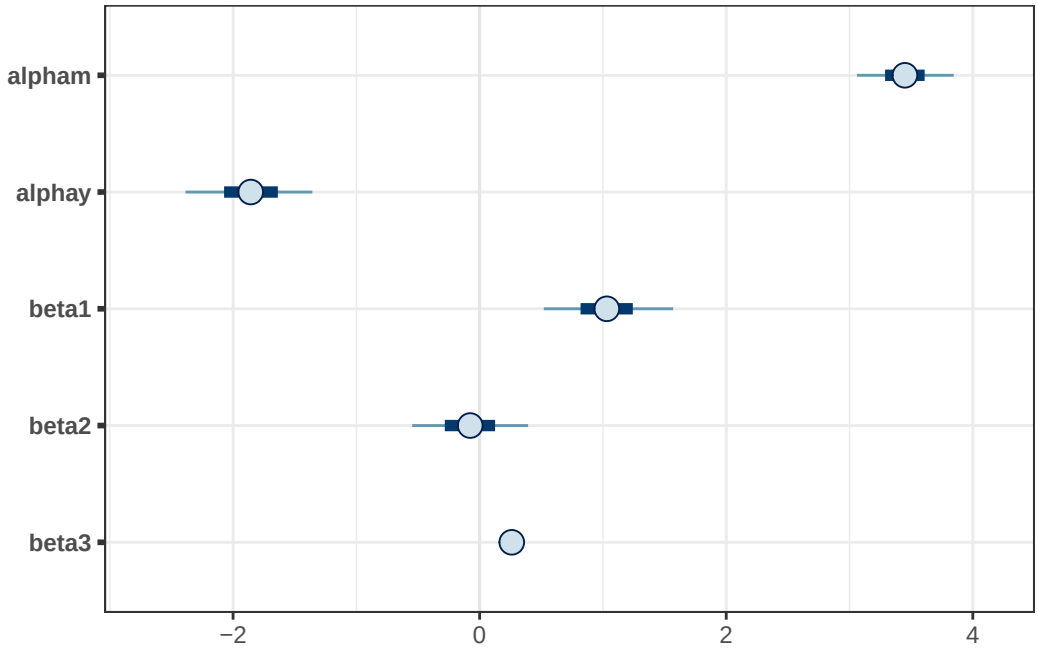


Figure 14.5: Estimated coefficients for the mediation model with the sensitivity analysis.

As you can see, the prior of the confounding effect attenuates the coefficients from the mediator to the outcome, but the path from the mediator to the outcome remains pretty much above zero.

You may also check out the `BayesGmed` package, which is also based on Stan. More descriptions are in the paper Yimer et al. (2023).

Part VIII

Week 10–11

15 Markov Chain Monte Carlo

Previously, we have seen a few examples with Bayesian inferences where the posterior distribution concerns only one parameter, like the Bernoulli and the Poisson model. We have also discussed the grid approximation and the conjugate prior approaches to obtain/approximate the posterior. In this note, we will discuss the simulation method and explain why we need a special class of methods called *Markov Chain Monte Carlo*. This note will consider mainly the **Metropolis algorithm**, which subsumes many other commonly used MCMC algorithms. Therefore, it is beneficial to build a solid foundation on what the basic version of the Metropolis algorithm is. You will also write your own Metropolis sampler to understand how it works.

But first, let's talk about the Monte Carlo method.

15.1 Monte Carlo Simulation

In a previous example, we see that with a conjugate prior (e.g., Beta), the posterior distribution is from the same distributional family (Beta). Thus, we can easily draw simulation samples from the posterior distribution using R. The more samples we draw, the better we can approximate the posterior distribution based on the simulation samples. It is the same logic to get a large sample to describe our population precisely; here, the posterior distribution, determined using mathematics, is considered the population, and the simulation draws are, well, a sample from that population. With 10,000 or 100,000 samples (draws), we can accurately describe our population (posterior).

For example, if we know that the posterior is a Beta$(15, 10)$ distribution, consider drawing 10, 100, 10,00, and 10,000 samples from it using the R function `rbeta`, and contrast the density estimated from the samples (in the histogram) with that of the actual Beta distribution (in red).

```
# Set the `seed` (initial point) for pseudo-random number generation algorithm
set.seed(2)
num_draws <- c(10, 100, 1000, 10000)
beta_draws <- data.frame(
    th = rbeta(sum(num_draws), shape1 = 15, shape2 = 10),
    sam = rep(paste(num_draws, "samples"), num_draws)
)
```

```
ggplot(beta_draws, aes(x = th)) +
    geom_histogram(aes(y = after_stat(density))) +
    stat_function(
        fun = dbeta, args = list(shape1 = 15, shape2 = 10),
        col = "red"
    ) +
    labs(x = expression(theta)) +
    facet_wrap(~sam)
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

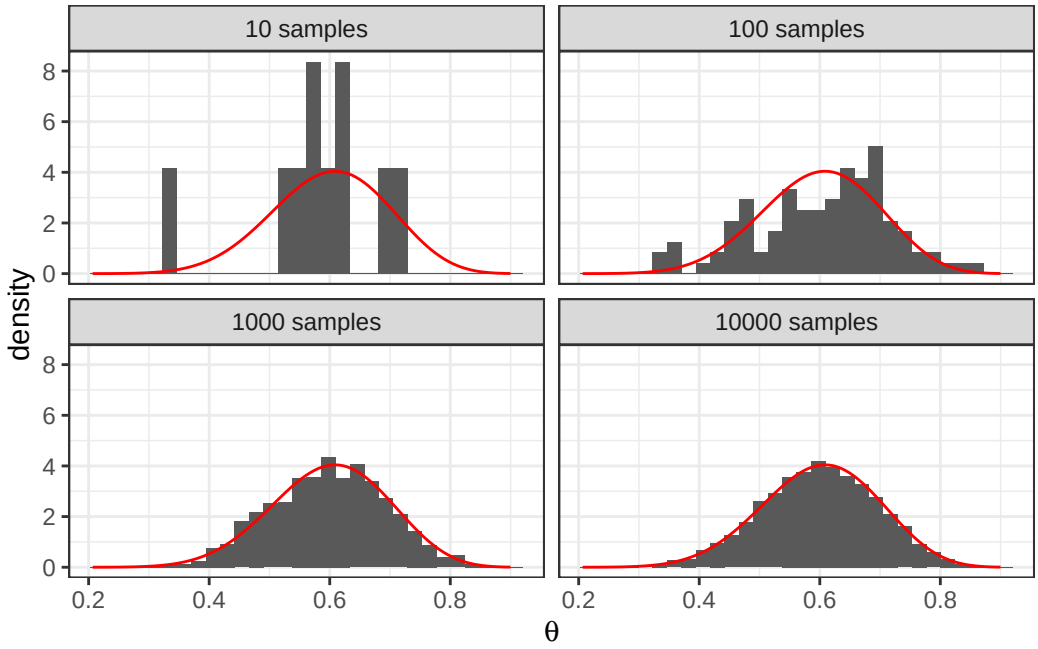


Figure 15.1: Monte Carlo simulation samples from the Beta(15, 10) distribution

The figure below shows the values when drawing 100 samples in time order:

```
beta_draws |>
    filter(sam == "100 samples") |>
    rowid_to_column("iter") |>
    ggplot(aes(y = th, x = iter)) +
    geom_line() +
    labs(y = expression(theta))
```

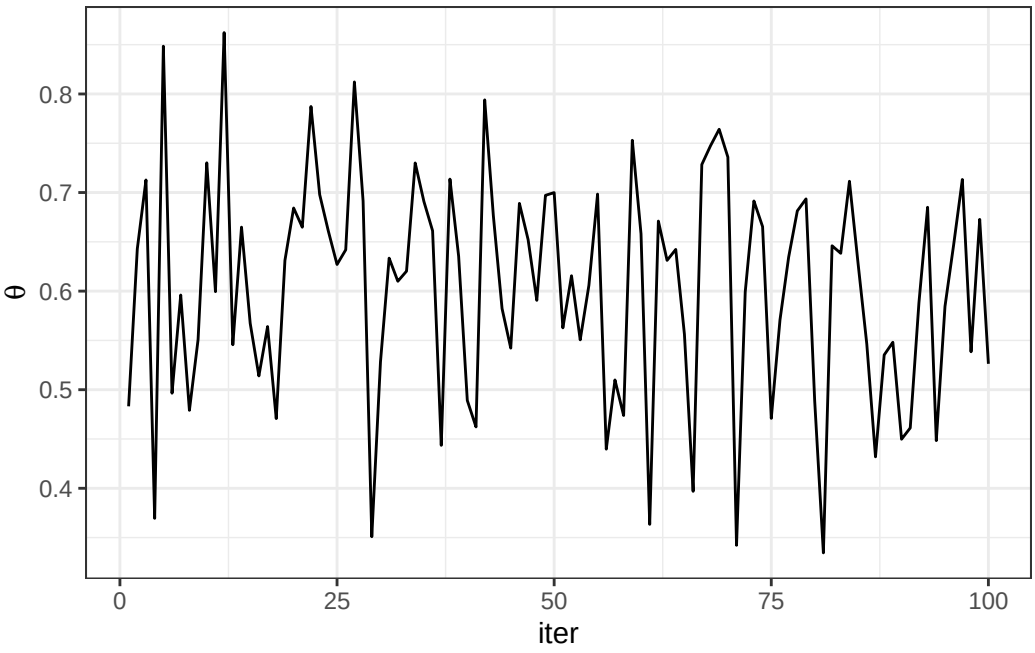


Figure 15.2: Trace plots of Monte Carlo samples.

So we can say that, when the number of posterior samples is very large, the sample distribution *converges* to the population density. The Monte Carlo method will work for many situations. Note, of course, the number of simulation samples, S, is controlled by the analysts; it is different from the sample size of the data, which is fixed and is a property of the observed data.

In addition, most descriptive statistics (e.g., mean, *SD*) of the simulation draws will converge to the corresponding values of the true posterior distribution. The graphs below show how the mean, median, *SD*, and skewness converge to the true values (red dashed lines) when the number of simulation samples increases.

```
beta_draws |>
    filter(sam == "1000 samples") |>
    rowid_to_column("iter") |>
    mutate(
        mean = cumsum(th) / row_number(),
        median = map_dbl(row_number(), ~ median(th[1:.x])),
        SD = map_dbl(row_number(), ~ sd(th[1:.x])),
        skewness = map_dbl(row_number(), ~ e1071::skewness(th[1:.x]))
    ) |>
    ungroup() |>
```

```r
    gather("stat", "val", mean:skewness) |>
    ggplot(aes(x = iter, y = val)) +
    geom_line() +
    geom_hline(
        data = data.frame(
            stat = c("mean", "median", "SD", "skewness"),
            val = c(
                15 / 25,
                qbeta(.50, 15, 10),
                sqrt(15 * 10 / (15 + 10)^2 / (15 + 10 + 1)),
                2 * (10 - 15) * sqrt(15 + 10 + 1) /
                    (15 + 10 + 2) / sqrt(15 * 10)
            )
        ),
        aes(yintercept = val), col = "red", linetype = "dashed"
    ) +
    facet_wrap(~stat, scales = "free") +
    labs(y = "")
```

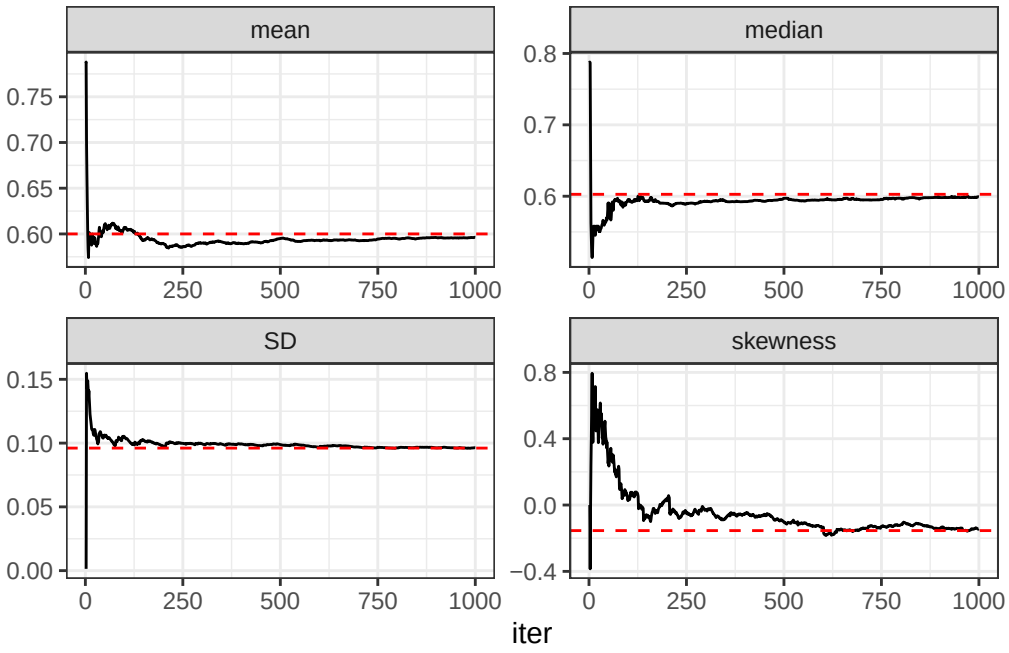


Figure 15.3: Sample statistics of the Monte Carlo samples.

15.2 Markov Chain Monte Carlo (MCMC): Drawing Dependent Samples

The above Monte Carlo simulation requires that (a) we know that the posterior distribution is exactly a beta distribution, and (b) R knows how to draw simulation samples from a beta distribution (with `rbeta`). As we progress through the class, it is more of an exception that we can use conjugate prior distribution, so in general, neither (a) nor (b) would hold. For example, if we instead use a normal distribution for the prior of θ, we may get something like

$$P(\theta \mid y) = \frac{\mathrm{e}^{-(\theta-1/2)^2}\theta^y(1-\theta)^{n-y}}{\int_0^1 \mathrm{e}^{-(\theta^*-1/2)^2}{\theta^*}^y(1-\theta^*)^{n-y}d\theta^*}$$

and it would be very hard, if possible, to draw simulation samples directly from the posterior. Luckily, MCMC provides a way to draw samples from the posterior distribution without the need to know everything about the posterior distribution. For example, the basic version of the Metropolis algorithm only requires that we know the *density ratio* of every two possible values θ_1 and θ_2. Thus, we don't need to deal with the integral in the denominator, as the integral does not depend on θ and will get canceled out when taking the ratio.

15.3 The Metropolis algorithm

The Metropolis algorithm can generally be used to draw samples from a distribution as long as the density ratio of any two points can be computed. Remember, in Bayesian inference, for two values in the posterior distribution, the ratio of the posterior densities at θ_1 and θ_2 is

$$\begin{aligned}\frac{P(\theta=\theta_2 \mid y)}{P(\theta=\theta_1 \mid y)} &= \frac{P(y \mid \theta=\theta_2)P(\theta=\theta_2)/P(y)}{P(y \mid \theta=\theta_1)P(\theta=\theta_1)/P(y)} \\ &= \frac{P(y \mid \theta=\theta_2)P(\theta=\theta_2)}{P(y \mid \theta=\theta_1)P(\theta=\theta_1)}.\end{aligned}$$

Therefore, even though we may not know $P(\theta=\theta_1 \mid y)$ as it involves $P(y)$ as the denominator, we can still compute the density ratio.

In addition, the Metropolis algorithm requires the use of a **proposal distribution**, which can be any symmetric distribution. Common choices are normal distribution or uniform distribution. For example, let's assume we will use a $N(0, 0.1)$ proposal distribution, with 0.1 being the standard deviation.

The steps of a Metropolis algorithm are:

1. Randomly start from a certain point in the parameter space, and call that point θ_0
2. Randomly generate a sampled value from a $N(\theta_0, 0.11)$ distribution. Call this proposed value θ^{prop}

3. Compute the density ratio $[P(\theta = \theta^{\text{prop}} \mid y)]/[P(\theta = \theta_0 \mid y)]$
4. If the ratio is larger than 1, accept θ^{prop} and include this value in the sample
5. If the ratio is smaller than 1, accept θ^{prop} with probability equal to the density ratio. For example, if the ratio is 0.7, one first generates a simulated value, u, from a uniform distribution between 0 and 1 (i.e., $U(0, 1)$). If u is smaller than the ratio, accept θ^{prop} and include it in the sample. Otherwise, reject the proposed value, and include θ_0 (again) in the sample
6. After accepting θ^{prop} or θ_0 in the sample, denote the accepted value as θ_0, and repeat steps 2 to 6.

Compared to the Monte Carlo method, which directly samples from a Beta distribution, the Metropolis algorithm does not require an R function to draw samples from the target distribution. The cost, however, is that the sampling process is not as *efficient* because the sampled values are dependent. We'll discuss this point later after seeing an example of the algorithm.

15.4 Shiny App

To see a visual demonstration, you may run the shiny app I created by typing in R

```
shiny::runGitHub("metropolis_demo", "marklhc")
```

15.5 Example 1: Estimating the Number of People Taking the Metro

This example uses data from the LA Barometer survey conducted by the USC Dornsife Center for Economic and Social Research. Specifically, I'm interested in the proportion of participants who took the Metro in the previous year among first-generation immigrants in LA county. You can see a press release on the data at https://dornsife.usc.edu/news/stories/3164/labarometer-mobility-in-los-angeles-survey/

```
uas_dat <- read_dta(here("data", "uas219_psyc573.dta"))
uas_dat |>
    filter(immigrant_status == 0) |>
    count(tr002s2)
```

```
# A tibble: 3 x 2
  tr002s2           n
  <dbl+lbl>     <int>
1     0 [0 No]     26
2     1 [1 Yes]   111
3 NA(a)           192
```

So in 338 participants who are first-generation immigrants, 86 said they had used the Metro.

Let's use a weakly informative prior of Beta(1.5, 2), which has a weight of 1.5 prior data points, with a weak belief that less than half of the people had used the Metro.

Model:

$$\text{usemetro}_i \sim \text{Bern}(\theta)$$

Prior:

$$\theta \sim \text{Beta}(1.5, 2)$$

```
prior_a <- 1.5
prior_b <- 2
```

Based on conjugacy, we know the posterior is Beta(87.5, 254). For pedagogical purposes, we will instead use a Metropolis sampler, which only requires the ratio of prior $\times$ likelihood for any two θ values.

15.5.1 MCMC sampling

```
num_yes <- 86
num_obs <- 86 + 252
# Define a function to compute values proportional to p(y | th) * p(th)
prior_times_lik <- function(th) {
    # Return 0 if th is out of range
    if (th < 0 || th > 1) return(0)
    pth <- dbeta(th, shape1 = prior_a, shape2 = prior_b)
    py_given_th <- th ^ num_yes * (1 - th) ^ (num_obs - num_yes)
    pth * py_given_th
}
# Define a function for generating data from the proposal distribution
generate_proposal <- function(th, sd = 0.1) {
    rnorm(1, mean = th, sd = sd)
}
# Initialize the Metropolis algorithm
```

```r
set.seed(2037)  # set the seed for reproducibility
num_draws <- 1000
num_warmup <- num_draws / 2
th_all_draws <- rep(NA, num_draws)
# Step 1: starting value
th_all_draws[1] <- 0.1
# counter for tracking acceptance rate
num_accepted <- 0
for (s in seq_len(num_draws - 1)) {
    current_th <- th_all_draws[s]
    # Step 2: Generate proposal
    proposed_th <- generate_proposal(current_th)
    # Step 3: Compute acceptance probability
    prob_accept <- min(
        1,
        prior_times_lik(proposed_th) /
            prior_times_lik(current_th)
    )
    # Steps 4 & 5: etermine whether to make the jump
    if (runif(1) < prob_accept) {
        th_all_draws[s + 1] <- proposed_th
        if (s + 1 >= num_warmup) {
            num_accepted <- num_accepted + 1
        }
    } else {
        th_all_draws[s + 1] <- current_th
    }
}
```

We can visualize the MCMC chain by plotting the iteration index on the x-axis and the sampled value on the y-axis:

```r
ggplot(
    data.frame(th = th_all_draws, iter = seq_along(th_all_draws)),
    aes(x = iter, y = th)
) +
    geom_line()
```

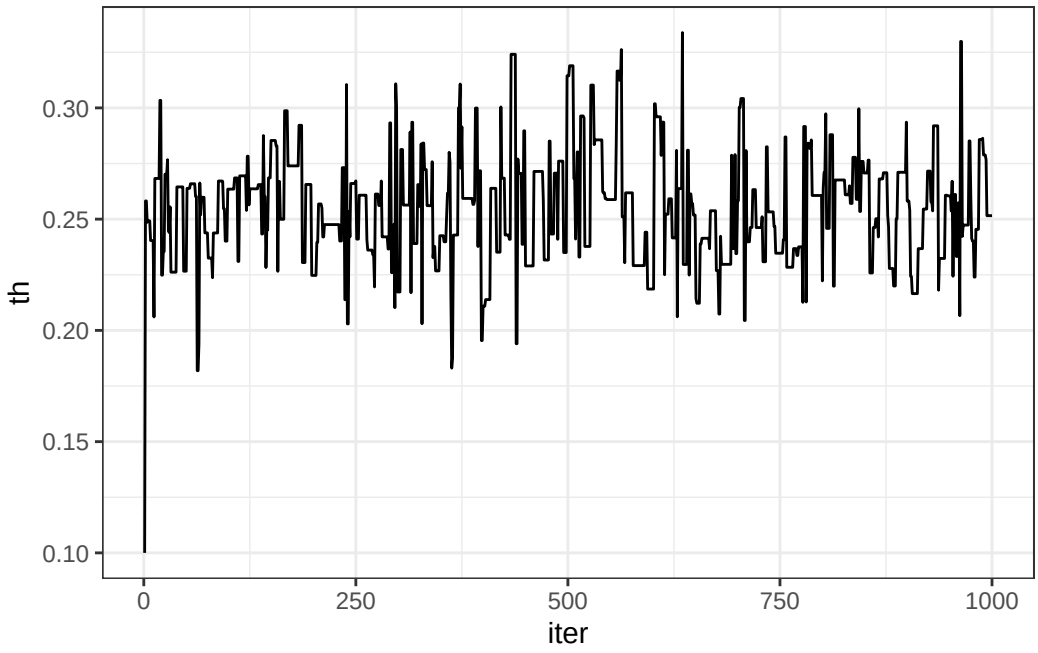


Figure 15.4: Trace plots of MCMC samples for the Metro example.

Each step in MCMC is called an *iteration*. The sampled values are *dependent*, meaning that the value at iteration s depends on the value at iteration $s-1$. This is a major difference from functions that simulate independent random samples, like `rbeta()` or `rnorm()`. The resulting sampled values will form a *Markov chain*, meaning that each sampled value is correlated with the previous value (e.g., if $\theta^{(s)}$ is large, $\theta^{(s+1)}$ is also large).

As shown above, the chain starts at 0.10 then quickly moves to the region around 0.25, the area with high posterior density. It then oscillates around that for the remaining iterations.

15.5.2 More on Markov Chain

A Markov chain describes how a variable transitions from one "state" to another. The current state depends on the previous state. A well-behaved Markov Chain is said to be *ergodic*, which means that it is (see Hoff, 2009, chapter 10):

- *irreducible*: at any state $\theta^{(s)}$, it can go to any value θ^* eventually. A reducible chain is one where some states cannot get to some other states; an example is when, at some point, the chain stays as a positive value forever and never gets back to the negative side.
- *aperiodic*: the chain does not have any periodic states. If it is a periodic chain, some values can only be visited every kth iteration.

- *recurrent*: after the chain visits a certain state θ^*, if the chain runs long enough, it eventually returns to the same state θ^*.

Under the above conditions, a Markov chain will converge to a *stationary distribution*. Thus, after a certain large amount of iterations, the draws from the chain can be considered a random (but correlated) sample of the stationary distribution. Moreover, one can prove that, with the Metropolis algorithm, the converging stationary distribution is the posterior distribution (see the discussion in Kruschke, 2015, chapter 7).

15.5.3 Warm-up/Burn-in

A Markov chain needs some iterations to get to the stationary distribution. Those iterations are usually called *warm-up* or *burn-in* (depending on the algorithm and the software) iterations and are usually discarded. In many software programs, the first half of the iterations are considered warm-ups, so even though we got 1,000 iterations, only 500 will be used:

```
num_warmup <- num_draws / 2
th_draws <- th_all_draws[- (1:num_warmup)]
```

15.5.4 Autocorrelation

The degree to which the value at iteration s is correlated with the value at $s-1$ (and at $s-2$, etc) can be measured by the autocorrelation. For example, below shows the lag-1 correlation:

```
ggplot(data.frame(current = th_draws,
                  previous = lag(th_draws)),
       aes(x = previous, y = current)) +
    geom_point() +
    geom_smooth()
```

```
`geom_smooth()` using method = 'loess' and formula = 'y ~ x'
```

```
Warning: Removed 1 rows containing non-finite values (`stat_smooth()`).
```

```
Warning: Removed 1 rows containing missing values (`geom_point()`).
```

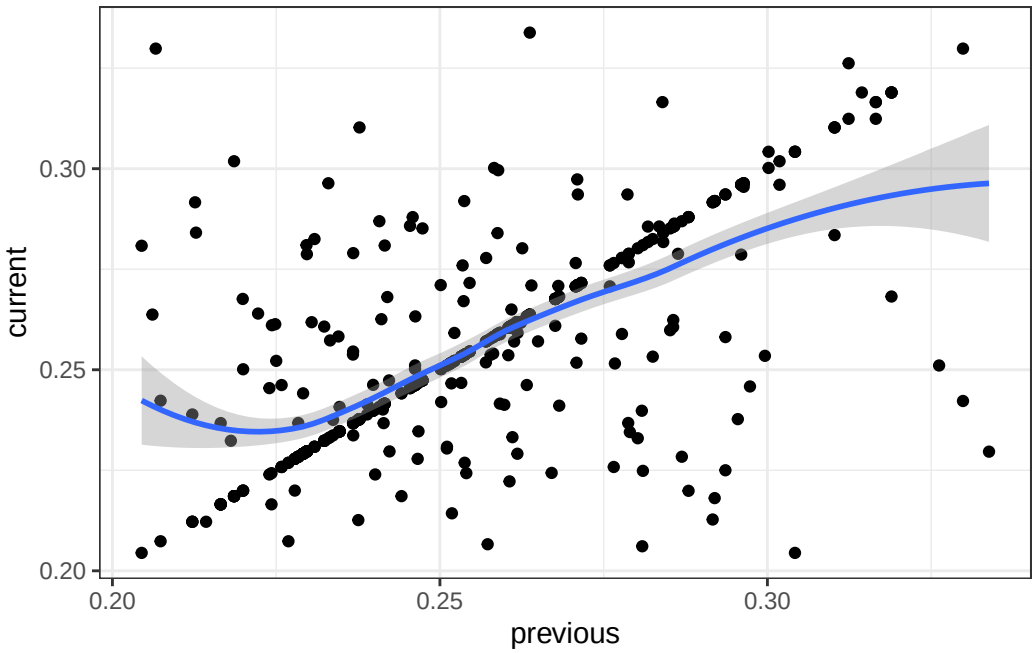


Figure 15.5: Scatterplot of observations at iteration s against observations at iteration s - 1, with MCMC samples.

Compared to samples from `rbeta()`

```
rbeta_draws <- rbeta(num_draws, shape1 = 87.5, shape2 = 254)
ggplot(data.frame(current = rbeta_draws,
                  previous = lag(rbeta_draws)),
       aes(x = previous, y = current)) +
    geom_point() +
    geom_smooth()
```

```
`geom_smooth()` using method = 'gam' and formula = 'y ~ s(x, bs = "cs")'
```

```
Warning: Removed 1 rows containing non-finite values (`stat_smooth()`).
```

```
Warning: Removed 1 rows containing missing values (`geom_point()`).
```

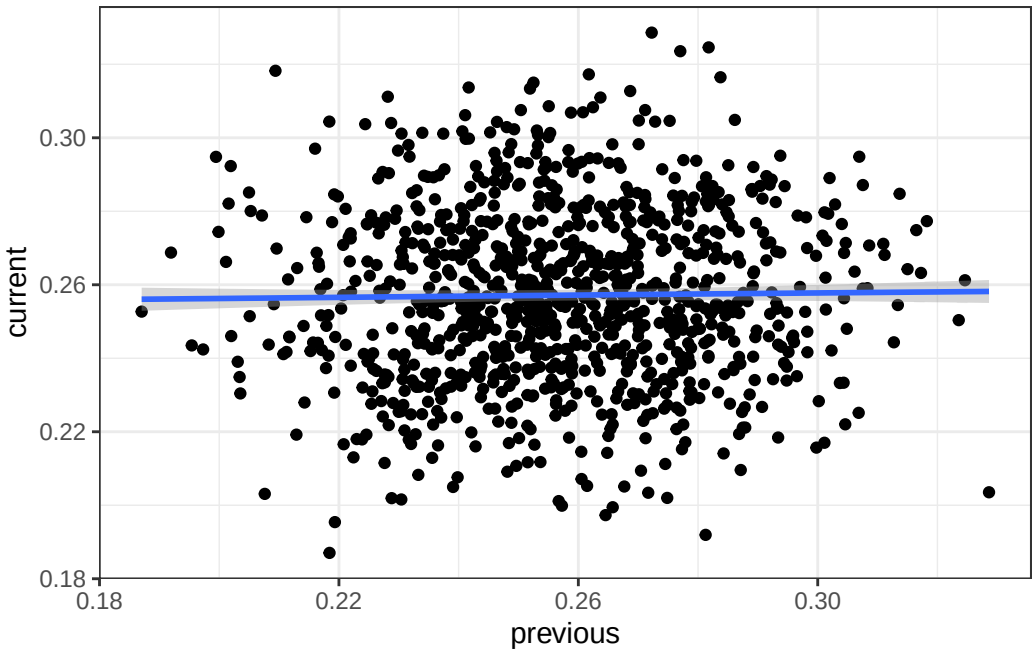


Figure 15.6: Scatterplot of observations at iteration s against observations at iteration s - 1, with independent Monte Carlo samples.

You can get the autocorrelation function plot (autocorrelation plot on the right):

```
mcmc_combo(data.frame(theta = th_draws),
    combo = c("trace", "acf")
)
```

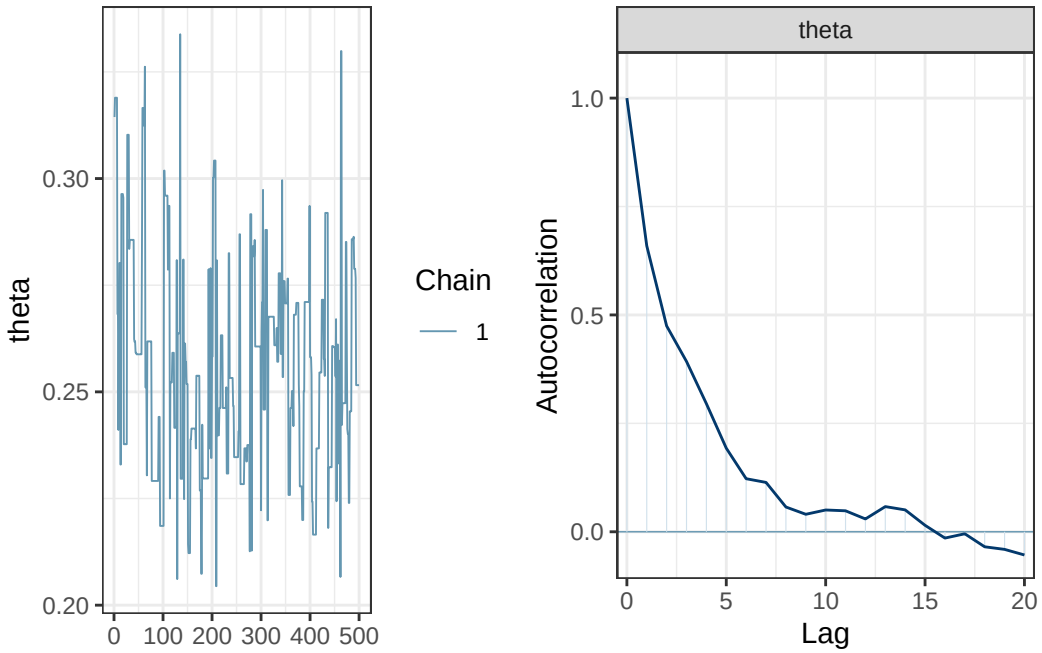


Figure 15.7: Trace plots and autocorrelation plots with MCMC samples.

which shows substantial autocorrelations until about nine iterations apart.

15.5.5 Acceptance Rate

When using the Metropolis algorithm, you want to monitor the acceptance rate and ensure it is within the optimal range. If you accept almost every time, it likely means that, in each iteration, the chain only jumps a tiny step (so that the acceptance ratio is close to 1 every time). As such, the chain will take many iterations to reach other regions of the stationary distribution, and consecutive draws are very strongly correlated. On the other hand, if the acceptance rate is very low, the chain gets stuck in the same location for many iterations before moving to a different state. For the basic Metropolis algorithm with one parameter, an optimal acceptance rate would be something between 40% to 50%.

> For Hamiltonian Monte Carlo to be discussed later, the optimal acceptance rate would be much higher, from 80% to 99%, or even higher.

```
# Acceptance rate
sum(num_accepted) / length(th_draws)
```

```
[1] 0.306
```

15.5.6 Effective sample size (ESS)

When iterations are dependent, each iteration contains overlapping information with the previous iterations. In other words, when one gets 500 dependent draws from the posterior, it only contains information equivalent to < 500 independent draws. The ESS quantifies the actual amount of information, so a chain with ESS $= n$ will contain roughly the same information as in n independent draws. In general, we want ESS to be at least 400 for the general purpose of summarizing the posterior. You can obtain ESS using the `posterior::ess_basic()` function:

```
ess_basic(th_draws)
```

```
[1] 84.42518
```

which is not sufficient for summarizing the posterior.

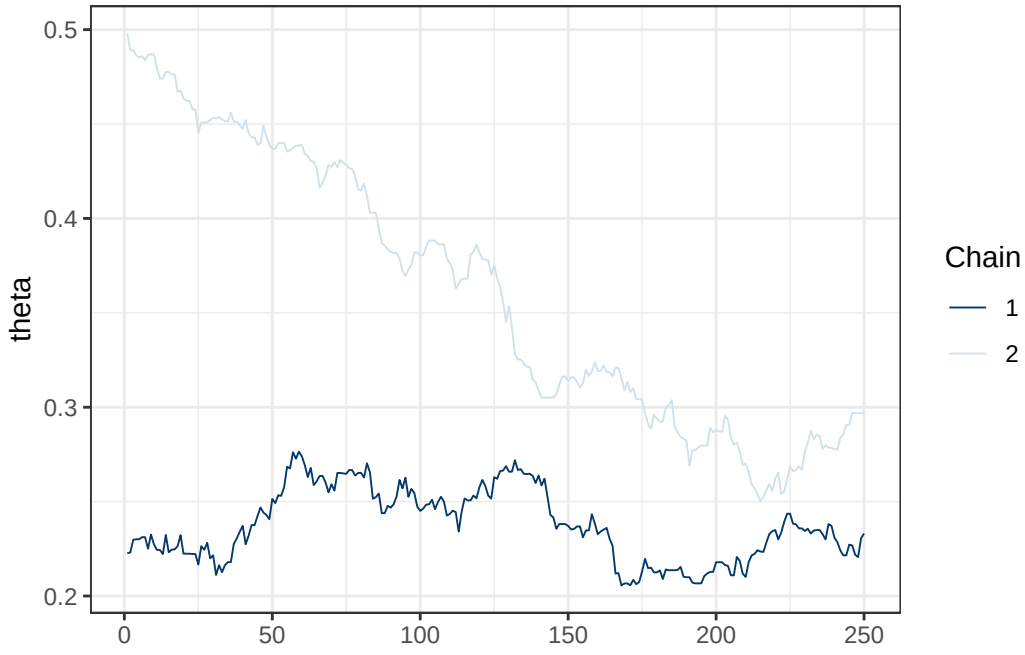
15.5.7 Multiple Chains

Because each state in a Markov chain depends on the previous states, the starting value(s) can influence the sampled values. Remember, in complex problems, one does not know how the posterior distributions would look. One solution to check the sensitivity to the starting value(s) is to use multiple chains, each with different starting values.

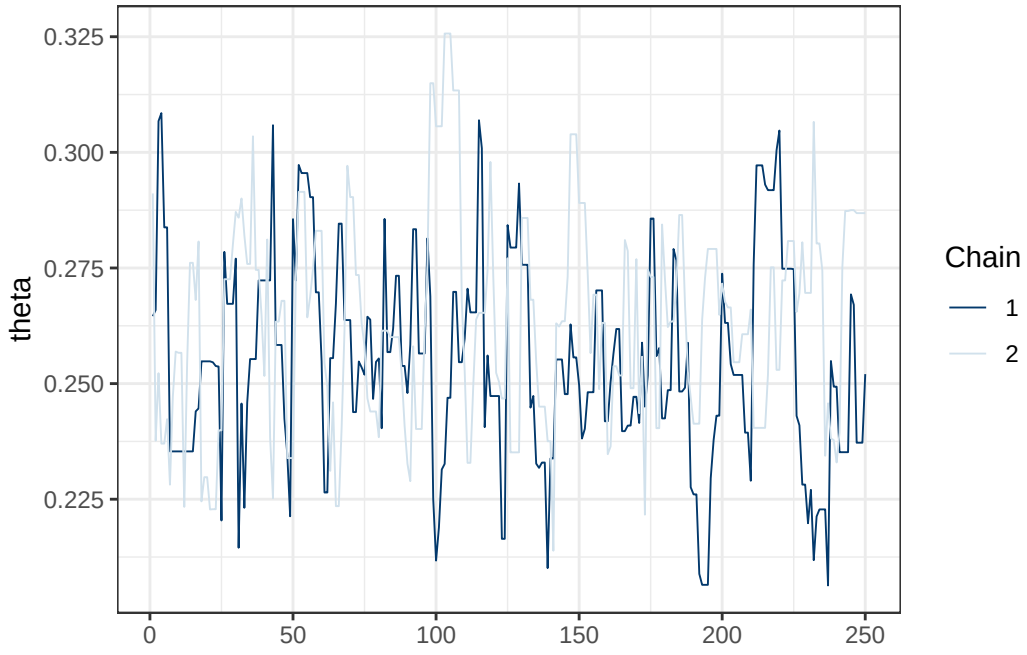
> If multiple chains sample the same target distribution, they should be *mixing* well, meaning they cross each other in a trace plot.

Below are examples of two chains with good/poor mixing.

15.5.8 Poor Mixing



15.5.9 Better Mixing



15.5.10 Full R Code With More Iterations

```
num_yes <- 86
num_obs <- 86 + 252
# Define a function to compute values proportional to p(y | th) * p(th)
prior_times_lik <- function(th) {
    # Return 0 if th is out of range
    if (th < 0 || th > 1) return(0)
    pth <- dbeta(th, shape1 = prior_a, shape2 = prior_b)
    py_given_th <- th ^ num_yes * (1 - th) ^ (num_obs - num_yes)
    pth * py_given_th
}
# Define a function for generating data from the proposal distribution
generate_proposal <- function(th, sd = 0.1) {
    rnorm(1, mean = th, sd = sd)
}
# Initialize the Metropolis algorithm
set.seed(2037)  # set the seed for reproducibility
num_chains <- 2
```

```
num_draws <- 10000
num_warmup <- num_draws / 2
th_all_draws <- matrix(NA, nrow = num_draws, ncol = num_chains)
th_all_draws[1, ] <- c(0.1, 0.9)  # starting value
# counter for tracking acceptance rate
num_accepted <- rep(0, num_chains)
for (s in seq_len(num_draws - 1)) {
    for (j in seq_len(num_chains)) {
        current_th <- th_all_draws[s, j]
        # Generate proposal
        proposed_th <- generate_proposal(current_th, sd = 0.05)
        # Compute acceptance probability
        prob_accept <- min(
            1,
            prior_times_lik(proposed_th) /
                prior_times_lik(current_th)
        )
        # Determine whether to make the jump
        if (runif(1) < prob_accept) {
            th_all_draws[s + 1, j] <- proposed_th
            if (s + 1 >= num_warmup) {
                num_accepted[j] <- num_accepted[j] + 1
            }
        } else {
            th_all_draws[s + 1, j] <- current_th
        }
    }
}
# Save the draws after warm-up
th_draws <- th_all_draws[- (1:num_warmup), ]
```

As shown below, the MCMC draws approximate the posterior distribution reasonably well.

```
ggplot(data.frame(th = c(th_draws)), aes(x = th)) +
    # Plot histogram, with density on y axis
    geom_histogram(binwidth = 0.0025, aes(y = after_stat(density))) +
    # Overlay the theoretical Beta distribution
    stat_function(
        fun = dbeta,
        args = list(
            shape1 = 86 + prior_a,
            shape2 = 252 + prior_b
```

```
        ),
        col = "red"
    ) +
    labs(x = expression(theta))
# Acceptance rate
sum(num_accepted) / length(th_draws)
```

```
[1] 0.4889
```

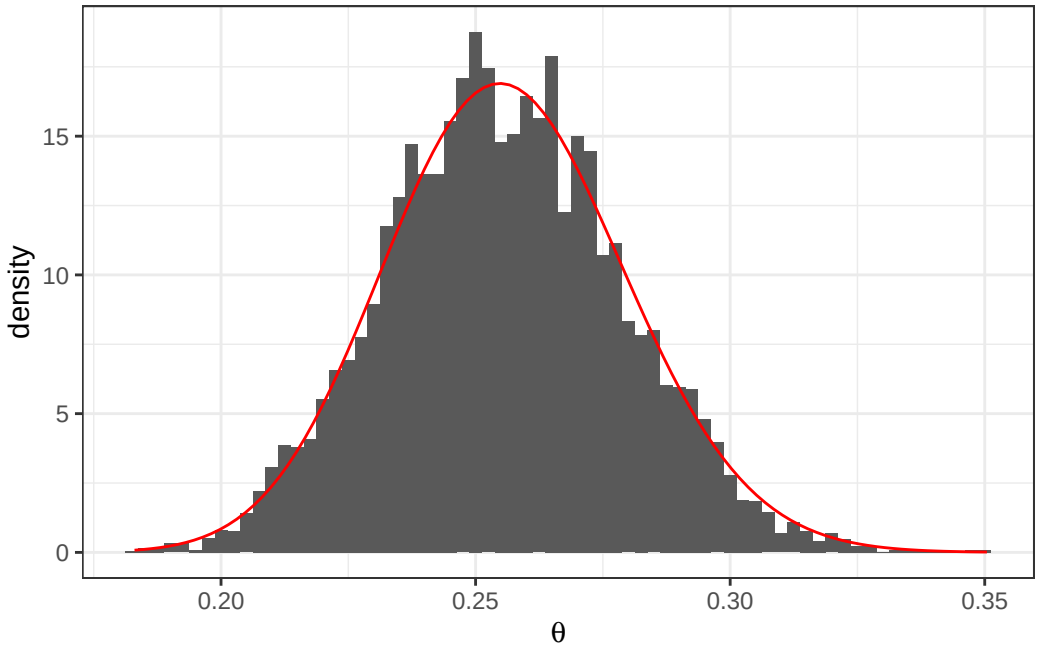


Figure 15.8: Comparing MCMC samples to the theoretical posterior distribution for the Metro example.

15.5.11 Convergence Check

The goal of checking for convergence of MCMC samples is to ensure that the draws are *representative* samples of the posterior distribution, and that they contain *sufficient information* to describe it. Convergence can be considered in two aspects:

- *Mixing*
- *Stationarity*

We'll see some tools in R for diagnosing convergence.

15.5.11.1 Trace Plot

Multiple chains have good *mixing* if they frequently cross each other. If two chains iterate in different regions of the posterior distribution and never cross each other, they don't mix well. You can check mixing using the trace plot. The below graph shows the two chains mixing well.

```
# Convert to `draws_array` object to use the following functions
th_draws_array <- draws_array(
    theta = th_draws,
    .nchains = num_chains
)
# Trace plot
mcmc_trace(th_draws_array)
```

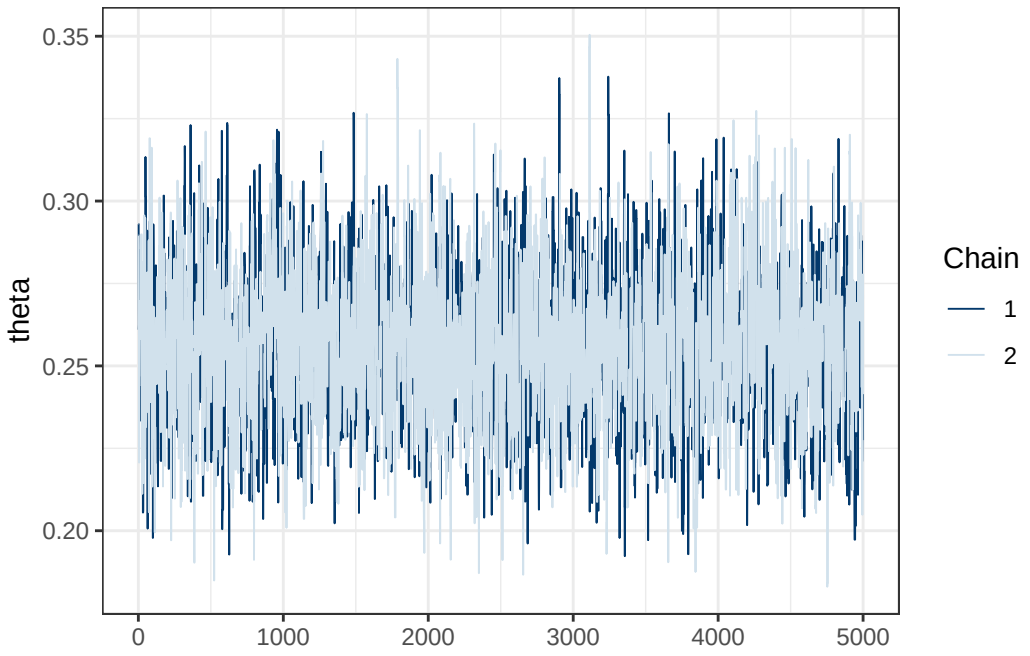


Figure 15.9: Trace plots of multiple chains.

15.5.11.2 Rank Histograms

Another useful tool is the rank histogram, recently proposed by Vehtari et al. (2021). The idea is first to convert the posterior values into ranks and then look at the distributions of the ranks across iterations. If the chains mix well and all explore the same target distribution, the

average rank in an interval of iterations should be similar for every chain. Therefore, the rank histogram should show something close to a uniform distribution, as shown below:

```
# Rank plot
mcmc_rank_hist(th_draws_array)
```

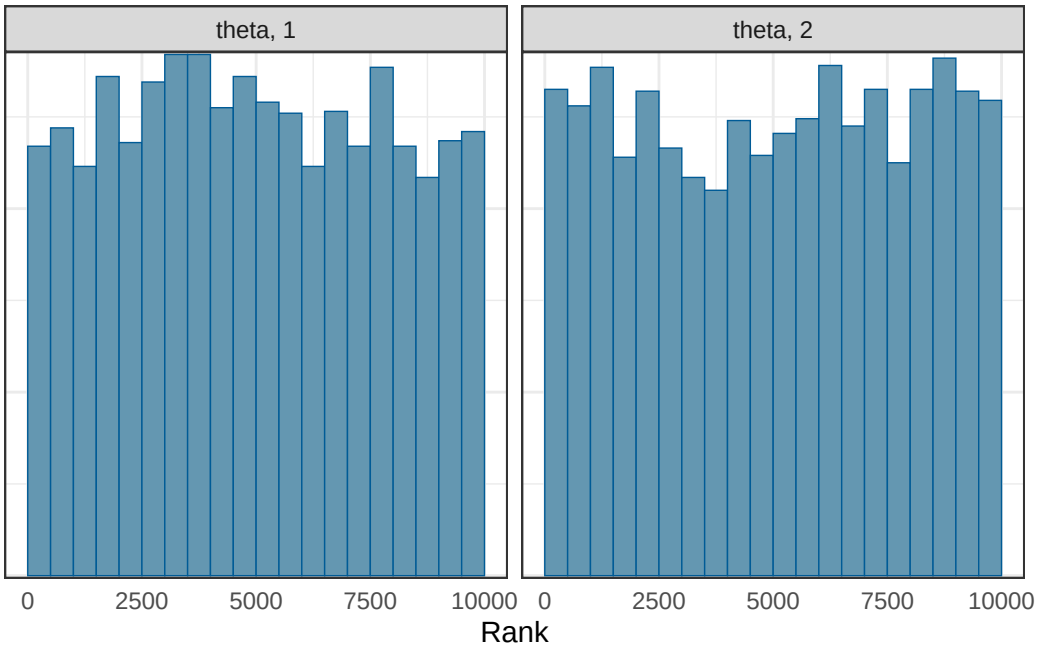


Figure 15.10: Rank histograms of two chains.

15.5.11.3 $\hat{R}$

A commonly used index in diagnosing convergence is $\hat{R}$, also called the potential scale reduction factor, proposed by Gelman & Rubin (1992) and later extended for multivariate distributions by Brooks & Gelman (1998). Vehtari et al. (2021) further improved it to account for unequal variances across chains using rank normalization and folding. $\hat{R}$ measures the ratio of the total variability combining multiple chains to the within-chain variability. When the Markov chains converge, each chain is based on the same posterior distribution, and they should have the same variance. Therefore, if the chains converge, there should be no between-chain variability, so $\hat{R}$ should be very close to 1.0.[1]

[1]Note that in Stan, $\hat{R}$ is computed by splitting each chain into half. So if you have two chains, $\hat{R}$ will be based on four groups.

While in older literature, the cutoff of $\hat{R} < 1.1$ was usually used, **Vehtari et al. (2021) recommended a safer criterion of $\hat{R} < 1.01$.**

You can use the `summarize_draws()` function from the `posterior` package, which provides summary statistics of the posterior and some convergence diagnostics.

```
summarize_draws(th_draws_array)
```

```
# A tibble: 1 x 10
  variable  mean median     sd    mad    q5   q95  rhat ess_bulk ess_tail
  <chr>    <dbl>  <dbl>  <dbl>  <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
1 theta    0.256  0.255 0.0233 0.0236 0.218 0.295  1.00    2368.    2465.
```

The numbers `ess_bulk` and `ess_tail` are two ways to compute ESS. `ess_bulk` says more about the center region of the posterior and is useful when assessing how accurate the mean of the posterior draws approximates the true posterior mean (or the posterior median). `ess_tail` is most useful for assessing how accurate the sample quantiles in the tail areas (e.g., 1st, 95th) approximate the true posterior quantiles. For example, the accuracy of the credible intervals would require a large `ess_tail`.

As recommended by Vehtari et al. (2021),

> ESS should be at least 400 for $\hat{R}$ to be useful in diagnosing convergence.

16 Gibbs Sampling

In the previous note, we learn about the Metropolis algorithm. While the algorithm is very general and easy to implement, it is inefficient because the effective sample size is only about 1/4 of the actual number of draws for a one-parameter model. The Metropolis algorithm usually gets stuck when there are multiple parameters. Therefore, until about 2010, many Bayesian analyses relied on a more efficient algorithm—the Gibbs sampler. The Gibbs sampler uses conjugate priors on the *conditional posterior* distributions to get proposal values with high acceptance probability (it's 100%). We'll also see the *normal* model with two parameters: mean and variance.

16.1 Data

The data set was from one of the studies reported in a paper published in *Psychological Science* in 2014. The authors compared participants' performance on conceptual questions after taking notes either using laptops or notebooks ("longhand"). Let's import the data directly from the Open Science Framework (https://osf.io/qrs5y/):

```
# Use haven::read_sav() to import SPSS data
nt_dat <- read_sav("https://osf.io/qrs5y/download")
```

One outcome variable the authors studied is the number of words in participants' notes. Here are the distributions of the variable `wordcount` for the two conditions (0 = laptop, 1 = longhand).

```
ggplot(nt_dat, aes(x = wordcount)) +
    geom_histogram(bins = 10) +
    facet_wrap(~ condition)
```

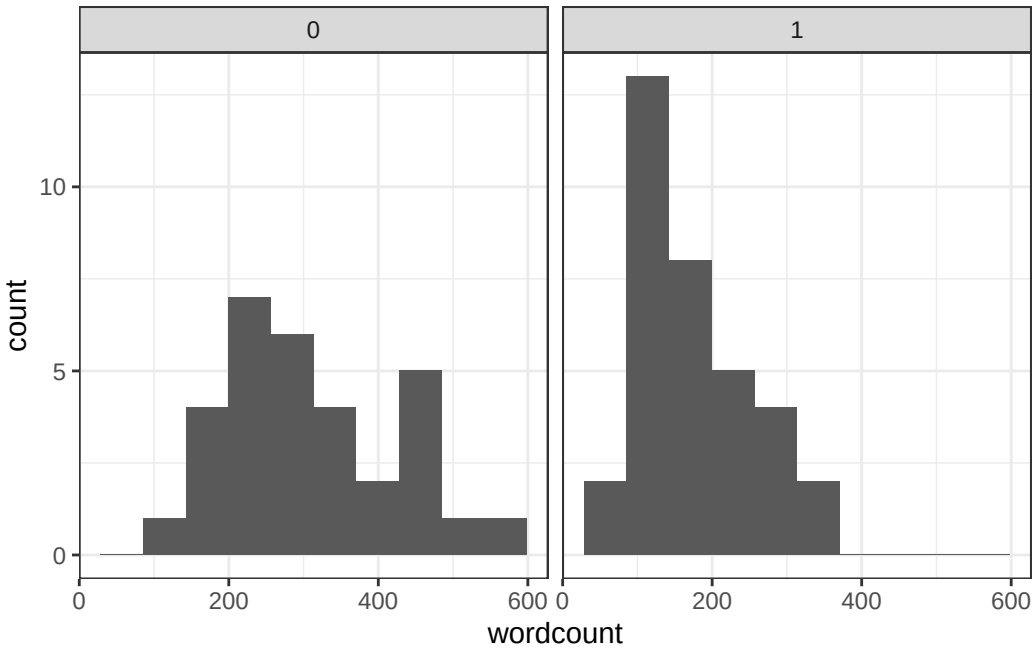


Figure 16.1: Number of words by experimental conditions.

The variable is somewhat skewed. We'll focus on the control group (`laptop`) first, so let's create a variable for that data. We'll also divide the count by 100.

> Often, in Bayesian analyses (and in frequentist ones as well), computer algorithms work best when the variables do not contain too many digits. In my experience, scaling variables to a range of -10 to 10 usually helps the computation.

```
(wc_laptop <- nt_dat$wordcount[nt_dat$condition == 0] / 100)
```

```
 [1] 4.20 4.61 5.72 4.47 3.34 1.27 2.65 3.40 2.43 2.55 2.73 2.26 3.16 2.47 3.25
[16] 1.67 4.49 4.77 1.67 5.19 3.00 2.98 1.59 2.23 4.39 2.29 1.52 2.13 3.11 3.82
[31] 2.62
```

16.2 The Normal Model

While only an approximation, the normal distribution is a popular choice for modeling variables that are relatively symmetric and have more than a few discrete values. The normal distribution has two parameters; in some situations, there are advantages to choosing a specific

parameterization. With the Gibbs sampler, we will parameterize it using the mean parameter, μ, and the variance parameter, σ^2. The model is

$$\text{wc\_laptop}_i \sim N(\mu, \sigma^2)$$

Note again that there are no subscripts to μ and σ^2, indicating exchangeability assumption.

16.3 Conjugate (Actually "Semiconjugate") Priors

It can be shown that when σ^2 is known, a conjugate prior to μ is a normal prior, meaning that the posterior is also normal. However, when σ^2 is unknown, the prior distribution needs to be a joint distribution of two parameters.

What we can do is consider the conditional distribution of a parameter. So instead of drawing a posterior sample from the joint posterior, $P(\mu, \sigma^2 \mid y)$, we consider each parameter separately, by drawing from the conditional of $P(\sigma^2 \mid \mu^{(s-1)}, y)$ first, and then from $P(\mu \mid \sigma^2 = {\sigma^2}^{(s)}, y)$ with ${\sigma^2}^{(s)}$ being the previous draw, and then continuing with $P(\sigma^2 \mid \mu^{(s)}, y)$. The advantage of doing so is that we can use a conjugate normal prior for μ when conditioning on σ^2. We also have a conjugate prior for σ^2 when conditioning on μ, which will be discussed later. Here is how the algorithm works:

1. Set an initial value for $\sigma^2(1)$
2. At iteration s, given sample ${\sigma^2}^{(s-1)}$, sample $\mu^{(s)}$ from the conditional posterior, $P(\mu \mid {\sigma^2}^{(s)}, y)$
3. Given $\mu^{(s)}$, sample ${\sigma^2}^{(s)}$ from the conditional posterior, $P(\sigma^2 \mid \mu^{(s-1)}, y)$
4. Repeat steps 2 and 3

It can be shown that with this *Gibbs* algorithm, the posterior draws will be from the joint posterior of $P(\mu, \sigma^2 \mid y)$.

Below I provide more details on conjugacy. The actual detail is not the most important for this class because, in practice, the software will likely handle the computation. You may want to, however, pay attention to the suggested meanings of the hyperparameters:

- μ_0: Prior mean
- τ_0^2: Prior variance (i.e., uncertainty) of the mean
- ν_0: Prior sample size for the variance
- σ_0^2: Prior expectation of the variance

16.3.1 For $\mu \mid \sigma^2$

A conjugate prior for $\mu \mid \sigma^2$ is $\mu \sim N(\mu_0, \tau_0^2)$, which gives the posterior conditional

$$\mu \mid \sigma^2, y \sim N(\mu_n, \tau_n^2),$$

where

$$\begin{aligned} \tau_n^2 &= \left(\frac{1}{\tau_0^2} + \frac{n}{\sigma^2} \right)^{-1} \\ \mu_n &= \tau_n^2 \left(\frac{\mu_0}{\tau_0^2} + \frac{n\bar{y}}{\sigma^2} \right) \end{aligned},$$

with n being the number of observations in the data and $\bar{y}$ being the sample mean of the data. The hyperparameters, μ_0 and τ_0^2, can be considered the prior mean and the prior variance of the mean, with a smaller prior variance indicating a stronger prior.

> Note that n (instead of N) is used here for the sample size to avoid confusion with the normal distribution.

16.3.2 For $\sigma^2 \mid \mu$

A conjugate prior for $\mu \mid \sigma^2$ is from the Inverse-Gamma family: $\sigma^2 \sim \text{Inv-Gamma}(\nu_0/2, \nu_0\sigma_0^2/2)$. You usually only hear about the Inverse-Gamma distribution in Gibbs sampling, mainly because of conjugacy. As the name suggested, the Inverse-Gamma distribution is the distribution of the *inverse* of a variable that follows a Gamma distribution. So we also write $1/\sigma^2 \sim \text{Gamma}(\nu_0/2, \nu_0\sigma_0^2/2)$.

> The Gamma distribution used here is also called a scaled χ^2 distribution by some authors, with $\text{Gamma}(\nu_0/2, \nu_0\sigma_0^2/2)$ being the same as $\chi^2(\nu_0, \sigma_0^2)$.

The posterior is also Inverse-Gamma, with

$$1/\sigma^2 \mid \mu^2, y \sim \text{Gamma}(\nu_n/2, \nu_n\sigma_n^2[\mu]/2),$$

where

$$\begin{aligned} \nu_n &= \nu_0 + n \\ \sigma_n^2(\mu) &= \frac{1}{\nu_n} \left[\nu_0\sigma_0^2 + (n-1)s_y^2 + \sum(\bar{y} - \mu)^2 \right] \end{aligned},$$

with $s_y^2 = \sum(y_i - \bar{y})^2/(n-1)$ being the sample variance of y. The hyperparameters, ν_0 and σ_0^2, can be considered the prior degrees of freedom and prior expected value of variance; ν_0 can be roughly considered as the prior sample size.

16.4 Prior, Model, and Posterior

We will use some weakly informative priors, written in the following equations:

Model:

$$\text{wc\_laptop}_i \sim N(\mu, \sigma^2)$$

Prior:

$$\mu \sim N(5, 10^2)$$
$$1/\sigma^2 \sim \text{Gamma}(1/2, [1][1]/2)$$

The priors are very weak. We also assume that the priors are independent, which is commonly the case. Here are some simulated data from these priors:

```
set.seed(2259)
num_draws <- 100
mu <- rnorm(num_draws, mean = 5, sd = 10)
inv_sigma2 <- rgamma(num_draws,
                     shape = 1 / 2, rate = 1 / 2)
num_obs <- length(wc_laptop)
# Initialize an S by N matrix to store the simulated data
y_tilde <- matrix(NA,
                  nrow = num_draws,
                  ncol = num_obs)
for (s in seq_len(num_draws)) {
    mu_s <- mu[s]
    sigma2_s <- 1 / inv_sigma2[s]
    y_tilde[s, ] <- rnorm(num_obs, mean = mu_s, sd = sqrt(sigma2_s))
}
# Plot the simulated data based on priors
ppd_dens_overlay(y_tilde)
```

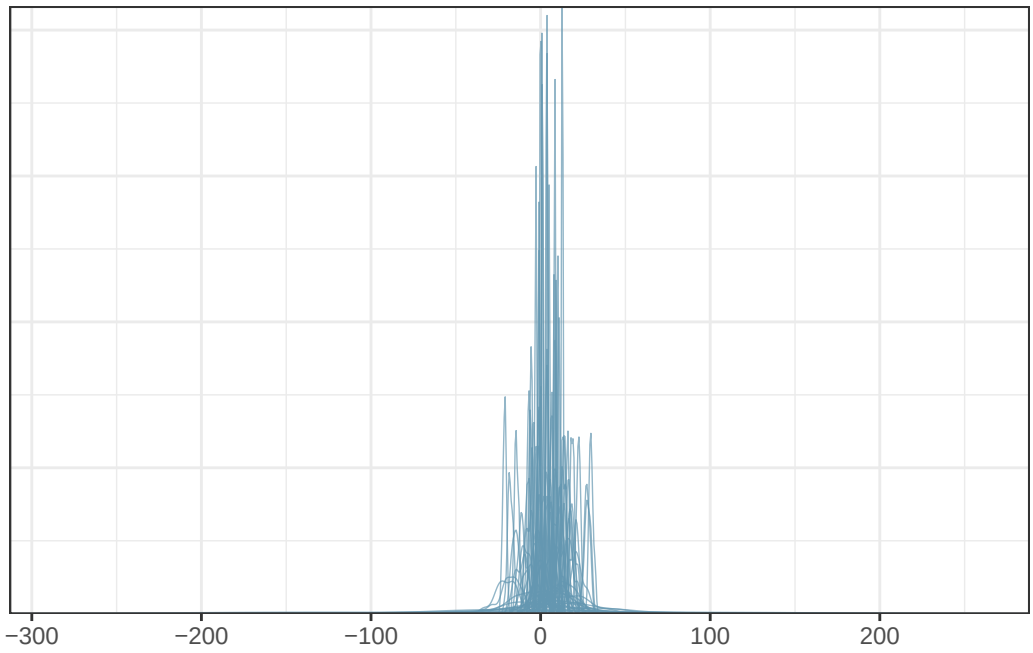


Figure 16.2: Prior predictive distributions.

The plot shows the types of data one can get. One can do better by avoiding the negative values if desired.

16.5 The Gibbs Sampler

The following is the full Gibbs sampler for the above normal model.

```
# Sufficient statistics from data
ybar <- mean(wc_laptop)  # sample mean
s2y <- var(wc_laptop)  # sample variance
n <- length(wc_laptop)  # sample size
# Hyperparameters
mu_0 <- 5
sigma2_0 <- 1
tau2_0 <- 10^2
nu_0 <- 1
# Initialize the Gibbs sampler
set.seed(2120)
num_draws <- 10000
```

```
num_warmup <- num_draws / 2
num_chains <- 2
# Initialize a 3-D array (S x # chains x 2 parameters)
post_all_draws <- array(
    dim = c(num_draws, num_chains, 2),
    dimnames = list(NULL, NULL, c("mu", "sigma2"))
)
# Step 1: starting values for sigma2
post_all_draws[1, 1, "sigma2"] <- 1  # for chain 1
post_all_draws[1, 2, "sigma2"] <- 3  # for chain 2
for (s in seq_len(num_draws - 1)) {
    for (j in seq_len(num_chains)) {
        sigma2_s <- post_all_draws[s, j, "sigma2"]
        # Step 2: Sample mu from the conditional posterior
        tau2_n <- 1 / (1 / tau2_0 + n / sigma2_s)
        mu_n <- tau2_n * (mu_0 / tau2_0 + n * ybar / sigma2_s)
        mu_new <- rnorm(1, mean = mu_n, sd = sqrt(tau2_n))
        post_all_draws[s + 1, j, "mu"] <- mu_new
        # Step 3: Sample sigma2 from the conditional posterior
        nu_n <- nu_0 + n  # you could put this line outside the loop
        sigma2_n <- 1 / nu_n *
            (nu_0 * sigma2_0 + (n - 1) * s2y + (ybar - mu_new)^2)
        sigma2_new <- 1 / rgamma(1,
            shape = nu_n / 2,
            rate = nu_n * sigma2_n / 2
        )
        post_all_draws[s + 1, j, "sigma2"] <- sigma2_new
    }
}
# Draws after warm-up
post_draws <- post_all_draws[- (1:num_warmup), , ]
```

16.6 Visualizing the Jumps

The plot below shows the jumps for 20 iterations in one chain, with the intermediate steps.

```
data.frame(
    mu = post_draws[c(1, rep(2:20, each = 2)), 1, "mu"],
    sigma2 = post_draws[c(rep(1:19, each = 2), 20), 1, "sigma2"]
) |>
```

```
    ggplot(aes(x = mu, y = sigma2)) +
    geom_path() +
    geom_point() +
    labs(x = expression(mu), y = expression(sigma^2))
```

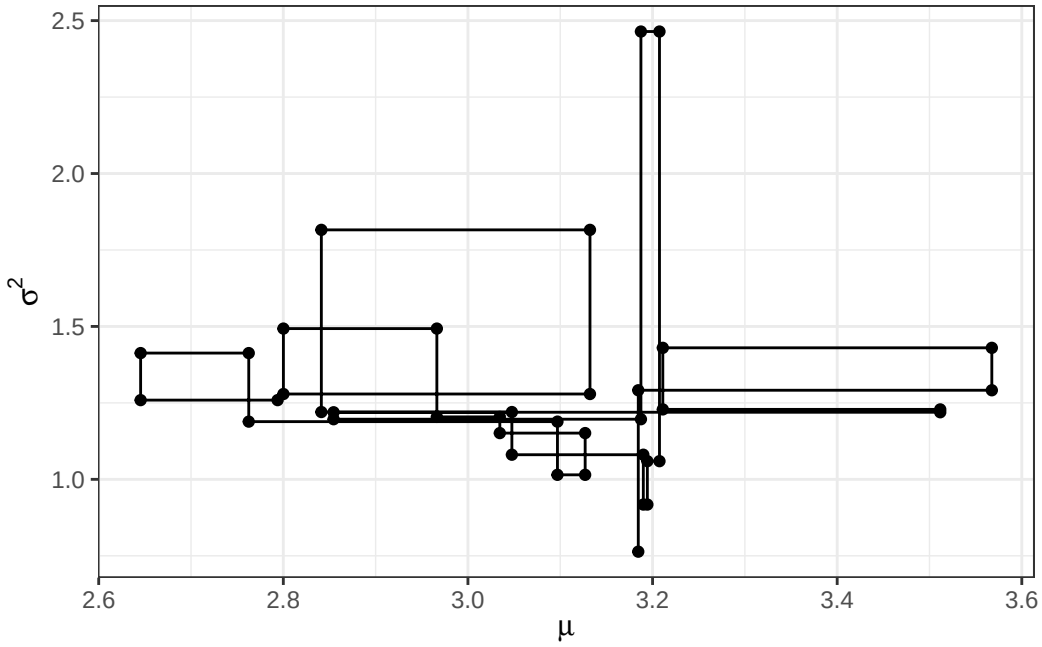
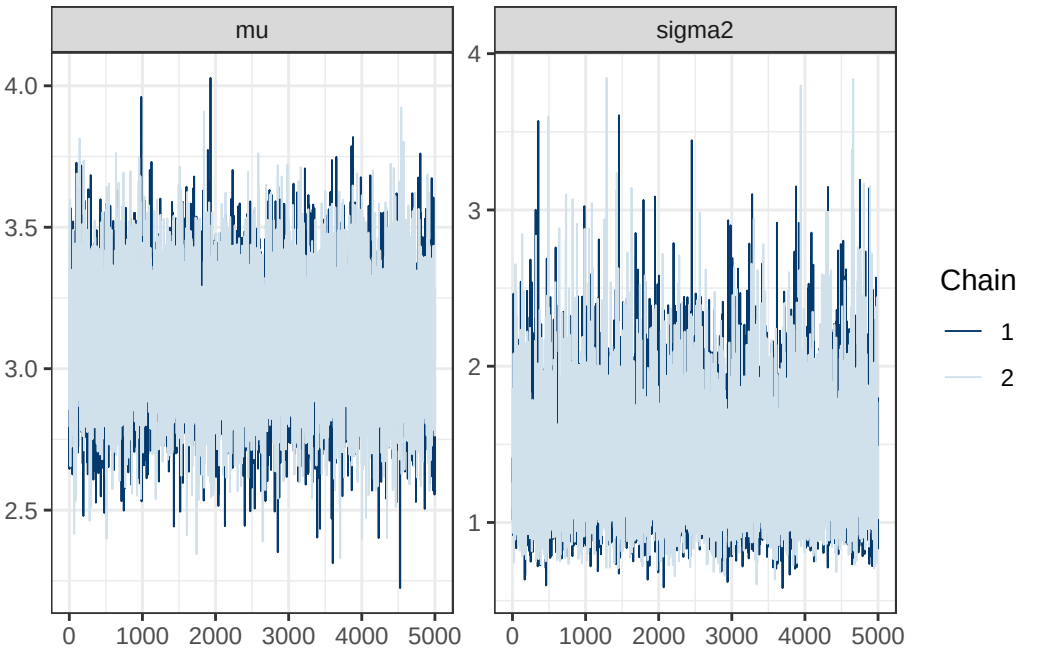


Figure 16.3: Jumps in the Gibbs sampler across iterations.

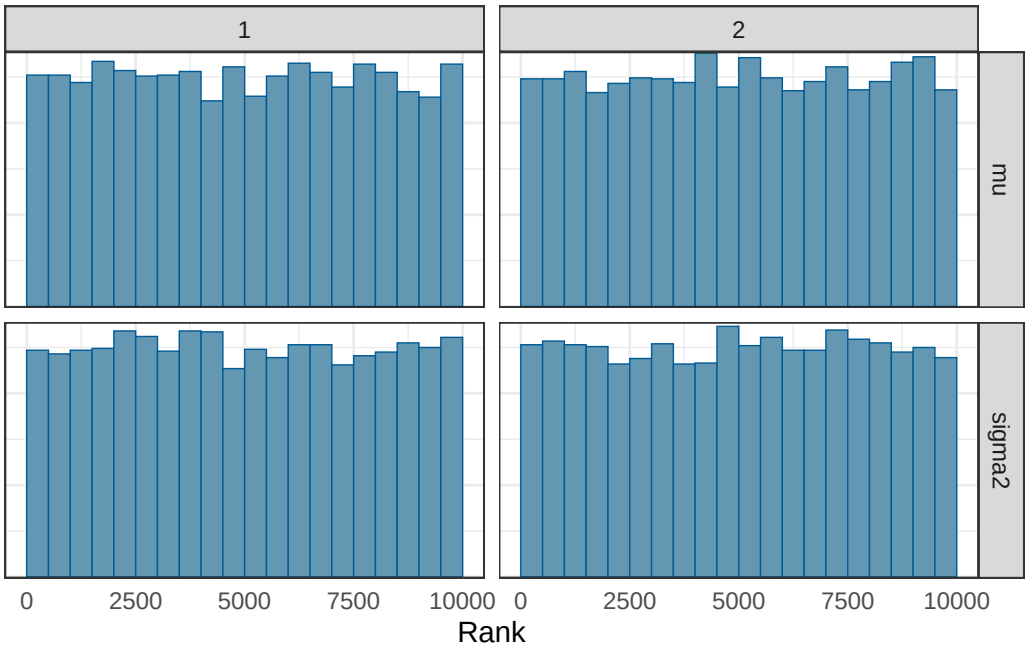
16.6.1 Convergence Check

```
# Convert to `draws_array` object to use the following functions
post_draws_array <- as_draws_array(post_draws)
# Trace plots
mcmc_trace(post_draws_array)  # good mixing
# Rank histograms
mcmc_rank_hist(post_draws_array)  # good mixing
```

```
# Summary (with rhat and ESS)
summarize_draws(post_draws_array) |>
    knitr::kable(digits = 2)
```



(a) Trace plots.



(b) Rank histograms.

Figure 16.4: Diagnostic plots for the Gibbs sampler.

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
mu	3.1	3.10	0.21	0.21	2.75	3.45	1	9928.49	9935.87
sigma2	1.4	1.33	0.38	0.34	0.90	2.11	1	10188.76	10135.62

As can be seen, the ESS is very high, indeed much higher than that obtained with the Metropolis algorithm.

16.6.2 Visualizing the Marginal and Joint Posterior

```
mcmc_areas(post_draws_array)  # marginal
```

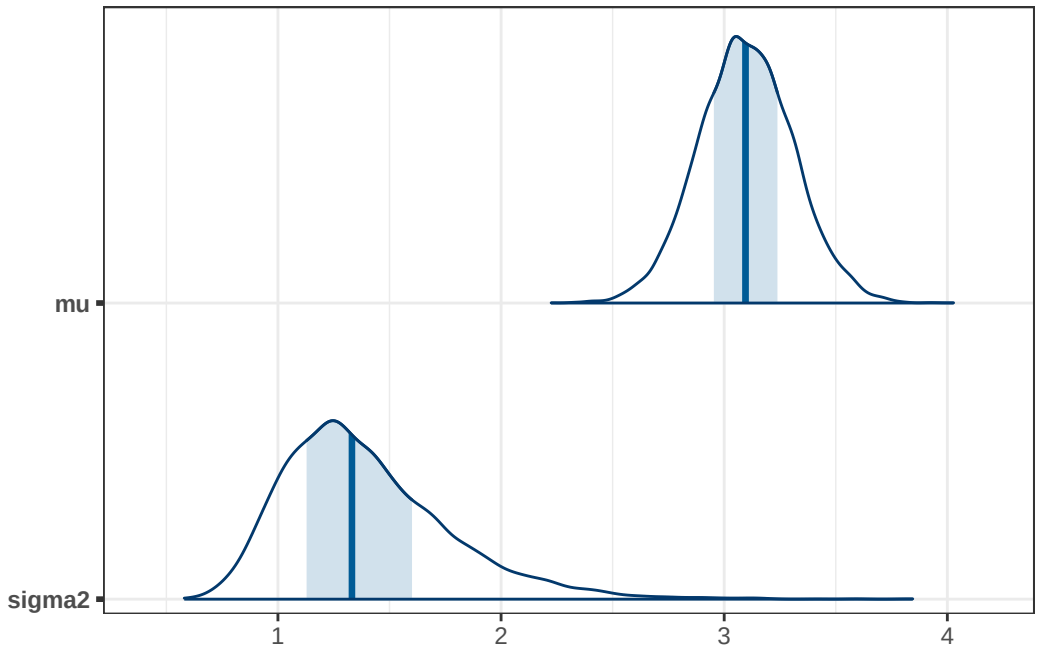


Figure 16.5: Marginal posterior distributions of model parameters.

```
mcmc_scatter(post_draws_array,  # joint
             size = 1, alpha = 0.3)  # make points smaller
```

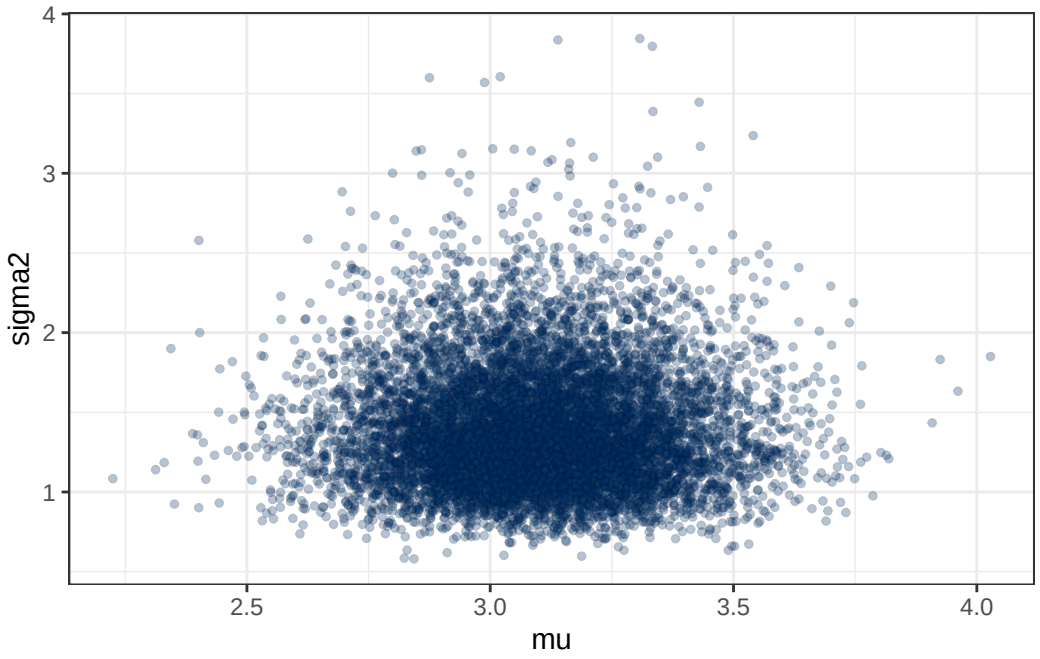


Figure 16.6: Joint posterior distributions of model parameters.

16.6.3 Posterior Predictive Check

We can check whether the simulated data based on the posterior look like the observed data.

```
num_draws <- 100
num_obs <- length(wc_laptop)
# Initialize an S by N matrix to store the simulated data
y_tilde <- matrix(NA,
                  nrow = num_draws,
                  ncol = num_obs)
for (s in seq_len(num_draws)) {
    mu_s <- post_draws[s, 1, "mu"]
    sigma2_s <- post_draws[s, 1, "sigma2"]
    y_tilde[s, ] <- rnorm(num_obs, mean = mu_s, sd = sqrt(sigma2_s))
}
# Plot the simulated data (in lighter lines)
# and the current data (in the darker line)
ppc_dens_overlay(wc_laptop, yrep = y_tilde)
```

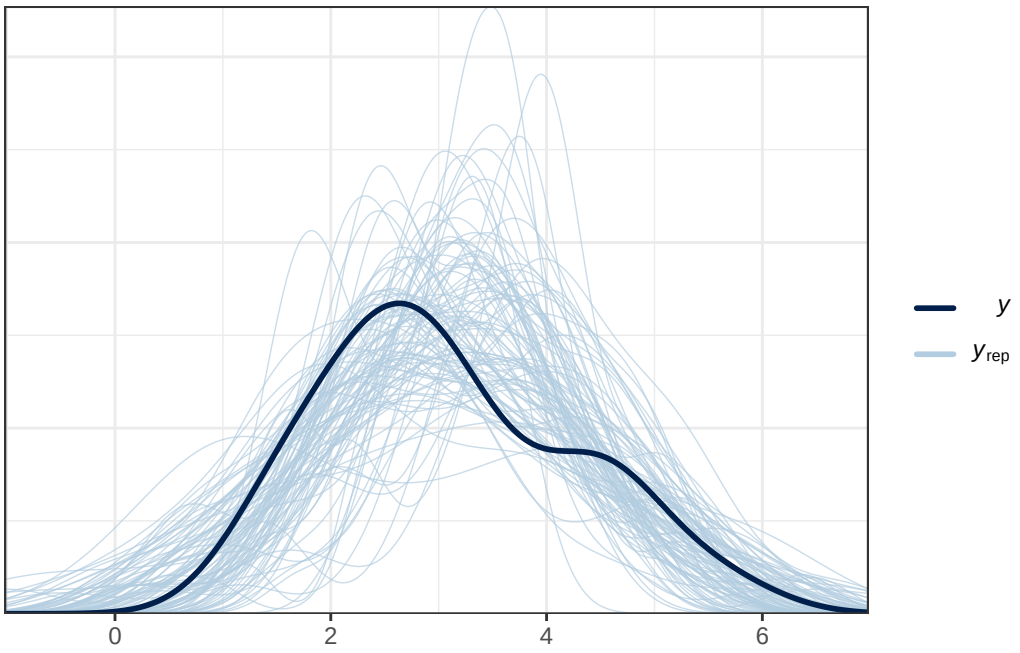


Figure 16.7: Posterior predictive check.

The simulated data are not too far off from the observed data. Just that the simulated data can also get negative values.

16.6.4 Limitations of Gibbs Sampler

The Gibbs sampler has been popular due to its computational efficiency for many problems. However, there are situations in which it works less well, such as when some parameters are highly correlated in the posterior, in which case a Gibbs sampler may get stuck. Another limitation is that Gibbs samplers require the use of conjugate priors. On the one hand, sometimes researcher beliefs may be better expressed in distributions other than the conjugate family. On the other hand, some conjugate families, such as the inverse Gamma distribution, are hard to work with and may yield suboptimal results in small sample situations.

16.7 The Metropolis-Hastings Algorithm

The Metropolis-Hastings (MH) algorithm is a generalization of the Metropolis algorithm, where it allows for more than one parameter and can use a proposal distribution that is not symmetric. It is less efficient than the Gibbs sampler but can accommodate non-conjugate prior distributions. Note that the proposal distribution needs to have the same dimension as the

posterior so that the proposal is a vector in the parameter space. For example, we need a bivariate proposal density with μ and σ.

Below is an example using a bivariate normal distribution for the proposal. While we can choose how correlated the variables are in the proposal, for simplicity, I just consider zero correlation and equal *SD* for both dimensions. I also parameterize the normal distribution by the mean, μ, and the standard deviation (instead of the variance), σ. The priors are:

$$\begin{aligned} \mu &\sim N(5, 10^2) \\ \sigma &\sim N^+(0, 3) \end{aligned},$$

where N^+ is a half-normal distribution because σ is non-negative. We'll revisit this for some later models.

Here is the code for the MH algorithm:

```
# Define a function to compute values proportional to p(y | th) * p(th)
prior_times_lik <- function(mu_sigma, y = wc_laptop) {
    mu <- mu_sigma[1]
    sigma <- mu_sigma[2]
    # Return 0 if sigma is out of range
    if (sigma < 0) return(0)
    # Joint prior = product of marginal priors
    pth <- dnorm(mu, mean = 5, sd = 10) *
        # half-normal is proportional to normal in [0, infinity)
        dnorm(sigma, sd = 3)
    # Likelihood
    py_given_th <- prod(dnorm(y, mean = mu, sd = sigma))
    pth * py_given_th
}
# Define a function for generating data from the proposal distribution
generate_proposal <- function(mu_sigma, sd = 0.1) {
    rnorm(length(mu_sigma), mean = mu_sigma, sd = sd)
}
# Initialize the Metropolis algorithm
set.seed(1051)  # set the seed for reproducibility
num_draws <- 10000
num_warmup <- num_draws / 2
num_chains <- 2
# Initialize a 3-D array (S x # chains x 2 parameters)
post_all_draws <- array(
    dim = c(num_draws, num_chains, 2),
    dimnames = list(NULL, NULL, c("mu", "sigma"))
)
```

```r
# Step 1: starting value
post_all_draws[1, 1, ] <- c(1, 1)  # for chain 1
post_all_draws[1, 2, ] <- c(8, 3)  # for chain 2
# counter for tracking acceptance rate
num_accepted <- rep(0, num_chains)
for (s in seq_len(num_draws - 1)) {
    for (j in seq_len(num_chains)) {
        current_par <- post_all_draws[s, j, ]
        # Generate proposal vector
        proposed_par <- generate_proposal(current_par, sd = 0.1)
        # Compute acceptance probability
        prob_accept <- min(
            1,
            prior_times_lik(proposed_par) /
                prior_times_lik(current_par)
        )
        # Determine whether to make the jump
        if (runif(1) < prob_accept) {
            post_all_draws[s + 1, j, ] <- proposed_par
            if (s + 1 >= num_warmup) {
                num_accepted[j] <- num_accepted[j] + 1
            }
        } else {
            post_all_draws[s + 1, j, ] <- current_par
        }
    }
}
# Draws after warm-up
post_draws <- post_all_draws[- (1:num_warmup), , ]
# Acceptance rate
sum(num_accepted) / length(post_draws)
```

```
[1] 0.3638
```

16.7.1 Convergence

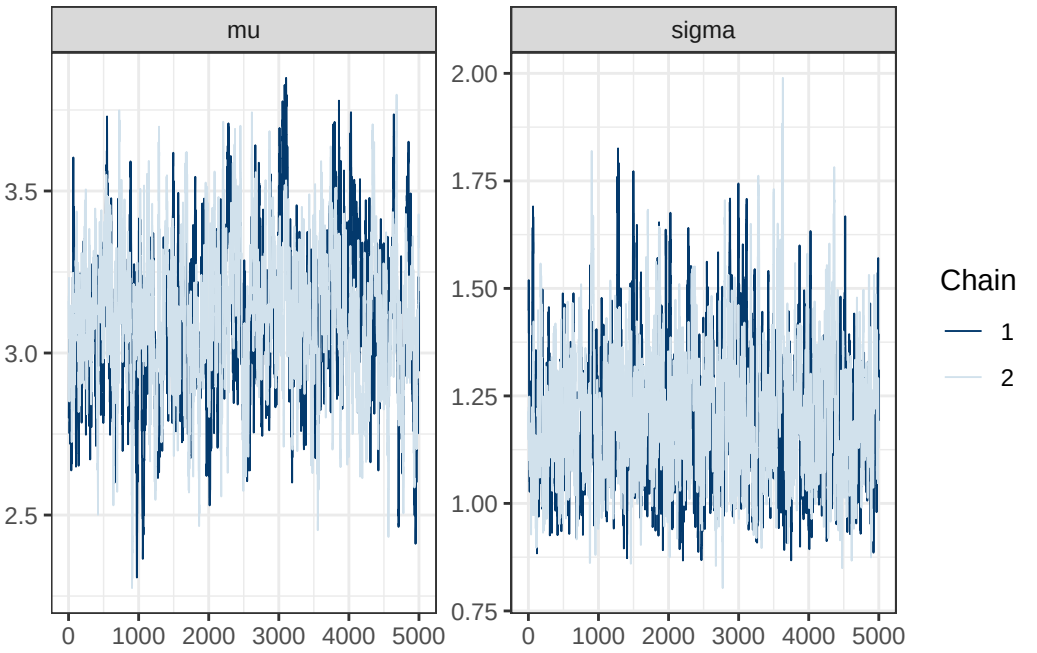
```r
# Convert to `draws_array` object to use the following functions
post_draws_array <- as_draws_array(post_draws)
# Trace plots
mcmc_trace(post_draws_array)  # good mixing
```

```r
# Rank histograms
mcmc_rank_hist(post_draws_array)  # good mixing
```

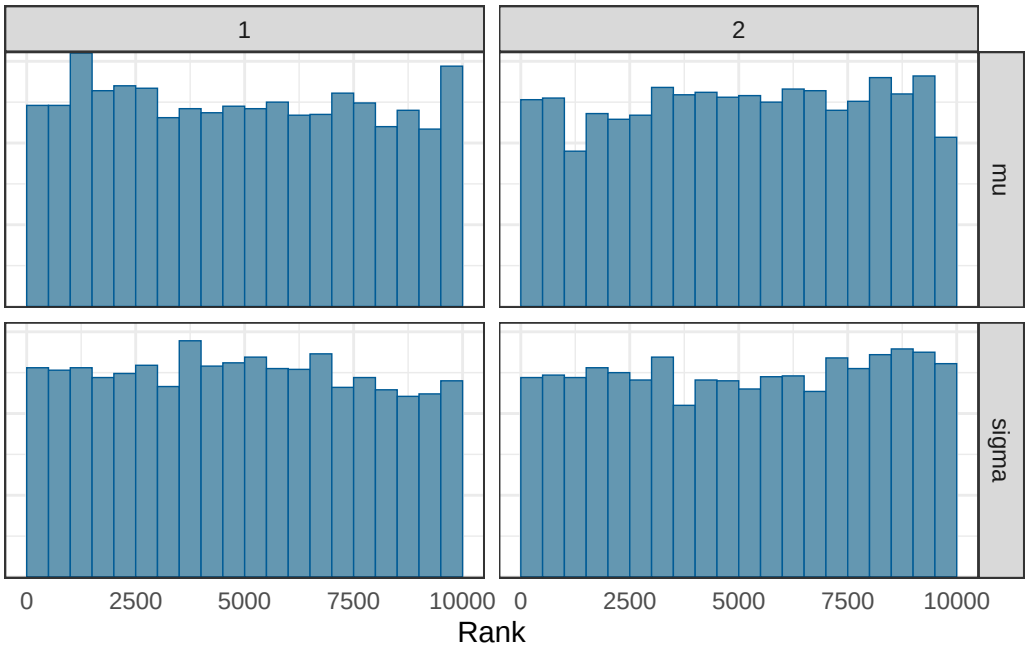
```r
# Summary (with rhat and ESS)
summarize_draws(post_draws_array) |>
    knitr::kable(digits = 2)
```

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
mu	3.11	3.11	0.23	0.23	2.72	3.49	1.01	304.66	426.00
sigma	1.20	1.19	0.15	0.15	0.98	1.48	1.00	694.50	733.81

As can be seen, ESS is much lower, so more iterations will be needed with MH.



(a) Trace plots.



(b) Rank histograms.

Figure 16.8: Diagnostic plots for the MH sampler.

17 Hamiltonian Monte Carlo

A more recent development in MCMC is the development of algorithms under the umbrella of *Hamiltonian Monte Carlo* or *hybrid Monte Carlo* (HMC). The algorithm is a bit complex, and my goal is to help you develop some intuition of the algorithm, hopefully, enough to help you diagnose the Markov chains.

1. It produces simulation samples that are much less correlated, meaning that if you get 10,000 samples from Metropolis and 10,000 samples from HMC, HMC generally provides a much higher effective sample size (ESS).
2. It does not require conjugate priors
3. When there is a problem in convergence, HMC tends to raise a clear red flag, meaning it goes really, really wrong.

So now, how does HMC work? First, consider a two-dimensional posterior below, which is the posterior of (μ, σ^2) from a normal model.

```
ybar <- 3.096129
s2y <- 1.356451
n <- 31
# Hyperparameters
mu_0 <- 5
sigma2_0 <- 1
kappa_0 <- 1 / 10^2
nu_0 <- 1
# Joint log density
lp_mu_sigma <- function(mu, sigma2) {
    kappa_n <- kappa_0 + n
    mu_n <- (kappa_0 * mu_0 + n * ybar) / kappa_n
    nu_n <- nu_0 + n
    sigma2_n <- (nu_0 * sigma2_0 + (n - 1) * s2y +
        kappa_0 * n / kappa_n * (ybar - mu_0)^2) / nu_n
    log_dens <- -(mu - mu_n)^2 / 2 / sigma2 * kappa_n +
        (-nu_n / 2 - 1) * log(sigma2) +
        (-nu_n * sigma2_n / 2 / sigma2)
    log_dens[is.nan(log_dens)] <- -Inf
    log_dens
```

```
}

num_gridpoints <- 51
mu_grid <- seq(2, to = 4, length.out = num_gridpoints)
sigma2_grid <- seq(0.5, to = 4.5, length.out = num_gridpoints)
grid_density <- exp(outer(mu_grid,
    Y = sigma2_grid,
    FUN = lp_mu_sigma
))
surf1 <- plot_ly(
    x = ~sigma2_grid, y = ~mu_grid, z = ~grid_density,
    type = "surface"
)
```

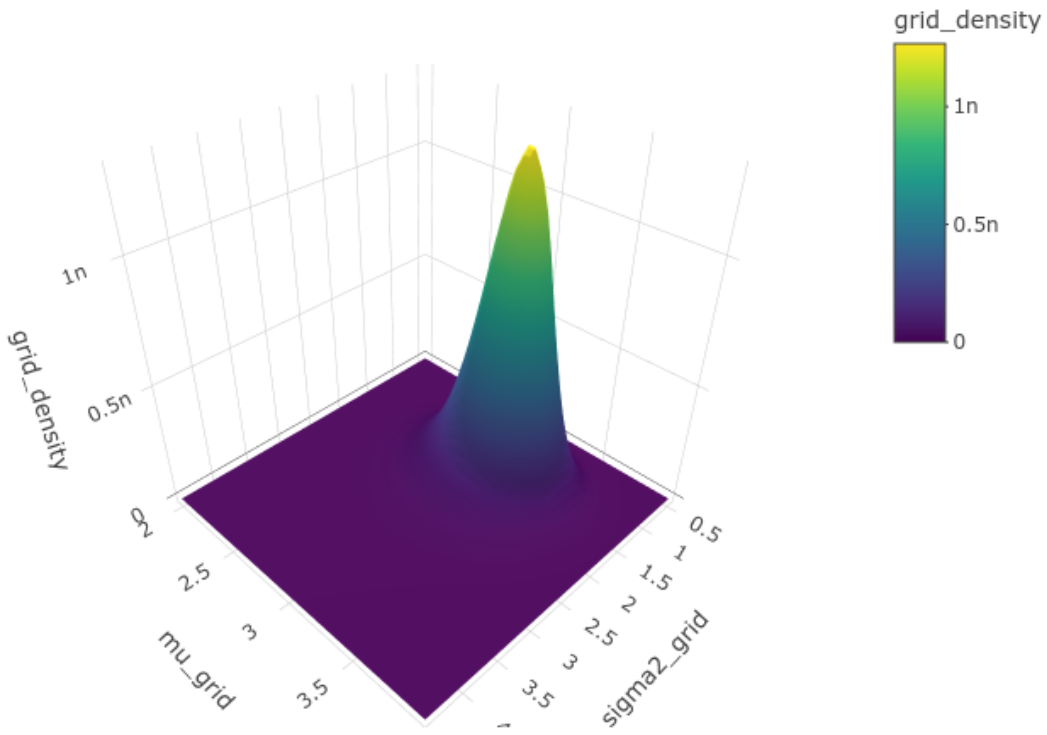


Figure 17.1: Joint posterior of (μ, σ^2) from a normal model.

The HMC algorithm improves from the Metropolis algorithm by simulating smart proposal values. It does so by using the *gradient* of the logarithm of the posterior density. Let's first

take the log of the joint density:

```
grid_logdensity <- outer(mu_grid,
    Y = sigma2_grid,
    FUN = lp_mu_sigma
)
surf2 <- plot_ly(
    x = ~sigma2_grid, y = ~mu_grid, z = ~grid_logdensity,
    type = "surface"
)
```

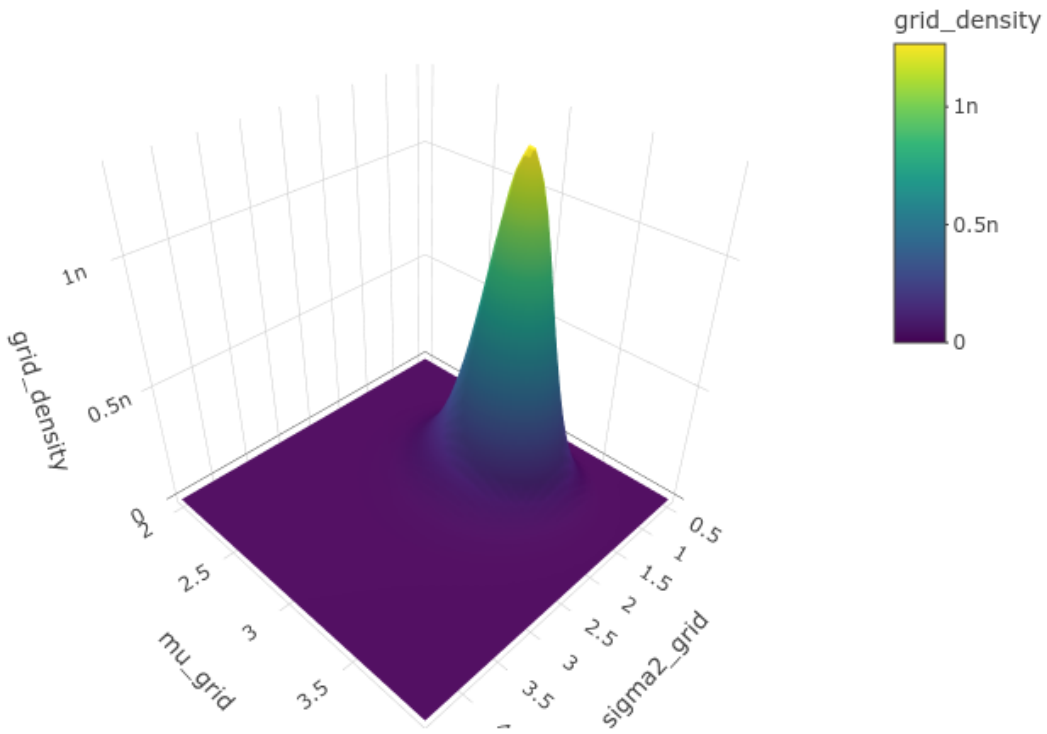


Figure 17.2: Gradient of (μ, σ^2) from a normal model.

Now, flip it upside-down.

```
grid_minuslogdensity <- - outer(mu_grid,
    Y = sigma2_grid,
    FUN = lp_mu_sigma
```

```
)
surf3 <- plot_ly(
    x = ~sigma2_grid, y = ~mu_grid, z = ~grid_minuslogdensity,
    type = "surface"
)
```

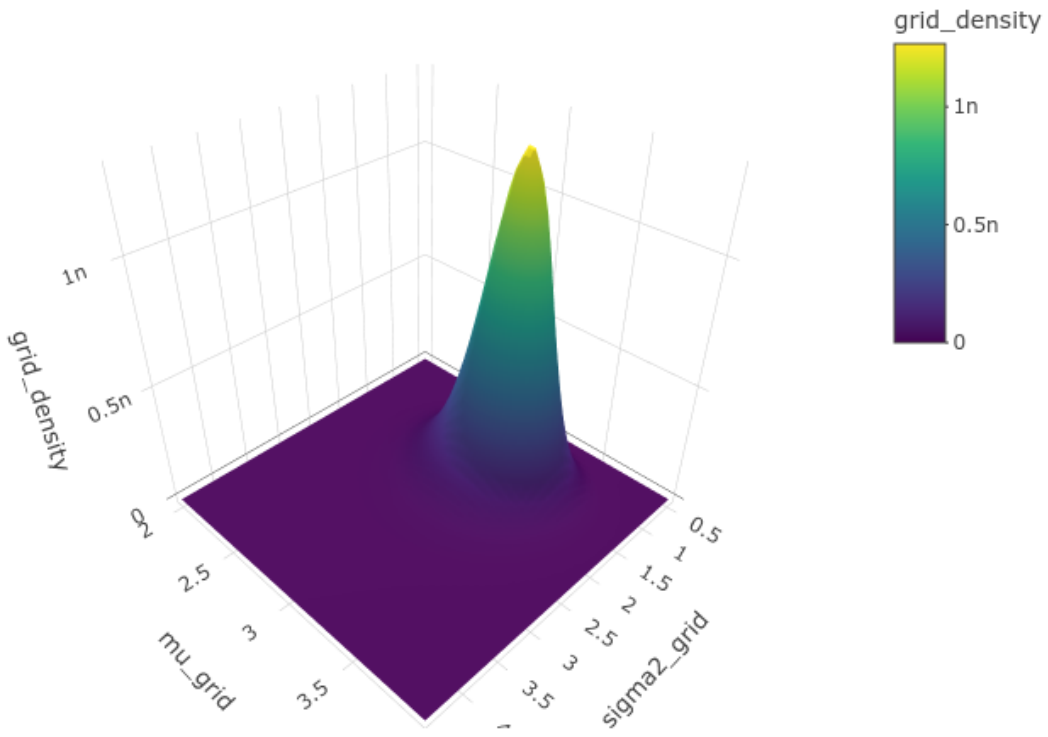


Figure 17.3: "Flipped" gradient of (μ, σ^2) from a normal model.

Imagine placing a marble on the above surface. With gravity, it is natural that the marble will have a tendency to move to the bottom of the surface. If you place the marble in a higher location, it will have a higher *potential energy* and tends to move faster towards the bottom, because that energy converts to a larger *kinetic energy*. If you place it close to the bottom, it will tend to move slower.

For simplicity, let's consider just one dimension with the following picture:

```
lp_sigma <- function(sigma2) {
    kappa_n <- kappa_0 + n
```

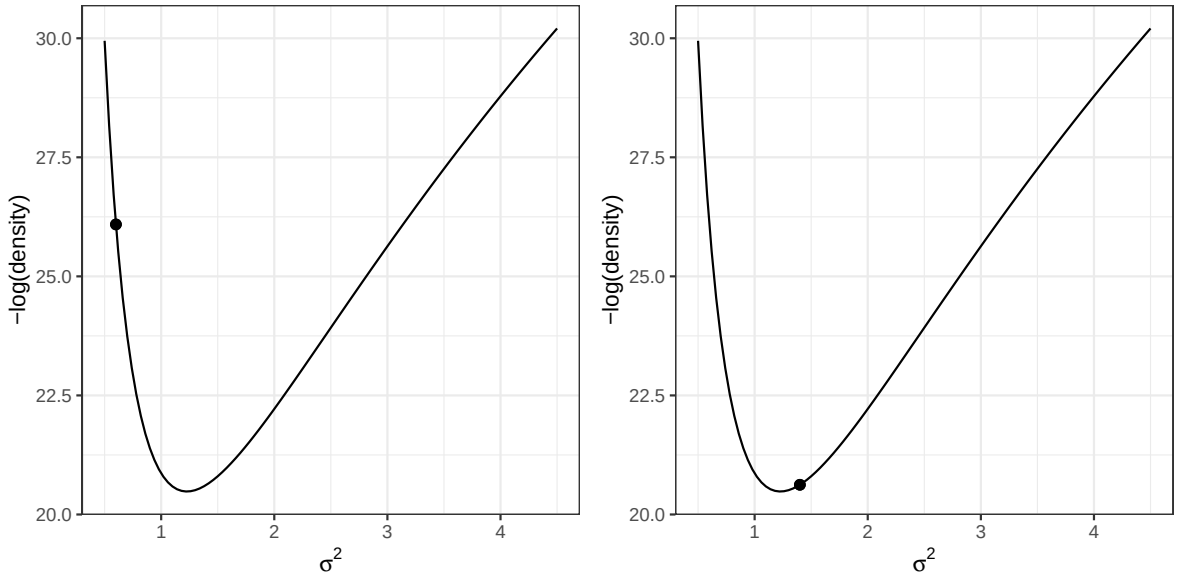
```
    nu_n <- nu_0 + n
    sigma2_n <- (nu_0 * sigma2_0 + (n - 1) * s2y +
        kappa_0 * n / kappa_n * (ybar - mu_0)^2) / nu_n
    log_dens <- (-nu_n / 2 - 1) * log(sigma2) +
        (-nu_n * sigma2_n / 2 / sigma2)
    log_dens[is.nan(log_dens)] <- -Inf
    log_dens
}
p2 <- ggplot(data = data.frame(x = c(0.5, 4.5)), aes(x = x)) +
    stat_function(fun = function(x) - lp_sigma(x)) +
    labs(x = expression(sigma^2),
         y = "-log(density)")
p2 +
    geom_point(
        x = 0.6, y = -lp_sigma(0.6),
        size = 2
    )
p2 +
    geom_point(
        x = 1.4, y = -lp_sigma(1.4),
        size = 2
    )
```

For the graph on the left, the marble (represented as a dot) has high potential energy and should quickly go down to the bottom; on the right, the marble has low potential energy and should move less fast.

> **i** If the sampler is near the bottom (i.e., the point with high posterior density), it tends to stay there.

But we don't want the marble to stay at the bottom without moving; otherwise, all our posterior draws will be just the posterior mode. In HMC, it moves the marble with a push, called *momentum*. The direction and the magnitude of the momentum will be randomly simulated, usually from a normal distribution. If the momentum is large, it should travel farther away; however, it also depends on the *gradient*, which is the slope in a one-dimension case.

> **i** HMC generates a proposed value by simulating the motion of an object on a surface, based on an initial momentum with a random magnitude and direction, and locating the object after a fixed amount of time.



(a) High potential energy

(b) Low potential energy

Figure 17.4: Marginal log posterior distribution of σ^2.

At the beginning of a trajectory, the marble has a certain amount of kinetic and potential energy, and the sum is the total amount of energy, called the *Hamiltonian*. Based on the conservation of energy, at any point in the motion, the Hamiltonian should remain constant.

17.1 Leapfrog Integrator

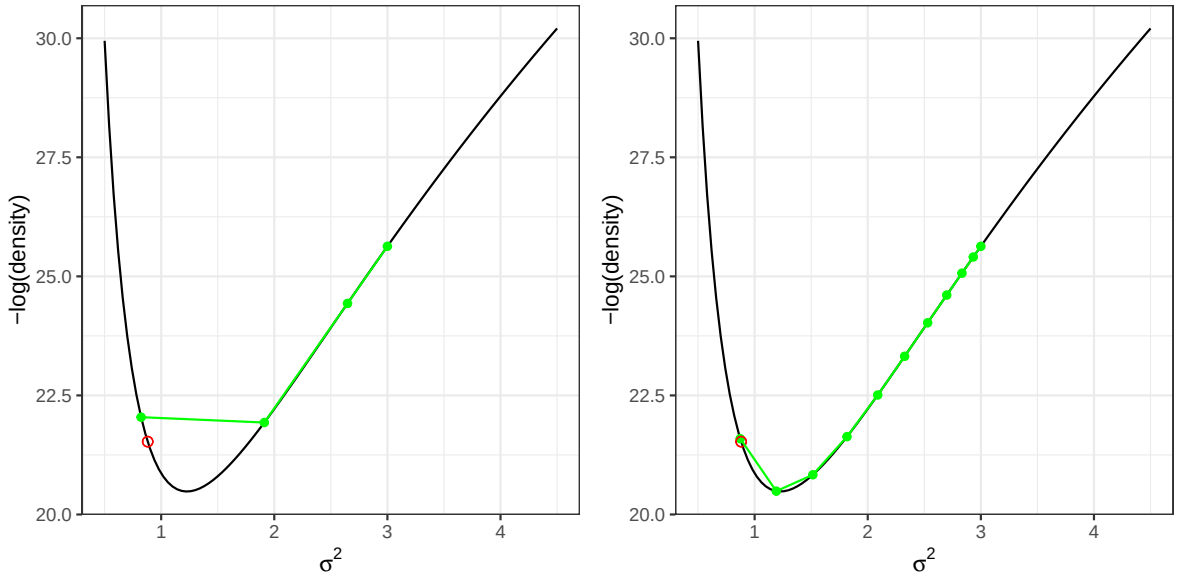
To simulate the marble's motion, one needs to solve a system of differential equations, which is not an easy task. A standard method is the so-called *leapfrog* integrator, which discretizes a unit of time into L steps. The following shows how it approximates the motion using $L = 3$ and $L = 10$ steps. The red dot is the target. As can be seen, larger L simulates the motion more accurately.

```
num_steps <- 3
leapfrog_df <- cbind(
    leapfrog_step(3, rho = -0.5, num_steps = num_steps),
    step = 0:num_steps
)
final_x <- leapfrog_step(3, rho = -0.5, num_steps = 1000)[1001, 1]
p2 + geom_point(
    data = leapfrog_df,
```

```
    aes(x = x, y = -lp_sigma(x)), col = "green"
) +
    geom_point(
        x = final_x, y = -lp_sigma(final_x),
        col = "red", size = 2, shape = 21
    ) +
    geom_path(
        data = leapfrog_df,
        aes(x = x, y = -lp_sigma(x)), col = "green"
    )
num_steps <- 10
leapfrog_df <- cbind(
    leapfrog_step(3, rho = -0.5, num_steps = num_steps),
    step = 0:num_steps
)
p2 + geom_point(
    data = leapfrog_df,
    aes(x = x, y = -lp_sigma(x)), col = "green"
) +
    geom_point(
        x = final_x, y = -lp_sigma(final_x),
        col = "red", size = 2, shape = 21
    ) +
    geom_path(
        data = leapfrog_df,
        aes(x = x, y = -lp_sigma(x)), col = "green"
    )
```

Suppose the simulated trajectory differs from the true trajectory by a certain threshold, like the one on the left. In that case, it is called a *divergent transition*, in which case the proposed value should not be trusted. In software like STAN, it will print out a warning about that. When the number of divergent transitions is large, one thing to do is increase L. If that does not help, it may indicate difficulty in a high-dimensional model, and reparameterization may be needed.

For more information on HMC, go to https://mc-stan.org/docs/reference-manual/mcmc.html. You can also find some sample R code at http://www.stat.columbia.edu/~gelman/book/software.pdf.



(a) 3 steps

(b) 10 steps

Figure 17.5: Simulated motion using the leapfrog integrator.

17.2 The No-U-Turn Sampler (NUTS)

Although HMC is more efficient by generating smarter proposal values, one performance bottleneck is that the motion sometimes takes a U-turn, like in some graphs above, in which the marble goes up (right) and then goes down (left), and eventually may stay in a similar location. The improvement of NUTS is that it uses a binary search tree that simulates both the forward and backward trajectory. The algorithm is complex, but to my understanding, it achieves two purposes: (a) finding the path that avoids a U-turn and (b) selecting an appropriate number of leapfrog steps, L. When each leapfrog step moves slowly, the search process may take a long time. With NUTS, one can control the maximum *depth* of the search tree.

See https://mc-stan.org/docs/reference-manual/mcmc.html#hmc-algorithm-parameters for more information on NUTS.

Part IX

Week 12

18 Generalized Linear Model

GLM (generalized linear model) is a general class of statistical models for predicting an outcome variable, Y. It accommodates Y in different types of measurement, such as continuous, counts, ordinal, or categorical. GLM is a generalization of the usual regression model that assumes linear associations and normally distributed errors.

Just to be careful, some scholars also use the abbreviation GLM to mean the *general* linear model, and the latter is actually the same as the linear model, which is a special case of the GLM we will discuss here. Here, we discuss the GLM (the generalized one) that is especially popular for modeling binary and count outcomes, but we will start with the linear regression case.

18.1 Overview of GLM

Under the GLM framework, with one predictor, we have models in the form

$$\begin{aligned} Y_i &\sim \text{Dist}(\mu_i, \tau) \\ g(\mu_i) &= \eta_i \\ \eta_i &= \beta_0 + \beta_1 X_i \end{aligned}$$

A GLM model has three components:

- Conditional distribution of Y (e.g., Dist = Normal, Poisson, Binomial, Bernoulli)[1]
- Linear predictor η, which is a linear combination of the predictor
- Link function $g(\cdot)$, which maps μ to η

In a GLM, one selects distributions like Dist = Normal, Poisson, Binomial, Bernoulli, etc. The distribution has a mean parameter μ_i and may have a dispersion parameter, τ. An intermediate step in GLM is transforming μ_i to η_i. η_i is called the *linear predictor*, which is the linear function of the predictors. In linear models, we directly model the conditional mean,

[1] Strictly speaking, GLM requires distributions that are in the *exponential family*, which will not include distributions like the t distribution, but here, we also include models that use distributions similar to those in the exponential family, like the Student's t distribution.

μ_i, as the same as η_i. However, to allow for the possibility of μ_i being a nonlinear function of the predictors, in GLM we transform μ_i by applying a *link function*, $g(\cdot)$, so that, even though we η_i to be linear in the coefficients, $\mu_i = g^{-1}(\eta_i)$ will be a nonlinear function of the coefficients as long as the link function is not linear. This step is needed to ensure the predicted values are not out of range.

Table 18.1 includes some commonly used GLMs.

Table 18.1: Commonly used GLMs

outcome type	Support	Distributions	Link
continuous	$[-\infty, \infty]$	Normal	Identity
count (fixed duration)	{0, 1, ...}	Poisson	Log
count (known # of trials)	{0, 1, ..., N}	Binomial	Logit
binary	{0, 1}	Bernoulli	Logit
ordinal	{0, 1, ..., K}	categorical	Logit
nominal	K-vector of {0, 1}	categorical	Logit
multinomial	K-vector of {0, 1, ..., K}	categorical	Logit

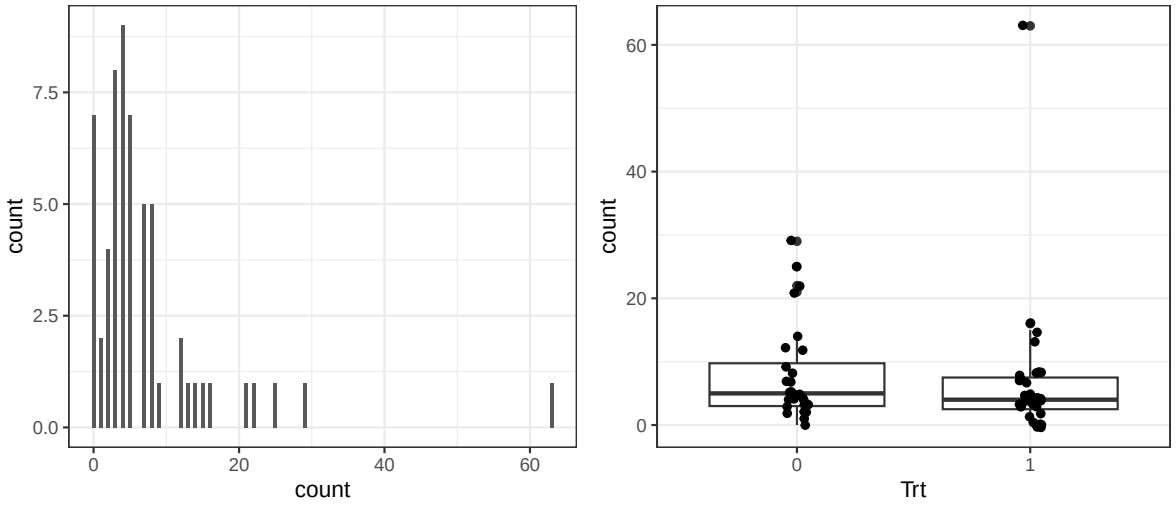
18.2 Poisson Regression

The Poisson GLM is used to model count outcomes. Count outcomes are non-negative discrete integers. Remember, with GLM, we are modeling the mean of the outcome, μ. Therefore, we need to make sure μ is non-negative, so we need a link function that can map η from the whole real line to non-negative numbers; by far, the most commonly used link function is the logarithmic transformation, $g(\mu) = \log(\mu)$.

Here's an example data set recording the effect of anticonvulsant therapy in epilepsy. The outcome variable is the number of seizures in the two-week window prior to the last of the four visits.

First check the distribution of the counts in Figure 18.1.

```
epilepsy4 <- dplyr::filter(epilepsy, visit == 4)
epilepsy4$Trt <- factor(epilepsy4$Trt)
ggplot(epilepsy4, aes(x = count)) +
    geom_bar(width = 0.5)
ggplot(epilepsy4, aes(x = Trt, y = count)) +
    geom_boxplot() +
    geom_jitter(width = 0.05)
```



(a) Overall counts

(b) By treatment conditions

Figure 18.1: Distribution of the number of seizures in the epilepsy data set

18.3 Model and Priors

Model:

$$\begin{aligned} \text{count}_i &\sim \text{Pois}(\mu_i) \\ \log(\mu_i) &= \eta_i \\ \eta_i &= \beta_0 + \beta_1 \text{Trt}_i \end{aligned}$$

Priors:

$$\begin{aligned} \beta_0 &\sim N(3, 2.5) \\ \beta_1 &\sim N(0, 1) \end{aligned}$$

Predicted seizure rate = $\exp(\beta_0 + \beta_1) = \exp(\beta_0)\exp(\beta_1)$ for Trt = 1; $\exp(\beta_0)$ for Trt = 0

β_1 = mean difference in **log** rate of seizure; $\exp(\beta_1)$ = ratio in rate of seizure

18.3.1 MCMC Sampling With `brms`

```
m2 <- brm(count ~ Trt,
    data = epilepsy4,
    family = poisson(link = "log"),
    prior = c(
        prior(normal(1, 3), class = "Intercept"),
        prior(normal(0, 1), class = "b")
    ),
    seed = 31143,
    file = "10_m2"
)
```

18.3.2 Interpretations

Because of the nonlinear link function, one needs to be careful in interpreting the coefficients. With the log link, it is common to obtain the exponentiated coefficient. With the exponentiated coefficient, for every unit difference in X, the predicted rate of seizure occurrence is **multiplied** by $\exp(\beta_1)$ times. Here is the usual step for obtaining the posterior distributions of the transformed parameters:

```
m2_summary <- as_draws(m2) |>
    mutate_variables(
        exp_beta0 = exp(b_Intercept),
        exp_beta1 = exp(b_Trt1)
    ) |>
    summarize_draws()
```

```
Loading required package: rstan
```

```
Loading required package: StanHeaders
```

```


rstan version 2.32.5 (Stan version 2.32.2)
```

```
For execution on a local, multicore CPU with excess RAM we recommend calling
options(mc.cores = parallel::detectCores()).
To avoid recompilation of unchanged Stan programs, we recommend calling
rstan_options(auto_write = TRUE)
For within-chain threading using `reduce_sum()` or `map_rect()` Stan functions,
change `threads_per_chain` option:
rstan_options(threads_per_chain = 1)
```

```
Attaching package: 'rstan'

The following objects are masked from 'package:posterior':

    ess_bulk, ess_tail

The following object is masked from 'package:tidyr':

    extract
```

```
knitr::kable(m2_summary, digits = 2)
```

Table 18.2: Posterior summary of the Poisson regression model

variable	mean	median	sd	mad	q5	q95	rhat	ess_bulk	ess_tail
b_Intercept	2.07	2.07	0.07	0.07	1.96	2.18	1	3472.02	2643.16
b_Trt1	-0.17	-0.17	0.10	0.10	-0.33	-0.01	1	3139.53	2637.42
Intercept	1.98	1.98	0.05	0.05	1.91	2.06	1	2930.65	2699.11
lprior	-3.01	-3.00	0.02	0.01	-3.04	-2.99	1	3326.32	2899.07
lp___	-334.41	-334.12	0.99	0.70	-336.27	-333.48	1	1838.59	2379.17
exp_beta0	7.95	7.93	0.52	0.53	7.13	8.84	1	3472.02	2643.16
exp_beta1	0.85	0.85	0.08	0.08	0.72	0.99	1	3139.53	2637.42

So here is a paragraph for the example:

> The model predicts that the mean seizure rate in two weeks for the control condition is 8, 90% CI [7.1, 8.8]; the exponentiated coefficient for the treatment indicator is 0.85, 90% CI [0.72, 0.99], meaning that on average, the treatment reduces seizure rate by 0.94% to 27.83%.

18.3.3 Rootogram

There is also a useful graphical tool, the rootogram (Figure 18.2), for diagnosing count models.

```
pp_check(m2, type = "rootogram", style = "hanging")
```

```
Using all posterior draws for ppc type 'rootogram' by default.
```

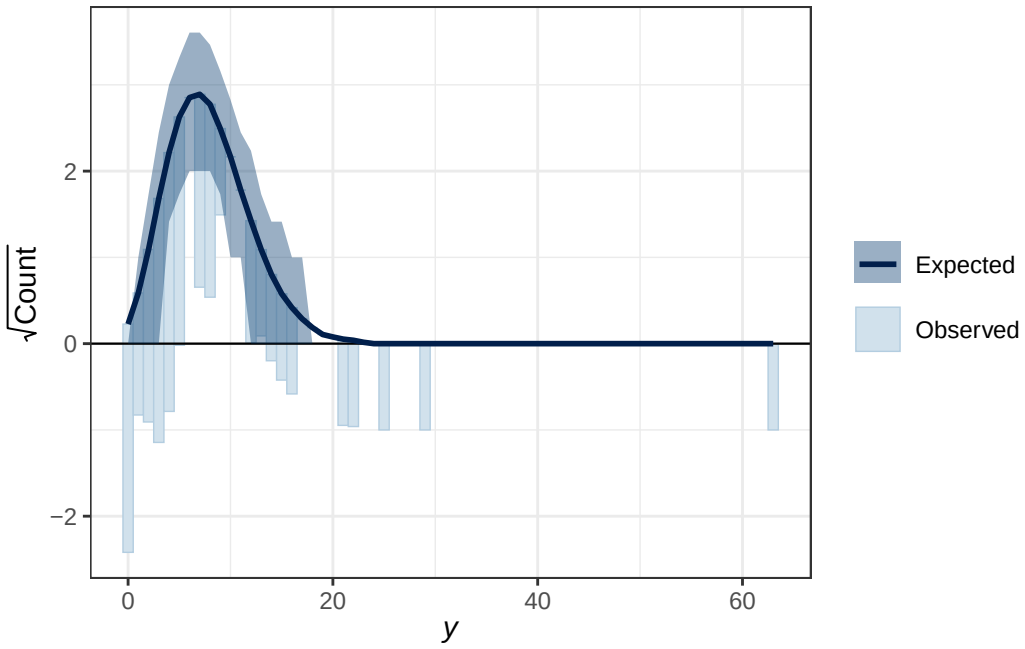


Figure 18.2: Rootogram for the Poisson regression model

If the fit is good, the bars should be close to touching the horizontal x-axis. Thus, the fit was not good in the above figure. Models that accommodate overdispersion and excessive zeros may be needed.

18.4 Negative Binomial Model

The negative binomial distribution is usually used to handle overdispersion in count data. The idea is that even with the same predictor value, each individual has a different rate of occurrence for an event, which is highly plausible for the epilepsy data. This class will not get into the details of the negative binomial, but you can check out this paper or this book.

```
m2_nb <- brm(count ~ Trt,
    data = epilepsy4,
    family = negbinomial(link = "log"),
    prior = c(
        prior(normal(1, 3), class = "Intercept"),
        prior(normal(0, 1), class = "b")
    ),
    seed = 31143,
```

```
    file = "10_m2_nb"
)
```

```
pp_check(m2_nb, type = "rootogram", style = "hanging")
```

```
Using all posterior draws for ppc type 'rootogram' by default.
```

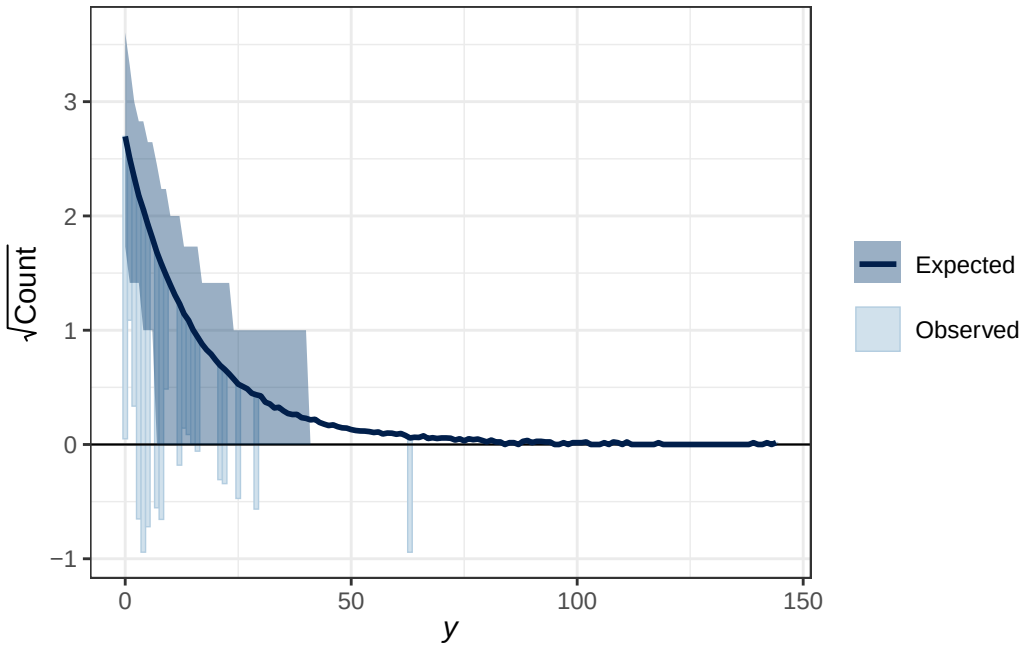


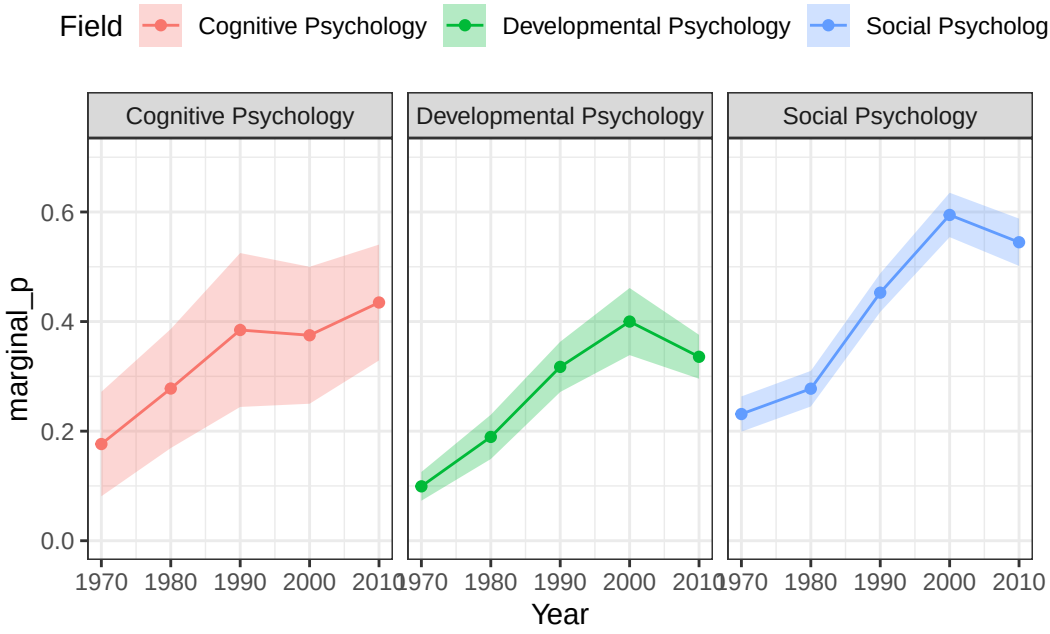
Figure 18.3: Rootogram for the Negative binomial model

18.5 Binary Logistic Regression

We will use an example from this paper: https://journals.sagepub.com/doi/abs/10.1177/0956797616645672, which examines how common it was for researchers to report marginal p values (i.e., $.05 < p \leq .10$). The outcome is whether a study reported one or more marginal p values (1 = Yes, 0 = No). The researchers also categorized the studies into three subfields (Cognitive Psychology, Developmental Psychology, Social Psychology), and there were a total of 1,535 studies examined from 1970 to 2010.

```r
# readxl package can be used to import excel files
datfile <- here("data", "marginalp.xlsx")
if (!file.exists(datfile)) {
    dir.create(here("data"), showWarnings = FALSE)
    download.file("https://osf.io/r4njf/download",
        destfile = datfile
    )
}
marginalp <- readxl::read_excel(datfile)
# Recode `Field` into a factor
marginalp <- marginalp |>
    # Filter out studies without any experiments
    filter(`Number of Experiments` >= 1) |>
    mutate(Field = factor(Field,
        labels = c(
            "Cognitive Psychology",
            "Developmental Psychology",
            "Social Psychology"
        )
    )) |>
    # Rename the outcome
    rename(marginal_p = `Marginals Yes/No`)
# Proportion of marginal p in each subfield across Years
marginalp |>
    ggplot(aes(x = Year, y = marginal_p)) +
    stat_summary(aes(fill = Field), geom = "ribbon", alpha = 0.3) +
    stat_summary(aes(col = Field), geom = "line") +
    stat_summary(aes(col = Field), geom = "point") +
    coord_cartesian(ylim = c(0, 0.7)) +
    facet_wrap(~ Field) +
    theme(legend.position = "top")
```

```
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
No summary function supplied, defaulting to `mean_se()`
```



18.5.1 Centering

The issue of centering applies to most regression models, including GLMs. Because the predictor `Year` has values 1970, 1980, etc, if we use this variable as a predictor, the intercept β_0 will be the predicted value of η when `Year` $= 0$, which is like 2,000 years before the data were collected. So instead, we usually want the value 0 to be something meaningful and/or a possible value in the data. So we will center the variable year by making 0 the year 1970. In addition, we will divide the values by 10 so that one unit in the new predictor means 10 years.

In other words, we will use a transformed predictor, `Year10` = (`Year` - 1970) / 10. So when `Year` = 1970, `Year10` = 0; when `Year` = 1990, `Year10` = 2.

```
marginalp <- marginalp |>
  mutate(Year10 = (Year - 1970) / 10)
# Check the recode
distinct(marginalp, Year, Year10)
```

```
# A tibble: 5 x 2
   Year Year10
  <dbl>  <dbl>
1  1980      1
```

```
2  1970       0
3  2000       3
4  1990       2
5  2010       4
```

For this example, I'll look at the subset of developmental psychology. You may want to try using the other subsets of the data for practice.

```
marginalp_dev <- filter(marginalp,
                        Field == "Developmental Psychology")
head(marginalp_dev)
```

```
# A tibble: 6 x 9
  Field            `Paper Title` Authors  Year Number of Experiment~1 marginal_p
  <fct>            <chr>         <chr>   <dbl>                  <dbl>      <dbl>
1 Developmental P~ A New Look a~ Christ~  2010                      1          1
2 Developmental P~ A Tale to Tw~ daniel~  2010                      1          1
3 Developmental P~ Associations~ Rachel~  2010                      1          1
4 Developmental P~ Attachment-b~ kathyr~  2000                      1          1
5 Developmental P~ Effects of A~ Timoth~  1990                      1          1
6 Developmental P~ Effortful co~ grazyn~  2000                      1          1
# i abbreviated name: 1: `Number of Experiments`
# i 3 more variables: `First or Only Marginal` <dbl>,
#   `Conventional Threshold` <dbl>, Year10 <dbl>
```

18.5.2 Model and Priors

As the name "logistic regression" suggested, the logistic function is used somewhere in the model. The logistic function, or the inverse logit function, is

$$\mu = g^{-1}(\eta) = \frac{\exp(\eta)}{1 + \exp(\eta)},$$

which is a transformation from η to μ. The link function, which is a transformation from μ to η, is the logit function,

$$\eta = g(\mu) = \log \frac{\mu}{1 - \mu},$$

which converts μ, which is in probability metric, to η, which is in log odds metric (odds = probability / [1 - probability]).

Model:

$$
\begin{aligned}
\text{marginal\_p}_i &\sim \text{Bern}(\mu_i) \\
\text{logit}(\mu_i) &= \eta_i \\
\eta_i &= \beta_0 + \beta_1 \text{Year10}_i
\end{aligned}
$$

Priors:

$$
\begin{aligned}
\beta_0 &\sim t_4(0, 2.5) \\
\beta_1 &\sim t_4(0, 1)
\end{aligned}
$$

There has been previous literature on what choices of prior on the β coefficients for logistic regressions would be appropriate (see this paper). β coefficients in logistic regression can be relatively large, unlike in normal regression. Therefore, it's pointed out that a heavy tail distribution, like Cauchy and t, would be more appropriate. Recent discussions have settled on priors such as t distributions with small degrees of freedom as a good balance between heavy tails and efficiency for MCMC sampling. I use $t_4(4, 0, 2.5)$ for β_0, which puts more density in [-2.5, 2.5] on the log odds unit. This means, in the year 1970, our belief is that the probability of marginally significant results would be somewhere between 0.08 to 0.92, which seems to cover a reasonable range. For β_1, I use $t_4(4, 0, 1)$, which suggests that a 10-year difference like corresponds to a difference in log odds between -1 and 1. While it's hard to interpret the difference in log odds, a quick rule of thumb is to divide β_1 by 4, which roughly corresponds to the maximum difference in probability for a unit difference in the predictor. So if $\beta_1 = 1$, the maximum difference in probability will be no more than 25 percentage points. So my prior says that it's unlikely that the probability of reporting marginal p values would increase or decrease by 25 percentage points every 10 years, which again is a weak prior. If you're uncertain, you can consider something weaker.

The priors are chosen to be weakly informative.

```
m4 <- brm(marginal_p ~ Year10,
    data = marginalp_dev,
    family = bernoulli(link = "logit"),
    prior = c(
        prior(student_t(4, 0, 1), class = "b"),
        prior(student_t(4, 0, 2.5), class = "Intercept")
    ),
    # Note: no sigma
    seed = 1340,
    file = "10_m4"
)
```

In `brms` we used `family = bernoulli()`. In other R functions, such as `glm`, they do not distinguish between bernoulli and Binomial and only recognize `family = binomial()`, as a Bernoulli variable is a binomial variable with $n = 1$.

18.5.3 Interpreting the results

Any nonlinear relationships will involve more work in interpretations, and the coefficients in logistic regressions are no exception.

18.5.3.1 Posterior predictions

A good way to start is to plot the model-implied association on the original unit of the data. The `conditional_effects()` function in `brms` comes in very handy, and I recommend you always start with this:

```
plot(
    conditional_effects(m4, prob = .90),
    points = TRUE,
    point_args = list(height = 0.01, width = 0.05, alpha = 0.05),
    plot = FALSE
)[[1]] +
    scale_x_continuous(
        breaks = 0:4,
        labels = c("1970", "1980", "1990", "2000", "2010")
    ) +
    xlab("Year")
```

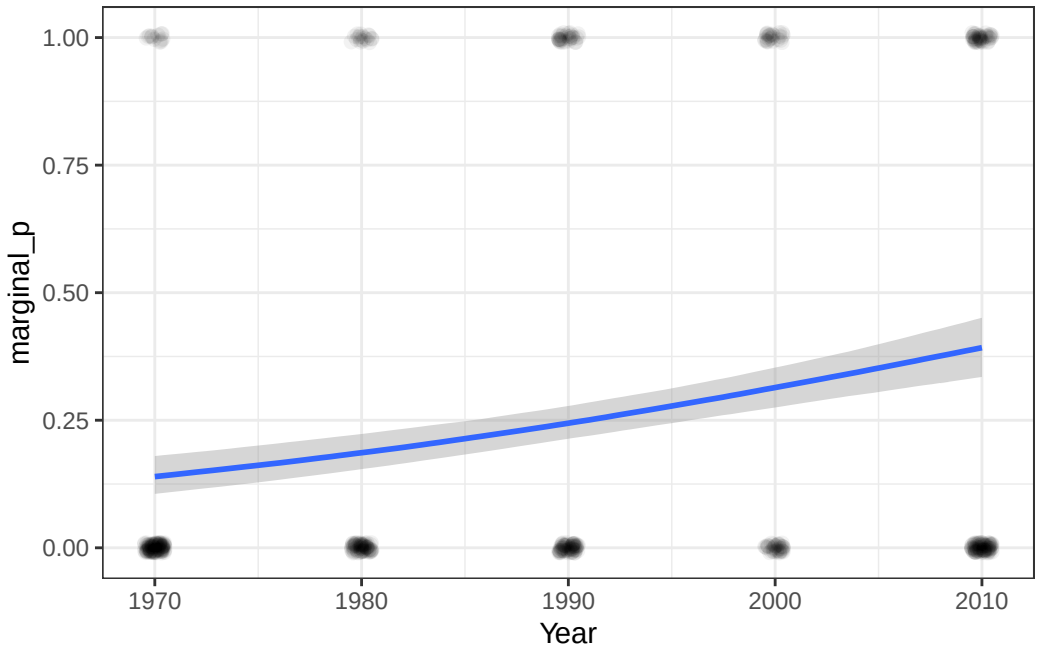


Figure 18.4: Predicted probabilities of marginal significant results over time.

As you can see, the logistic model implies a somewhat nonlinear association between `Year10` and the outcome. From the graph, when `Year10` = 2, which is the Year 1990, the predicted probability of marginal significant results is about 25%, with a 90% credible interval of about 21 to 28%. We can get that using

```
posterior_epred(m4, newdata = list(Year10 = 2)) |>
    summarise_draws()
```

```
# A tibble: 1 x 10
  variable  mean median     sd    mad    q5   q95  rhat ess_bulk ess_tail
  <chr>    <dbl>  <dbl>  <dbl>  <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
1 ...1     0.245  0.244 0.0195 0.0191 0.214 0.278  1.00    2460.    2529.
```

18.5.3.2 Intercept

From the equation, when all predictors are zero, we have

$$\text{logit}(\mu_i) = \beta_0.$$

Therefore, the intercept is the log odds that a study reported a marginally significant p value when `Year10` = 0 (i.e, in 1970), which was estimated to be -1.8, 90% CI [-2.1, -1.5]. As log

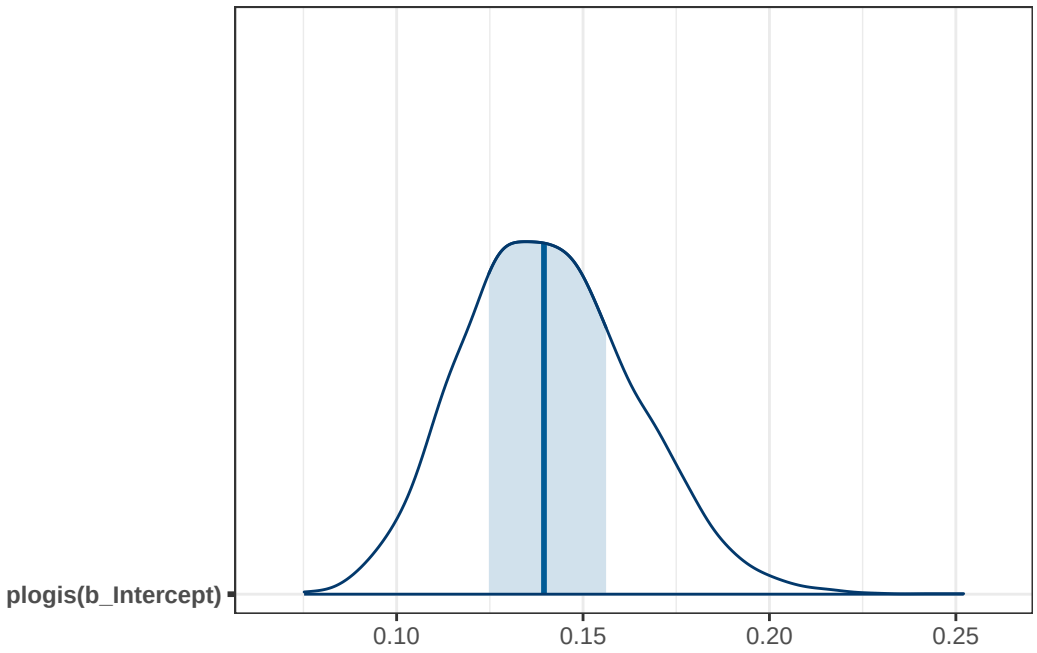
odds are not as intuitive as probability, it is common to interpret instead $\hat{\mu} = \text{logistic}(\beta_0)$, which is the conditional probability of being `marginal_p` $= 1$ in 1970. For Bayesian, that means obtaining the posterior distribution of $\text{logistic}(\beta_0)$, which can be done by

```
m4_draws <- as_draws(m4)
m4_draws <- m4_draws |>
    mutate_variables(logistic_beta0 = plogis(b_Intercept))
m4_draws |>
    subset(variable = "logistic_beta0") |>
    summary()
```

```
# A tibble: 1 x 10
  variable        mean median     sd    mad    q5   q95  rhat ess_bulk ess_tail
  <chr>          <dbl>  <dbl>  <dbl>  <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
1 logistic_beta0 0.141  0.140 0.0230 0.0230 0.106 0.180  1.00    2100.    2030.
```

The `bayesplot` package allows you to plot transformed parameters quickly:

```
mcmc_areas(m4, pars = "b_Intercept",
           transformations = list("b_Intercept" = "plogis"),
           bw = "SJ")
```



18.5.3.3 Interpreting $\exp(\beta_1)$ as odds ratio

The slope, β_1, represents the difference in the predicted log odds between two observations with a unit difference in the predictor. For example, for two individuals with a unit difference in `Year10` (i.e., 10 years), we have

$$\text{logit}(\mu_{\text{marginal\_p=1}}) - \text{logit}(\mu_{\text{marginal\_p=0}}) = \beta_1.$$

Again, the difference in log odds are hard to interpret, so we will exponentiate to get

$$\frac{\text{odds}_{\text{marginal\_p=1}}}{\text{odds}_{\text{marginal\_p=0}}} = \exp(\beta_1).$$

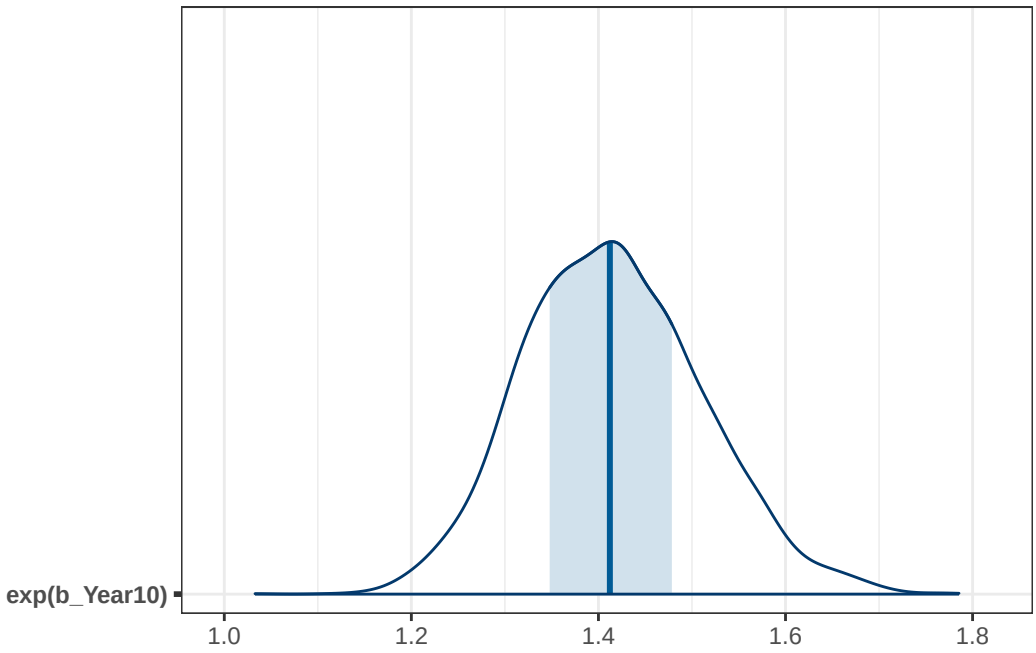
The fraction on the left-hand side is the *odds ratio* of reporting a marginal p value associated with a unit difference in `Year10` (i.e., 10 years). An odds of 1.0 means that the probability of success and failure is equal; an odds > 1 means success is more likely than failures; and an odds < 1 means success is less likely than failures. Again, for Bayesian, we can obtain the posterior distribution of $\exp(\beta_1)$ by

```
m4_draws <- m4_draws |>
    mutate_variables(exp_beta1 = exp(b_Year10))
m4_draws |>
    subset(variable = "exp_beta1") |>
    summary()
```

```
# A tibble: 1 x 10
  variable   mean median     sd    mad    q5   q95  rhat ess_bulk ess_tail
  <chr>     <dbl>  <dbl>  <dbl>  <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
1 exp_beta1  1.42   1.41 0.0954 0.0968  1.27  1.58  1.00    2688.    2698.
```

Using the posterior mean, we predict that the odds of reporting a marginal p value for a study that is 10 years later is multiplied by 1.4 times, 90% CI [1.3, 1.6]; in other words, every 10 years, the odds increased by 41.5852521%. Here's the posterior density plot for the odds ratio:

```
mcmc_areas(m4, pars = "b_Year10",
           transformations = list("b_Year10" = "exp"),
           bw = "SJ")
```



Odds ratio (OR) is popular as the multiplicative effect is constant, thus making interpretations easier. Also, in medical research and some other research areas, OR can be an excellent approximation of the relative risk, which is the probability ratio of two groups, of some rare diseases or events. However, odds and odds ratios are never intuitive metrics for people, and in many situations, a large odds ratio may be misleading as it may represent a very small effect. Therefore, in general, I would recommend you to interpret coefficients in probability units, even though that means more work.

18.5.3.4 Interpreting Coefficients in Probability Units

Another way to interpret the results of the logistic regression coefficient is to examine the change in probability. Because the predicted probability is a nonlinear function of the predictors, a unit difference in the predictor has different meanings depending on the values of X you chose for interpretations. You can see that in the `conditional_effects()` plot earlier.

Consider the change in the predicted probability of reporting a marginal p value with `Year10` $= 0$ (1970), `Year10` $= 1$ (1980), to `Year10` $= 4$, respectively:

```
m4_pred <- posterior_epred(m4, list(Year10 = 0:4))
colnames(m4_pred) <- paste0("Year10=", 0:4)
summarise_draws(m4_pred)
```

```
# A tibble: 5 x 10
```

```
  variable  mean median     sd    mad    q5   q95  rhat ess_bulk ess_tail
  <chr>    <dbl>  <dbl>  <dbl>  <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
1 Year10=0 0.141  0.140 0.0230 0.0230 0.106 0.180  1.00    2062.    2024.
2 Year10=1 0.187  0.186 0.0211 0.0212 0.154 0.223  1.00    2072.    2150.
3 Year10=2 0.245  0.244 0.0195 0.0191 0.214 0.278  1.00    2460.    2529.
4 Year10=3 0.314  0.314 0.0235 0.0233 0.275 0.353  1.00    3601.    2610.
5 Year10=4 0.393  0.392 0.0351 0.0349 0.335 0.451  1.00    3948.    2653.
```

As you can see, the predicted difference in probability is smaller when comparing `Year10` = 0 and 1, but is larger when comparing `Year10` = 3 and 4.

> **The "divide by 4 rule"**
>
> A quick approximation is to divide the coefficient by 4 to get an upper bound on the change in probability associated with a unit change in the predictor. In our example, this corresponds to 0.3454722 / 4 = 0.086368, which is very close to the predicted difference in probability from `Year10` = 3 to `Year10` = 4.

18.5.4 Posterior Predictive Check

```
pp_check(
    m4,
    type = "error_binned"
)
```

```
Using 10 posterior draws for ppc type 'error_binned' by default.
```

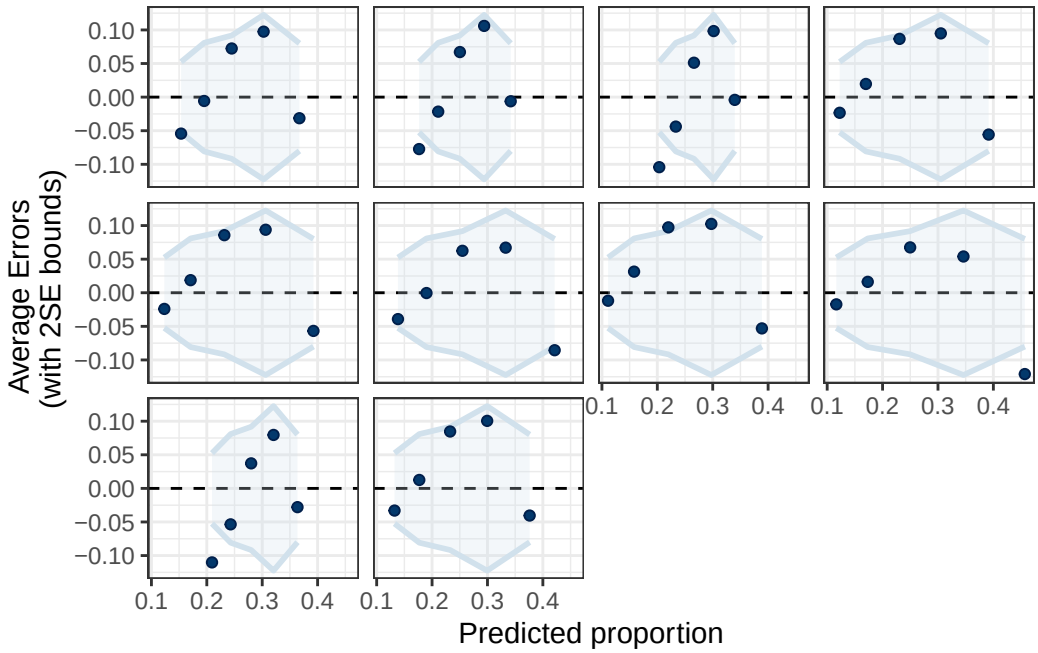


Figure 18.5: Posterior Predictive Check for the binary logistic model.

The linear model is not the best fit.

18.5.5 Linear Spline

Use `bs()` to specify a linear spline (degree = 1) with one turning point (knots = 3).

```
library(splines)
m5 <- brm(marginal_p ~ bs(Year10, degree = 1, knots = 3),
    data = marginalp_dev,
    family = bernoulli(link = "logit"),
    prior = prior(student_t(4, 0, .875), class = "b"),
    # Note: no sigma
    seed = 1340,
    file = "10_m5"
)
```

18.5.6 Posterior Prediction

```
plot(
    conditional_effects(m5),
    points = TRUE,
    point_args = list(height = 0.01, width = 0.05, alpha = 0.05)
)
```

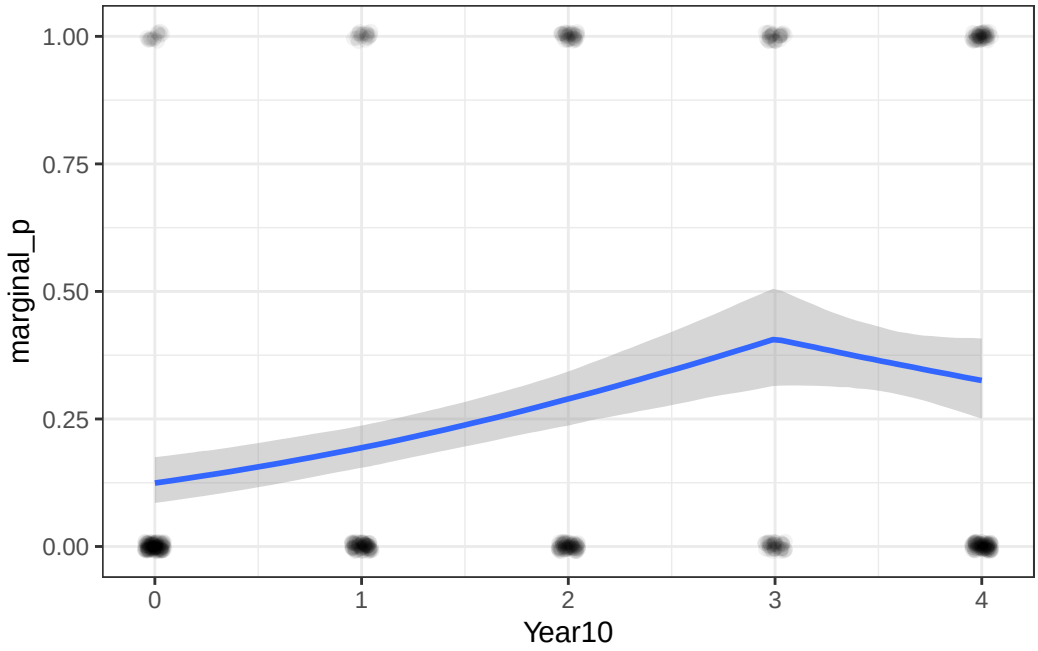


Figure 18.6: Predicted probabilities of marginal significant results over time with the spline model.

```
pp_check(
    m5,
    type = "error_binned",
    x = "Year10"
)
```

```
Using 10 posterior draws for ppc type 'error_binned' by default.
```

```
Warning: The following arguments were unrecognized and ignored: x
```

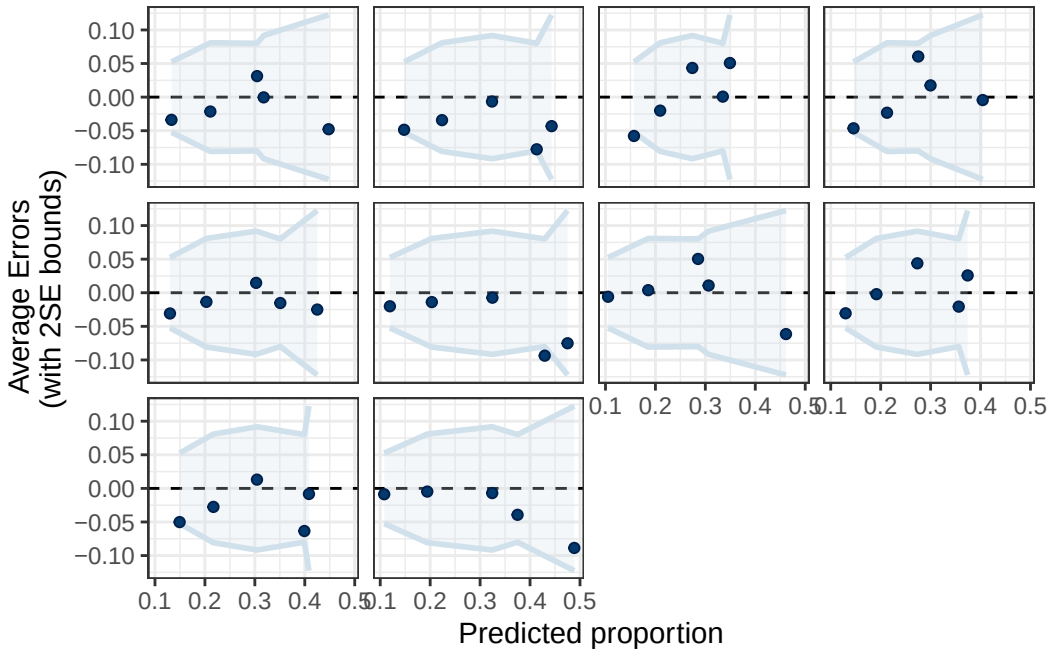


Figure 18.7: Posterior Predictive Check for the binary logistic model with a linear spline.

18.5.7 Model Comparison

```
msummary(list(linear = m4, `linear spline` = m5),
         estimate = "{estimate} [{conf.low}, {conf.high}]",
         statistic = NULL, fmt = 2)
```

```
Warning:
`modelsummary` uses the `performance` package to extract goodness-of-fit
statistics from models of this class. You can specify the statistics you wish
to compute by supplying a `metrics` argument to `modelsummary`, which will then
push it forward to `performance`. Acceptable values are: "all", "common",
"none", or a character vector of metrics names. For example: `modelsummary(mod,
metrics = c("RMSE", "R2")` Note that some metrics are computationally
expensive. See `?performance::performance` for details.
 This warning appears once per session.
```

The linear spline is better according to the information criteria.

	linear	linear spline
b_Intercept	−1.82 [−2.20, −1.46]	−1.95 [−2.37, −1.55]
b_Year10	0.35 [0.22, 0.48]	
b_bsYear10degreeEQ1knotsEQ31		1.57 [0.93, 2.27]
b_bsYear10degreeEQ1knotsEQ32		1.22 [0.69, 1.77]
Num.Obs.	535	535
R2	0.049	0.050
ELPD	−292.9	−290.1
ELPD s.e.	11.2	11.1
LOOIC	585.8	580.2
LOOIC s.e.	22.5	22.2
WAIC	585.8	580.2
RMSE	0.43	0.42

19 Generalized Linear Model (II)

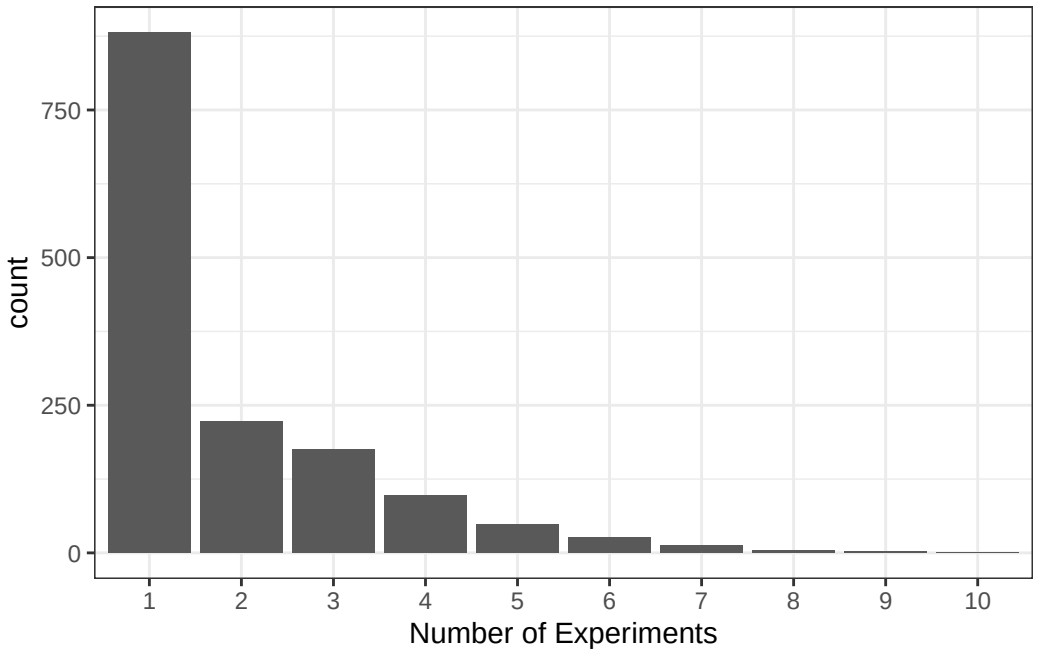
```
datfile <- here("data", "marginalp.xlsx")
marginalp <- readxl::read_excel(datfile)
# Recode `Field` into a factor
marginalp <- marginalp |>
    # Filter out studies without any experiments
    filter(`Number of Experiments` >= 1) |>
    mutate(Field = factor(Field,
        labels = c(
            "Cognitive Psychology",
            "Developmental Psychology",
            "Social Psychology"
        )
    )) |>
    # Rename the outcome
    rename(marginal_p = `Marginals Yes/No`)
marginalp <- marginalp |>
  mutate(Year10 = (Year - 1970) / 10)
marginalp_dev <- filter(marginalp,
                        Field == "Developmental Psychology")
```

19.1 Flexible Non-Linear Models

The `brms` package has a special syntax for non-linear models for more complex relationships. More information can be found in https://cran.r-project.org/web/packages/brms/vignettes/brms_nonlinear.html.

As an example, in the `marginalp` data, some studies have more than one experiment:

```
ggplot(marginalp, aes(x = `Number of Experiments`)) +
    geom_bar() +
    scale_x_discrete(limits = as.character(c(1, 2, 3, 4, 5, 6, 7, 8, 9, 10)))
```



It seems sensible that the probability of reporting at least one marginally significant result would be higher when there are more experiments. And if the number of experiments increases over time, this variable is a potential confound for the relationship between time and the probability of marginally significant results.

One can instead explicitly incorporate the number of experiments in the model. Assuming that the probability of reporting marginal significant result in one experiment is p, and assume that, within a study, the chance of reporting marginal significant results in different experiments is constant and independent, then the probability of reporting at least one marginal p value in a study with n experiments is

$$1 - (1 - p_m)^n \tag{19.1}$$

We will see how to incorporate this into `brms` using the non-linear syntax. But first, let's use the non-linear syntax to refit our binary logistic model.

19.1.1 Binary Logistic Using the Non-Linear Syntax

Recall that our model can be written as

$$\begin{aligned} \text{marginal\_p}_i &\sim \text{Bern}(\mu_i) \\ \mu_i &= \text{logit}^{-1}(\beta_0 + \beta_1 \text{Year10}_i) \end{aligned}$$

We can translate the above model into the non-linear syntax:

```
f1 <- bf(
    # mu = logit^{-1}(beta0 + beta1 * Year10)
    marginal_p ~ inv_logit(b0 + b1 * Year10),
    # b0 and b1 are constant numbers
    b0 + b1 ~ 1,
    # nl = TRUE means we are using the non-linear syntax
    nl = TRUE
)
```

> ! Because we already incorporate the inverse link function (inverse logit) in the syntax, we should use `family = bernoulli(link = "identity")`.

```
# Reft m4 using the non-linear syntax
m4b <- brm(f1,
    data = marginalp_dev,
    family = bernoulli(link = "identity"),
    prior = c(
        prior(student_t(4, 0, 1), nlpar = "b1"),
        prior(student_t(4, 0, 2.5), nlpar = "b0")
    ),
    file = "10_m4b"
)
m4b
```

```
 Family: bernoulli
  Links: mu = identity
Formula: marginal_p ~ inv_logit(b0 + b1 * Year10)
         b0 ~ 1
         b1 ~ 1
   Data: marginalp_dev (Number of observations: 535)
  Draws: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup draws = 4000

Regression Coefficients:
             Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
b0_Intercept    -1.81      0.19    -2.18    -1.45 1.00     1248     1451
b1_Intercept     0.34      0.07     0.21     0.47 1.00     1281     1562

Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
```

```
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

The results are basically the same as `m4` in the previous note, as they are the same model.

19.1.2 Custom Model Incorporating Number of Experiments

Now, we can modify the above model by incorporating Equation 19.1. Just substite $p_m =$ `inv_logit(b0 + b1 * Year10)`:

```
f2 <- bf(
    marginal_p ~ 1 - (1 - inv_logit(b0 + b1 * Year10))^nexp,
    b0 + b1 ~ 1,
    nl = TRUE
)
```

```
# Rename `Number of Experiments`
marginalp_dev$nexp <- marginalp_dev$`Number of Experiments`
m4c <- brm(f2,
    data = marginalp_dev,
    family = bernoulli(link = "identity"),
    prior = c(
        prior(student_t(4, 0, 1), nlpar = "b1"),
        prior(student_t(4, 0, 2.5), nlpar = "b0")
    ),
    file = "10_m4c"
)
```

We can now plot the model-implied probabilities of marginal significant results over time, for one experiment.

```
conditional_effects(
    m4c,
    effects = "Year10",
    conditions = data.frame(
        nexp = 1
    )
)
```

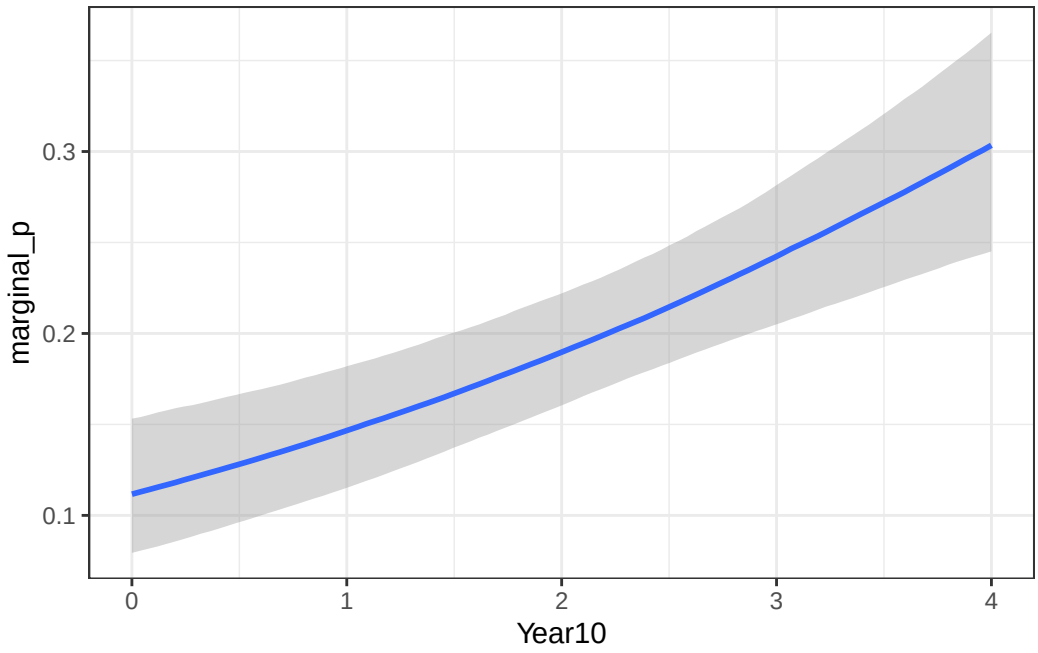


Figure 19.1: Predicted probabilities of marginal significant results over time for one experiment.

19.2 Binomial Logistic Regression

Two Equivalent Models

When the probability is assumed equal across trials, the following are equivalent:

- Individual data: Bernoulli
- Grouped data: Binomial

19.2.1 Model

$$\begin{aligned} \text{marginal\_p}_j &\sim \text{Bin}(N_j, \mu_j) \\ \text{logit}(\mu_j) &= \eta_j \\ \eta_j &= \beta_0 + \beta_1 \text{Year10}_j \end{aligned}$$

Priors:

$$\beta_0 \sim t_3(0, 2.5)$$
$$\beta_1 \sim t_4(0, 1)$$

```
# Grouping data should only be done for observations with
# the same predicted probabilities
marginalp_dev_grouped <-
    marginalp_dev |>
    group_by(Year10) |>
    summarize(
        marginal_p = sum(marginal_p),  # number of "successes"
        n = n()  # number of trials
    )
```

```
m5_bin <- brm(
    marginal_p | trials(n) ~ bs(Year10, degree = 1, knots = 3),
    data = marginalp_dev_grouped,
    family = binomial(link = "logit"),
    prior = prior(student_t(4, 0, 1), class = "b"),
    # Note: no sigma
    seed = 1340,
    file = "10_m5_bin"
)
```

```
pp_check(m5_bin, type = "intervals", x = "Year10")
```

```
Using all posterior draws for ppc type 'intervals' by default.
```

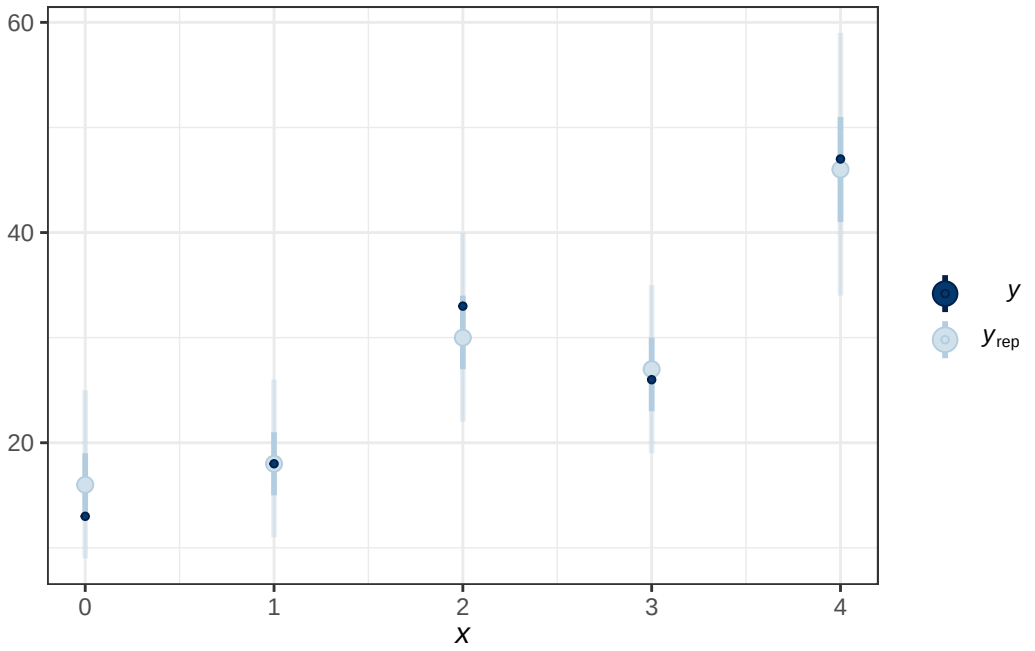


Figure 19.2: Posterior predictive check using the predicted and observed counts.

19.3 Ordinal Regression

The example here is based on this paper: https://journals.sagepub.com/doi/full/10.1177/2515245918823199. The data come from the 2006 U.S. General Social Survey (GSS), where the codebook can be found at https://www.thearda.com/data-archive?tab=2&fid=GSS2006. The data can be imported from OSF:

```
stemcell <- read.csv("https://osf.io/vxw73/download")
stemcell <- stemcell |>
    mutate(
        belief = factor(belief,
            levels = c("moderate", "fundamentalist", "liberal")
        )
    )
```

The predictor is religious belief, and the outcome is the attitude toward stem cell research:

> Recently, there has been controversy over whether the government should provide any funds at all for scientific research that uses stem cells taken from human embryos. Would you say the government . . .

- 1 = Definitely, should fund such research
- 2 = Probably should fund such research
- 3 = Probably should not fund such research
- 4 = Definitely should not fund such research

```
stemcell |>
    ggplot(aes(x = rating)) +
    geom_bar() +
    facet_wrap(~ belief)
```

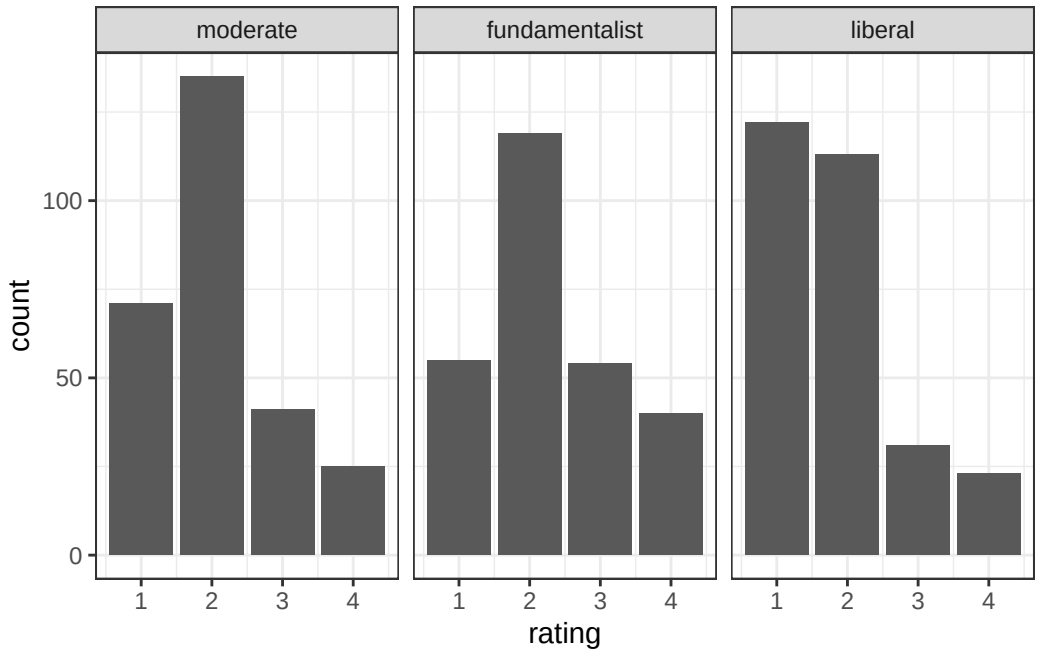


Figure 19.3: Distribution of opinion ratings on whether the government should fund stem-cell research by religious belief.

19.4 Model

$$
\begin{aligned}
\text{rating}_i &\sim \text{Categorical}(\pi_i^1, \pi_i^2, \pi_i^3, \pi_i^4) \\
\pi_i^1 &= \text{logit}^{-1}(\tau^1 - \eta_i) \\
\pi_i^2 &= \text{logit}^{-1}(\tau^2 - \eta_i) - \text{logit}^{-1}(\tau^1 - \eta_i) \\
\pi_i^3 &= \text{logit}^{-1}(\tau^3 - \eta_i) - \text{logit}^{-1}(\tau^2 - \eta_i) \\
\pi_i^4 &= 1 - \text{logit}^{-1}(\tau^3 - \eta_i) \\
\eta_i &= \beta_1 \text{fundamentalist}_i + \beta_2 \text{liberal}_i
\end{aligned}
$$

Priors:

$$
\begin{aligned}
\tau^1, \tau^2, \tau^3 &\sim t_3(0, 2.5) \\
\beta_1 &\sim N(0, 1)
\end{aligned}
$$

```
m6 <- brm(
    rating ~ belief,
    data = stemcell,
    family = cumulative(link = "logit"),
    prior = prior(std_normal(), class = "b"),
    seed = 1340,
    file = "10_m6"
)
```

19.4.1 Posterior Predictive Check

```
pp_check(m6, type = "bars_grouped", group = "belief",
         ndraws = 100)
```

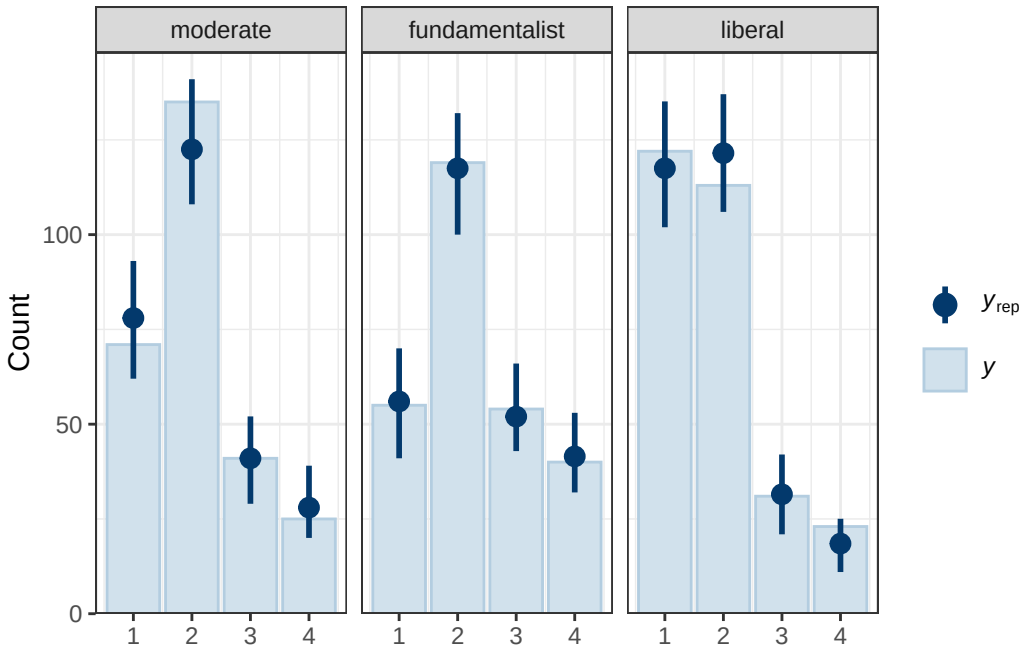


Figure 19.4: Posterior Predictive Check for the ordinal regression model.

The fit was reasonable.

19.4.2 Plot

```
conditional_effects(m6, categorical = TRUE)
```

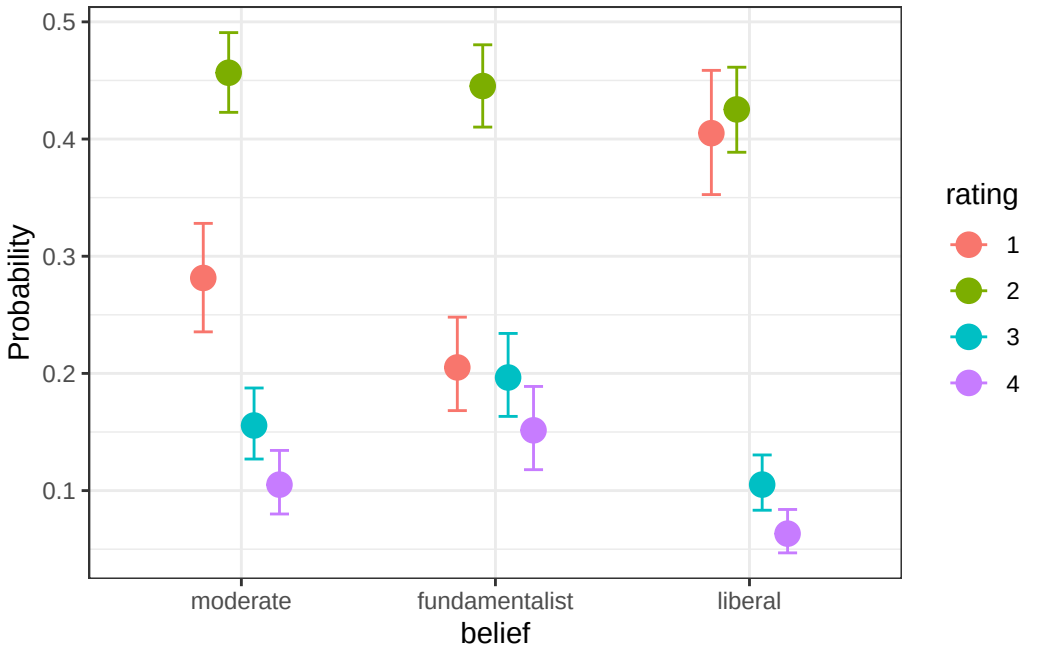


Figure 19.5: Model-predicted probabilities based on the ordinal regression model.

19.5 Nominal Logistic Regression

Ordinal regression is a special case of nominal regression with the proportional odds assumption.

19.5.1 Model

$$
\begin{aligned}
\text{rating}_i &\sim \text{Categorical}(\pi_i^1, \pi_i^2, \pi_i^3, \pi_i^4) \\
\pi_i^1 &= \frac{1}{\exp(\eta_i^2) + \exp(\eta_i^3) + \exp(\eta_i^4) + 1} \\
\pi_i^2 &= \frac{\exp(\eta_i^2)}{\exp(\eta_i^2) + \exp(\eta_i^3) + \exp(\eta_i^4) + 1} \\
\pi_i^3 &= \frac{\exp(\eta_i^3)}{\exp(\eta_i^2) + \exp(\eta_i^3) + \exp(\eta_i^4) + 1} \\
\pi_i^4 &= \frac{\exp(\eta_i^4)}{\exp(\eta_i^2) + \exp(\eta_i^3) + \exp(\eta_i^4) + 1} \\
\eta_i^2 &= \beta_0^2 + \beta_1^2 \text{fundamentalist}_i + \beta_2^2 \text{liberal}_i \\
\eta_i^3 &= \beta_0^3 + \beta_1^3 \text{belief}_i + \beta_2^3 \text{liberal}_i \\
\eta_i^4 &= \beta_0^4 + \beta_1^4 \text{belief}_i + \beta_2^4 \text{liberal}_i
\end{aligned}
$$

As you can see, it has two additional parameters for each predictor column.

```
m7 <- brm(
    rating ~ belief,
    data = stemcell,
    family = categorical(link = "logit"),
    prior = prior(std_normal(), class = "b", dpar = "mu2") +
        prior(std_normal(), class = "b", dpar = "mu3") +
        prior(std_normal(), class = "b", dpar = "mu4"),
    seed = 1340,
    file = "10_m7"
)
```

19.5.2 Model Comparison

```
msummary(list(`ordinal (proportional odds)` = m6, norminal = m7),
         estimate = "{estimate} [{conf.low}, {conf.high}]",
         statistic = NULL, fmt = 2)
```

```
Warning:
`modelsummary` uses the `performance` package to extract goodness-of-fit
statistics from models of this class. You can specify the statistics you wish
to compute by supplying a `metrics` argument to `modelsummary`, which will then
push it forward to `performance`. Acceptable values are: "all", "common",
```

Table 19.1: Comparison of the ordinal and nominal regression models.

	ordinal (proportional odds)	norminal
b_Intercept[1]	−0.94 [−1.18, −0.72]	
b_Intercept[2]	1.04 [0.81, 1.28]	
b_Intercept[3]	2.14 [1.86, 2.44]	
b_belieffundamentalist	0.41 [0.12, 0.72]	
b_beliefliberal	−0.55 [−0.85, −0.25]	
b_mu2_Intercept		0.63 [0.38, 0.90]
b_mu3_Intercept		−0.57 [−0.94, −0.20]
b_mu4_Intercept		−1.05 [−1.48, −0.65]
b_mu2_belieffundamentalist		0.12 [−0.29, 0.54]
b_mu2_beliefliberal		−0.69 [−1.06, −0.33]
b_mu3_belieffundamentalist		0.52 [0.00, 1.04]
b_mu3_beliefliberal		−0.77 [−1.32, −0.24]
b_mu4_belieffundamentalist		0.70 [0.13, 1.26]
b_mu4_beliefliberal		−0.58 [−1.18, 0.01]
Num.Obs.	829	829
R2	0.043	
ELPD	−1019.2	−1020.9
ELPD s.e.	15.5	15.6
LOOIC	2038.5	2041.8
LOOIC s.e.	31.1	31.2
WAIC	2038.5	2041.8

```
"none", or a character vector of metrics names. For example: `modelsummary(mod,
metrics = c("RMSE", "R2")` Note that some metrics are computationally
expensive. See `?performance::performance` for details.
 This warning appears once per session.
```

Part X

Week 13

20 Multilevel Models

In this note, we'll talk about multilevel models. To start, we have already seen a basic version of a multilevel—when discussing hierarchical models with partial pooling. There, we consider a binomial model with a parameter θ_j for each person, and consider a common distribution for all the θ parameters. A multilevel model is a model where we can have one or more cluster-specific parameters for each cluster (e.g., person, group, etc.), and these parameters are assumed to come from some common distributions.

We will use a within-subject example in this note, starting with a few data points to fit a model equivalent to a repeated-measure ANOVA, and then generalize to a multilevel regression model with varying intercepts and slopes. The latter is also called a growth curve model.

Naming of Multilevel Models

Multilevel models are very general and have been used in many different areas of research. Depending on the field of study, they are also called by the following names (not an exhaustive list):

- Hierarchical linear models
- Mixed-effects models
- Random-coefficients models

Special Cases of Multilevel Models

The following are some special cases or specific applications of multilevel models:

- Dependent-sample t-test
- Random-effect ANOVA
- Repeated-measure ANOVA
- Variance components models
- Growth curve models
- Generalizability theory
- Random-effect meta-analysis

20.1 Examples of Clustering

There are many different forms of clustering in data across different disciplines, including

- Students in schools
- Clients nested within therapists within clinics
- Employees nested within organizations
- Citizens nested within employees
- Repeated measures nested within persons

They can be represented in network graphs like Figure 20.1 (students within schools):

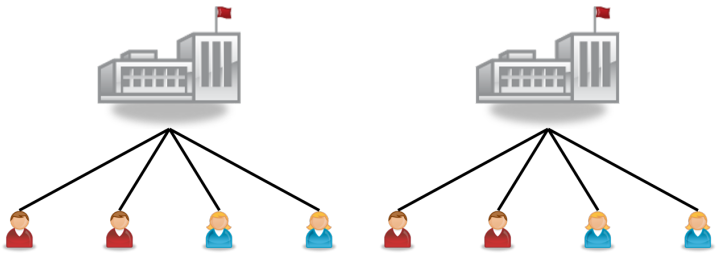


Figure 20.1

Sometimes, there is more than one level of clustering, like students clustered by middle and high schools. This is called a *crossed* structure, as shown in Figure 20.2, where we say that students are cross-classified by both middle and high schools. Another typical example in psychological experiments is when participants see multiple stimuli, each as an item, so the observations are cross-classified by both persons and items.

The scenario of repeated measures nested within persons is particularly relevant, as essentially all longitudinal data are multilevel and should be modelled accordingly. It allows one to build individualized models to look at within-person changes, as well as between-person differences of those changes. Techniques such as dependent-sample t-test, repeated-measures ANOVA, growth curve modeling, and time-series analyses, can all be represented in the multilevel modeling framework. Therefore, some authors, such as @ mcelreath2020, suggest that MLM should be the default model we use for analyses rather than regression.

20.2 Data

We will use the data set `sleepstudy` from the `lme4` package, a popular package for frequentist multilevel modeling. The data set contains 18 participants, each with 10 observations. It examines the change in average reaction time daily with increasing sleep deprivation. See `?lme4::sleepstudy` for more of the description. Here is a plot of the the `Reaction` variable:

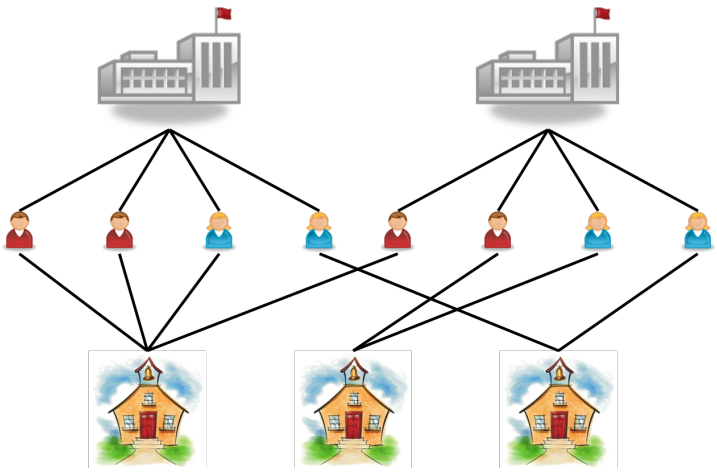


Figure 20.2

```
data(sleepstudy, package = "lme4")
hist(sleepstudy$Reaction)
```

Figure 20.3: Distribution of reaction times (ms)

This data set has clustering because it is repeated measures nested within persons. For the initial example, we will only take the first three time points (Days 1-3).

```
sleep3 <- sleepstudy |>
    filter(Days %in% 1:3)
head(sleep3)  # first two people
```

```
  Reaction Days Subject
1 258.7047    1     308
2 250.8006    2     308
3 321.4398    3     308
4 205.2658    1     309
5 202.9778    2     309
6 204.7070    3     309
```

> **Long-Format Data**
>
> Note that the data above is in *long format*, which is typically required for multilevel analysis. Here, each row of the data represents one observation, so there are multiple rows for each person. This is in contrast to *wide format*, where each row represents one person and has multiple columns for each observation.

Here is a *spaghetti plot* of each individual over the three days:

```
ggplot(sleep3, aes(x = Days, y = Reaction)) +
    geom_point(size = 0.5) +
    geom_line(aes(group = Subject)) +
    scale_x_continuous(breaks = 1:3) +
    ylab("Reaction Time (ms)")
```

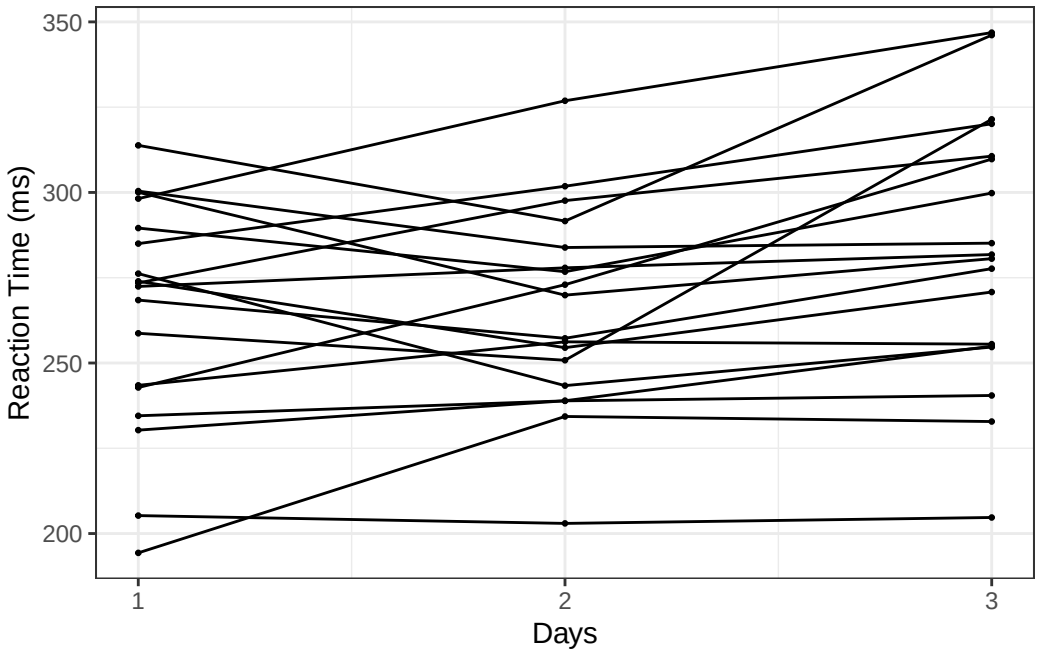


Figure 20.4: Reaction time change over three days.

The plot shows a general increasing trend of reaction time.

20.3 Analysis 1: Time as Nominal

This analysis is analogous to a repeated-measure ANOVA. Here, our interest is simply whether there are any differences across time, without any assumption on any linear or nonlinear trends. In other words, we treat time as a nominal variable.

20.3.1 Model

We use Reaction_{ij} to represent the reaction time for the jth person on the ith day.

$$\begin{aligned} \text{Reaction}_{ij} &\sim N(\mu_{ij}, \sigma) \\ \mu_{ij} &\sim N(\gamma_i, \tau) \end{aligned}$$

- μ_{ij}: the expected reaction time for person j on day i.
- σ: the within-person error.
- γ_i: the mean reaction time across participants on day i.

- τ: the between-person variance on a particular day.

> **Assumptions**
>
> The above model assumes:
>
> - Normality
> - Homogeneity of error variance across observations
> - Homogeneity of variance across persons

```
# Treat Days as a nominal variable
sleep3$Days_cat <- factor(sleep3$Days)
m1 <- brm(Reaction ~ 0 + Days_cat + (1 | Subject),
    data = sleep3,
    seed = 2225,
    file = "11_m1")
m1
```

```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: Reaction ~ 0 + Days_cat + (1 | Subject)
   Data: sleep3 (Number of observations: 54)
  Draws: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup draws = 4000

Multilevel Hyperparameters:
~Subject (Number of levels: 18)
              Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sd(Intercept)    31.56      6.16    21.58    45.07 1.00      869     1371

Regression Coefficients:
          Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Days_cat1   264.32      8.43   248.27   281.08 1.00      600      719
Days_cat2   265.21      8.37   248.87   282.11 1.00      632      640
Days_cat3   282.98      8.37   266.77   299.18 1.00      615      702

Further Distributional Parameters:
      Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sigma    16.70      2.17    13.28    21.77 1.00     2120     2344

Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
```

```
scale reduction factor on split chains (at convergence, Rhat = 1).
```

The model estimates the mean reaction time on each day, as well as the between-person and within-person variances. One can visualize the means:

```
conditional_effects(m1)
```

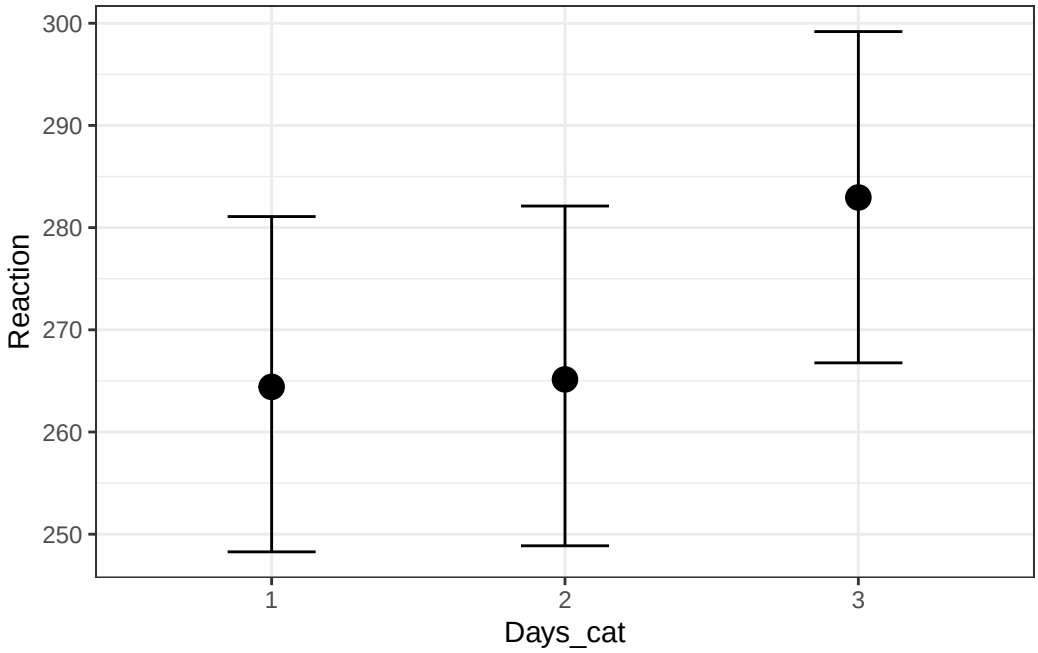


Figure 20.5: Model predicted mean reaction times over three days.

One can compare this model to one where the mean reaction time is assumed equal across days:

```
m0 <- brm(Reaction ~ 1 + (1 | Subject),
    data = sleep3,
    seed = 2225,
    file = "11_m0")
loo(m0, m1)
```

```
Warning: Found 2 observations with a pareto_k > 0.7 in model 'm1'. We recommend
to set 'moment_match = TRUE' in order to perform moment matching for
problematic observations.
```

```
Output of model 'm0':

Computed from 4000 by 54 log-likelihood matrix.

         Estimate   SE
elpd_loo   -245.9  5.9
p_loo        15.4  2.8
looic       491.7 11.9
------
MCSE of elpd_loo is 0.2.
MCSE and ESS estimates assume MCMC draws (r_eff in [0.4, 1.6]).

All Pareto k estimates are good (k < 0.7).
See help('pareto-k-diagnostic') for details.

Output of model 'm1':

Computed from 4000 by 54 log-likelihood matrix.

         Estimate  SE
elpd_loo   -239.2 4.6
p_loo        17.4 2.4
looic       478.3 9.2
------
MCSE of elpd_loo is NA.
MCSE and ESS estimates assume MCMC draws (r_eff in [0.4, 1.6]).

Pareto k diagnostic values:
                         Count Pct.    Min. ESS
(-Inf, 0.7]   (good)     52    96.3%   115
   (0.7, 1]   (bad)       2     3.7%   <NA>
   (1, Inf)   (very bad)  0     0.0%   <NA>
See help('pareto-k-diagnostic') for details.

Model comparisons:
   elpd_diff se_diff
m1  0.0       0.0
m0 -6.7       3.4
```

LOO indicates that allowing a different mean reaction time for each day fits the data better.

20.4 Analysis 2: Growth Curve

We will now use all 10 time points, and try to fit a line/curve to the time trend. Figure 20.6 shows the changes across participants.

```
ggplot(sleepstudy, aes(x = Days, y = Reaction)) +
    geom_point(size = 0.5) +
    geom_smooth() +
    # presented by person
    facet_wrap(~Subject, ncol = 6)
```

```
`geom_smooth()` using method = 'loess' and formula = 'y ~ x'
```

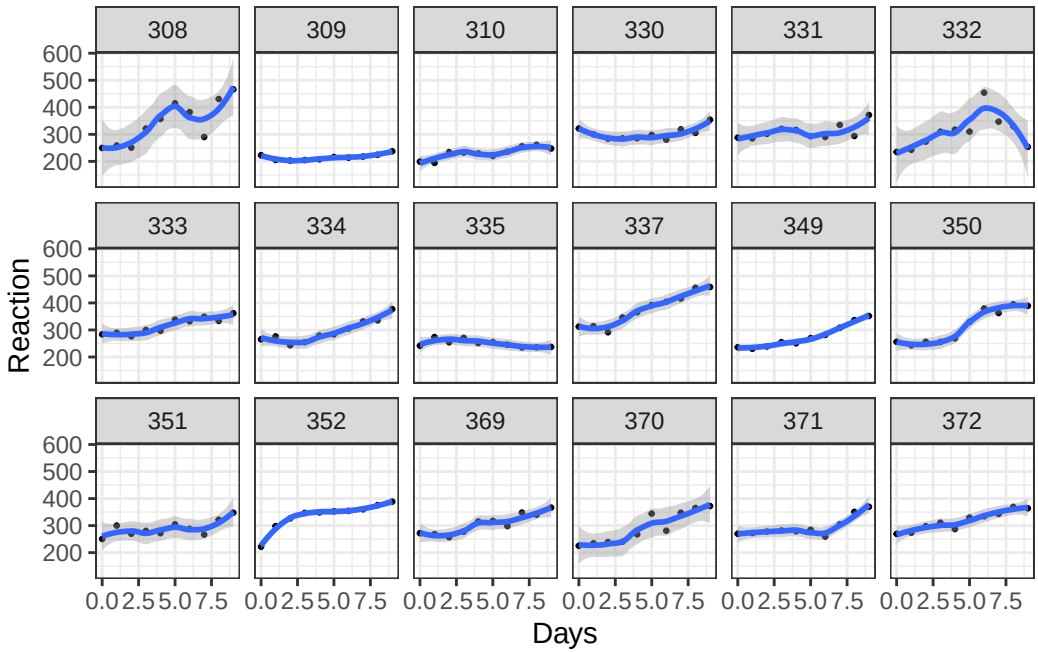


Figure 20.6: Individual trajectories across days.

As you can see, most people experience increases in reaction time, although there are certainly differences across individuals, such that each person has a different trajectory.

20.4.1 Intraclass correlation

With multilevel data, the first question is how much variation in the outcome is at each level. This is quantified by the *intraclass correlation*, which, for a two-level model, is defined by

$$\rho = \frac{\tau^2}{\tau^2 + \sigma^2}$$

where τ is the between-level *SD*, which is the *SD* of the cluster means (i.e., the variability of mean response time across persons in this example), and σ is the within-level *SD* (i.e., variability within a person, which is assumed constant across persons).

How Things Look With Different ICCs

The ICC represents the proportion of variance of the outcome that is due to between-level (e.g., between-group, between-person) differences

```
set.seed(1)
fake_dat1 <- data.frame(
    person = as.character(rep(1:8, 25)),
    y = rnorm(200,
        mean = rnorm(8, mean = 50, sd = 0.1),
        sd = 10
    )
)

pbase <- ggplot(fake_dat1, aes(x = person, y = y)) +
    geom_jitter(width = 0.1, col = "darkgrey") +
    stat_summary(
        geom = "point", fun = mean,
        size = 4, shape = 24, fill = "red"
    ) +
    ylim(20, 80) +
    theme(axis.text.y = element_blank())
pbase

fake_dat2 <- data.frame(
    person = as.character(rep(1:8, 25)),
    y = rnorm(200,
        mean = rnorm(8, mean = 50, sd = sqrt(20)),
        sd = sqrt(80)
    )
)
pbase %+% fake_dat2
```

Figure 20.8 shows substantial between-person variation for the `sleepstudy` data.

```
ggplot(sleepstudy, aes(x = Subject, y = Reaction)) +
    geom_jitter(width = 0.1, col = "darkgrey") +
    stat_summary(
        geom = "point", fun = mean,
        size = 4, shape = 24, fill = "red"
    )
```

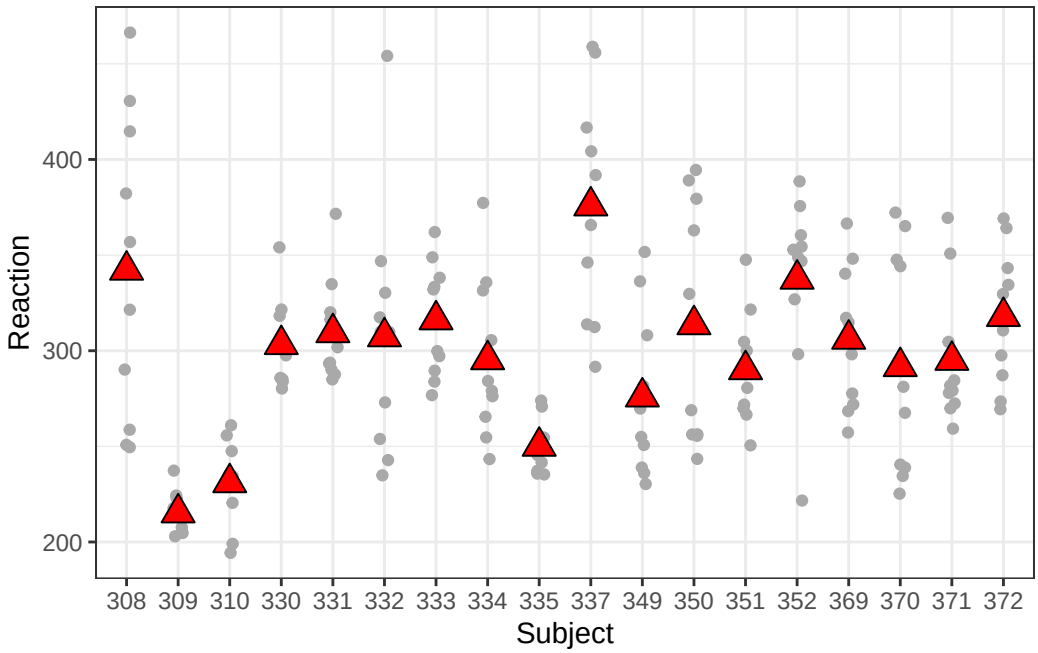


Figure 20.8: ICC for the `sleepstudy` data.

20.4.1.1 Computing ICC: Varying-intercept model

To compute the ICC, we need first to fit a multilevel model, which in this case is the *varying intercept* model:

$$\begin{aligned} \text{Reaction}_{ij} &\sim N(\mu_j, \sigma) \\ \mu_j &\sim N(\gamma, \tau) \end{aligned}$$

where μ_j is the mean reaction for the jth person.

We'll rescale `Reaction` by 10:

```r
sleepstudy <- sleepstudy |>
    mutate(Reaction10 = Reaction / 10)
```

To use weakly informative priors, we will set

$$\gamma \sim N(0, 50)$$
$$\sigma \sim t^{+}(4, 0, 5)$$
$$\tau \sim \text{Gamma}(2, 1/5)$$

```r
m2 <- brm(Reaction10 ~ (1 | Subject), data = sleepstudy,
          prior = c(# for intercept
            prior(normal(0, 50), class = "Intercept"),
            # for tau
            prior(gamma(2, 0.2), class = "sd"),
            # for sigma
            prior(student_t(4, 0, 5), class = "sigma")),
          # Higher adapt_delta is usually needed for MLM
          control = list(adapt_delta = .95),
          seed = 2107,
          file = "11_m2")
m2
```

```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: Reaction10 ~ (1 | Subject)
   Data: sleepstudy (Number of observations: 180)
  Draws: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup draws = 4000

Multilevel Hyperparameters:
~Subject (Number of levels: 18)
              Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sd(Intercept)     3.94      0.87     2.61     6.05 1.01      959     1207

Regression Coefficients:
          Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Intercept    29.81      1.00    27.78    31.82 1.01      662     1199

Further Distributional Parameters:
      Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sigma     4.45      0.25     3.98     4.96 1.00     3691     2506
```

```
Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

Now use the posterior draws of τ and σ to compute the posterior for the ICC:

```
icc_draws <- as_draws(m2, variable = c("sd_Subject__Intercept", "sigma")) |>
    mutate_variables(
        icc = sd_Subject__Intercept^2 / (sd_Subject__Intercept^2 + sigma^2)
    )
summary(icc_draws)
```

```
# A tibble: 3 x 10
  variable           mean median    sd   mad    q5   q95  rhat ess_bulk ess_tail
  <chr>             <dbl>  <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>    <dbl>    <dbl>
1 sd_Subject__Inte~ 3.94   3.81  0.873 0.761 2.77  5.58   1.01     959.     1207.
2 sigma             4.45   4.44  0.251 0.250 4.05  4.87   1.00    3691.     2506.
3 icc               0.432  0.426 0.104 0.104 0.271 0.613  1.01     947.     1339.
```

```
mcmc_dens(icc_draws, pars = "icc")
```

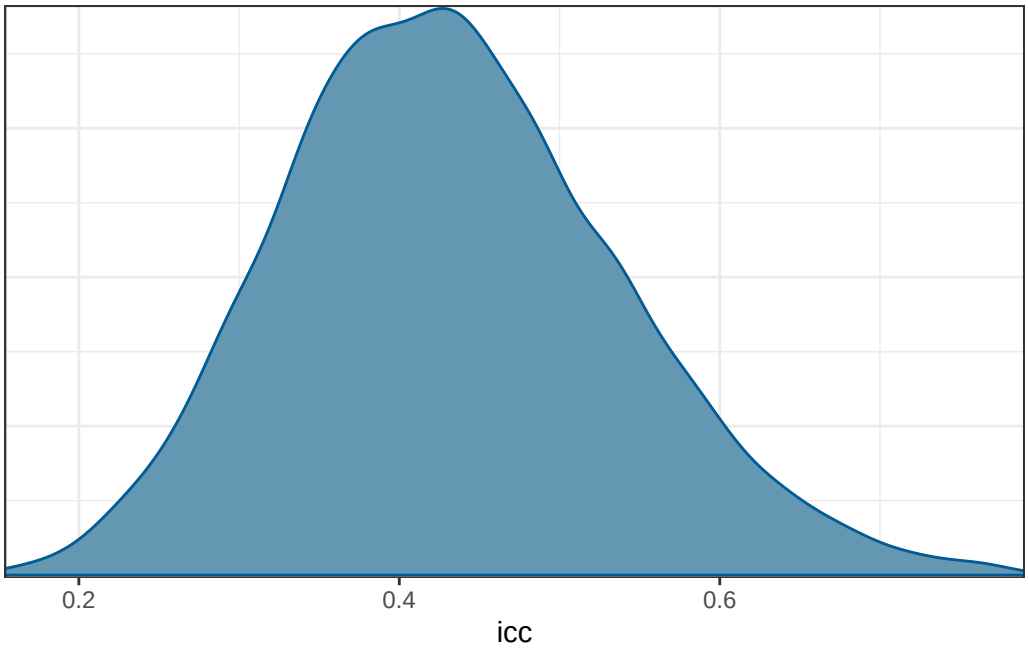


Figure 20.9: Posterior distribution of the ICC for reaction time.

Interpretations

The model suggested that the average reaction time across individuals and measurement occasions was 298ms, 90% CI [281ms, 314ms]. It was estimated that 43.22%, 90% CI [27.12%, 61.31%] of the variations in reaction time was attributed to between-person differences.

Is MLM Needed?

This is a commonly asked question. Based on Lai & Kwok (2015), you can compute the design effect index, which shows the inflation in the variability of the estimates due to clustering. It is recommended to account for clustering if the design effect is larger than 1.1. It is defined as:

$$\text{Deff} = 1 + (n - 1)\rho$$

where n is the (average) number of observations in each cluster, and in our case it is 10. Therefore, the design effect in `sleepstudy` for `Reaction` is

$$\text{Deff} = 1 + (10 - 1)(0.432219)$$

which is 4.889971, so we do need to account for the clustering.

20.5 Varying Coefficients

The strength of a multilevel model is that it can allow researchers to build models that allow for cluster-specific coefficients. In our example data, this is analogous to fitting separate models for each person, but instead of only using 10 data points for each model, MLM pools information from other people as it believes that we can learn something about one person by looking at data from other people.

For example, for each person, we'll fit a regression model using `Days` to predict `Reaction10`. Using our previous notations,

$$\begin{aligned} \text{Reaction10}_i &\sim N(\mu_i, \sigma) \\ \mu_i &= \beta_0 + \beta_1 \text{Days}_i \end{aligned}$$

However, because we have more than one person, we'll use the subscript j to denote the person, so that the model becomes

$$\begin{aligned} \text{Reaction10}_{ij} &\sim N(\mu_{ij}, \sigma_j) \\ \mu_{ij} &= \beta_{0j} + \beta_{1j} \text{Days}_{ij} \end{aligned}$$

which suggests that all three of β_0, β_1, and σ can be different across persons. We'll first start with varying β_0, or *varying intercepts*.

20.5.1 Varying Intercepts

With varying intercepts model, we assumed that only β_0 is different across persons, but β_1 and σ are common parameters that do not change across persons. This is called a *random intercept model* in (frequentist) MLM literature. Specifically, the model and priors are:

$$
\begin{aligned}
&\text{Repeated-measure level:} \\
&\qquad \text{Reaction10}_{ij} \sim N(\mu_{ij}, \sigma) \\
&\qquad \mu_{ij} = \beta_{0j} + \beta_1 \text{Days}_{ij} \\
&\text{Person level:} \\
&\qquad \beta_{0j} \sim N(\mu^{[\beta_0]}, \tau^{[\beta_0]}) \\
&\text{Priors:} \\
&\qquad \mu^{[\beta_0]} \sim N(0, 50) \\
&\qquad \tau^{[\beta_0]} \sim \text{Gamma}(2, 0.2) \\
&\qquad \beta_1 \sim N(0, 10) \\
&\qquad \sigma \sim t^+(4, 0, 5)
\end{aligned}
$$

where the β_{0j}s follow a common normal distribution with hyperparameters $\mu^{[\beta_0]}$ and $\tau^{[\beta_0]}$. Thus, $\mu^{[\beta_0]}$ is the *grand intercept*, or the average intercept across persons, and $\tau^{[\beta_0]}$ is the *SD* of those intercepts.

The model can be fitted in `brms`:

```
m3 <- brm(Reaction10 ~ Days + (1 | Subject),
    data = sleepstudy,
    prior = c( # for intercept
        prior(normal(0, 50), class = "Intercept"),
        # for slope
        prior(normal(0, 10), class = "b"),
        # for tau
        prior(gamma(2, 0.2), class = "sd"),
        # for sigma
        prior(student_t(4, 0, 5), class = "sigma")
    ),
    control = list(adapt_delta = .95),
    seed = 2107,
```

```
    file = "11_m3"
)
```

```
m3
```

```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: Reaction10 ~ Days + (1 | Subject)
   Data: sleepstudy (Number of observations: 180)
  Draws: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup draws = 4000

Multilevel Hyperparameters:
~Subject (Number of levels: 18)
              Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sd(Intercept)     4.11      0.82     2.85     6.04 1.00      765     1360

Regression Coefficients:
          Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Intercept    25.23      1.07    23.16    27.27 1.00      589      929
Days          1.05      0.08     0.89     1.21 1.00     2906     2862

Further Distributional Parameters:
      Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sigma     3.12      0.17     2.81     3.49 1.00     2370     2541

Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

Let's check the fit of the model to the data, first to the overall data and then to each individual.

20.5.1.1 Fit of Overall data

```
pp_check(m3, type = "intervals", x = "Days",
         re_formula = NA) +
    geom_smooth(se = FALSE, col = "blue") +
    geom_smooth(aes(y = y_obs), se = FALSE, col = "red", linetype = "dashed")
```

```
Using all posterior draws for ppc type 'intervals' by default.

`geom_smooth()` using method = 'loess' and formula = 'y ~ x'

Warning: The following aesthetics were dropped during statistical transformation: ymin,
ymax
i This can happen when ggplot fails to infer the correct grouping structure in
  the data.
i Did you forget to specify a `group` aesthetic or to convert a numerical
  variable into a factor?

`geom_smooth()` using method = 'loess' and formula = 'y ~ x'

Warning: The following aesthetics were dropped during statistical transformation: ymin,
ymax
i This can happen when ggplot fails to infer the correct grouping structure in
  the data.
i Did you forget to specify a `group` aesthetic or to convert a numerical
  variable into a factor?
```

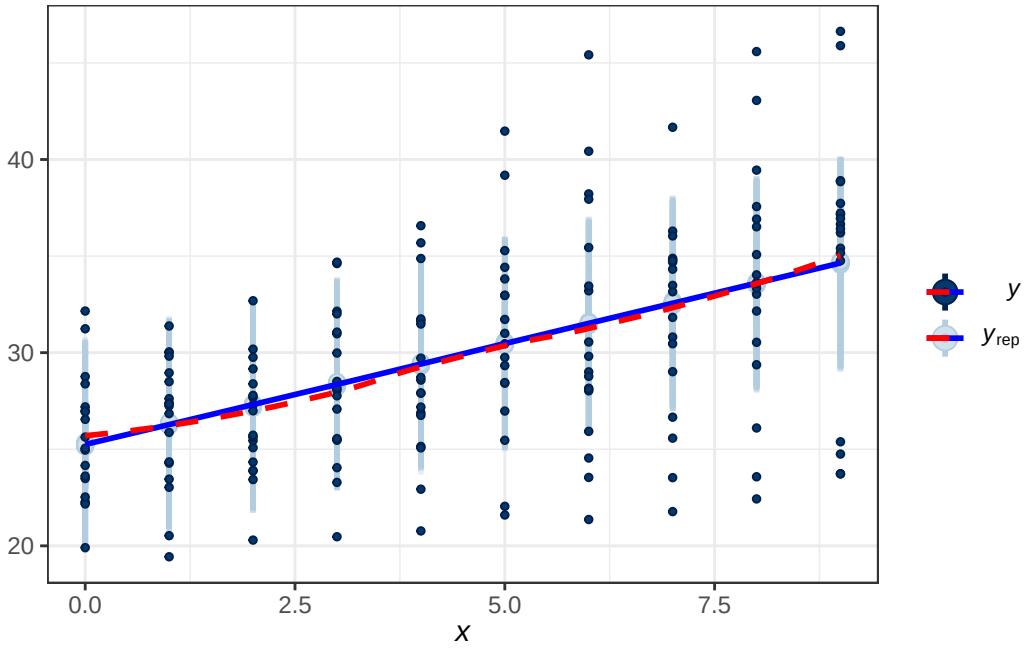


Figure 20.10: Marginal model plot of the overall data.

As can be seen, the estimated coefficient for `Days`, which was assumed constant for everyone, fit the overall data. However, does it fit each individual?

20.5.1.2 Fit of Individuals

```
ce_m3 <- conditional_effects(m3,
    re_formula = NULL,
    conditions = data.frame(Subject = unique(sleepstudy$Subject))
)
# Add original outcome variable
plot(ce_m3, points = TRUE, ncol = 6, plot = FALSE)[[1]] +
    geom_smooth(
        data = attr(ce_m3[[1]], "points"),
        aes(x = Days, y = resp__),
        se = FALSE, col = "red",
        linewidth = 0.8, alpha = 0.5,
        inherit.aes = FALSE
    )
```

```
`geom_smooth()` using method = 'loess' and formula = 'y ~ x'
```

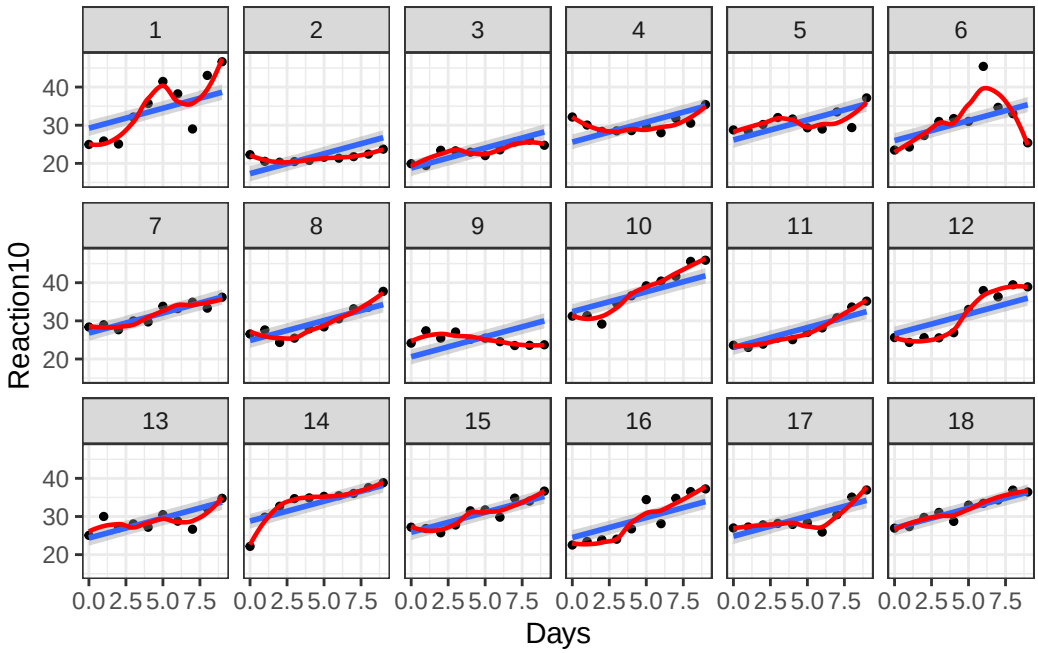


Figure 20.11: Marginal model plot by individuals, with only varying intercepts.

Obviously, it only fits a few individuals, but not all. So let's also allow β_1 to vary.

20.5.2 Varying Slopes

We'll now also allow β_1 to vary across clusters, with the following model:

$$
\begin{aligned}
&\text{Repeated-measure level:} \\
&\qquad \text{Reaction10}_{ij} \sim N(\mu_{ij}, \sigma) \\
&\qquad \mu_{ij} = \beta_{0j} + \beta_{1j}\text{Days}_{ij} \\
&\text{Person level:} \\
&\qquad \begin{bmatrix} \beta_{0j} \\ \beta_{1j} \end{bmatrix} \sim N_2 \left(\begin{bmatrix} \mu^{[\beta_0]} \\ \mu^{[\beta_1]} \end{bmatrix}, \mathbf{T} \right)
\end{aligned}
$$

where

$$
\mathbf{T} = \begin{bmatrix} {\tau^{[\beta_0]}}^2 & \\ \tau^{\beta 10} & {\tau^{[\beta_1]}}^2 \end{bmatrix}
$$

Note that N_2 denotes a bivariate normal (i.e., 2-dimensional multivariate normal) distribution, because now we can talk about how β_0 and β_1 are associated at the person level. Generally, I

don't interpret the covariance between them because it largely depends on how the variables were centered, but we should allow them to be correlated. The parameter $\tau^{\beta 10}$ thus denotes their covariance.

> **i** Programs using Gibbs sampling, such as `MCMCglmm`, use an inverse-Wishart distribution as a prior for the covariance matrix $\mathbf{T}$, but it has been shown to usually lead to biased and inefficient estimates.

To estimate $\mathbf{T}$, recent recommendations, as implemented in `brms`, suggest decomposing $\mathbf{T}$ into a correlation matrix and the scaling matrices, and using an LKJ prior to the correlation matrix. We explain the LKJ prior in Important 1. Let's first do the decomposition:

$$\mathbf{T} = \text{diag}(\tau)\Omega\text{diag}(\tau),$$

where $\mathbf{T} = [\tau_1, \tau_2, ...]$ is a vector containing the scale parameters (i.e., *SD*) of the varying coefficients, and Ω is the correlation matrix of the varying coefficients.

Important 1: LKJ Prior

The LKJ Prior is a probability distribution for correlation matrices. A correlation matrix has 1 on all the diagonal elements. For example, a 2×2 correlation matrix is

$$\begin{bmatrix} 1 & \\ 0.35 & 1 \end{bmatrix}$$

where the correlation is 0.35. Therefore, with two variables, there is one correlation; with three or more variables, the number of correlations will be $q(q-1)/2$, where q is the number of variables.

For a correlation matrix of a given size, the LKJ prior has one shape parameter, η, where $\eta = 1$ corresponds to a uniform distribution of the correlations such that any correlations are equally likely, $\eta \geq 1$ favors a matrix closer to an identity matrix so that the correlations are closer to zero, and $\eta \leq 1$ favors a matrix with larger correlations. For a 2×2 matrix, the distribution of the correlation, ρ, with different

The resulting model and priors are:

$$
\begin{aligned}
&\text{Repeated-measure level:} \\
&\qquad \text{Reaction10}_{ij} \sim N(\mu_{ij}, \sigma) \\
&\qquad \mu_{ij} = \beta_{0j} + \beta_{1j}\text{Days}_{ij} \\
&\text{Person level:} \\
&\qquad \begin{bmatrix} \beta_{0j} \\ \beta_{1j} \end{bmatrix} \sim N_2\left(\begin{bmatrix} \mu^{[\beta_0]} \\ \mu^{[\beta_1]} \end{bmatrix}, \mathbf{T}\right) \\
&\qquad \mathbf{T} = \text{diag}(\tau)\Omega\text{diag}(\tau) \\
&\text{Priors:} \\
&\qquad \mu^{[\beta_0]} \sim N(0, 50) \\
&\qquad \mu^{[\beta_1]} \sim N(0, 10) \\
&\qquad \tau^{[\beta_m]} \sim \text{Gamma}(2, 0.2),\ m = 0, 1 \\
&\qquad \Omega \sim \text{LKJ}(1) \\
&\qquad \sigma \sim t^{+}(4, 0, 5)
\end{aligned}
$$

```
m4 <- brm(Reaction10 ~ Days + (Days | Subject),
    data = sleepstudy,
    prior = c( # for intercept
        prior(normal(0, 50), class = "Intercept"),
        # for slope
        prior(normal(0, 10), class = "b"),
        # for tau_beta0 and tau_beta1
        prior(gamma(2, 0.2), class = "sd", group = "Subject"),
        # for correlation
        prior(lkj(1), class = "cor"),
        # for sigma
        prior(student_t(4, 0, 5), class = "sigma")
    ),
    control = list(adapt_delta = .95),
    seed = 2107,
    file = "11_m4"
)
```

```
m4
```

```
 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: Reaction10 ~ Days + (Days | Subject)
```

```
   Data: sleepstudy (Number of observations: 180)
  Draws: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup draws = 4000

Multilevel Hyperparameters:
~Subject (Number of levels: 18)
                    Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sd(Intercept)           2.83      0.70     1.68     4.41 1.00     1637     2216
sd(Days)                0.69      0.16     0.44     1.09 1.00     1875     2371
cor(Intercept,Days)     0.06      0.31    -0.52     0.67 1.00     1108     1623

Regression Coefficients:
          Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Intercept    25.12      0.78    23.55    26.66 1.00     2342     2378
Days          1.04      0.18     0.70     1.41 1.00     1745     2239

Further Distributional Parameters:
      Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sigma     2.59      0.16     2.29     2.92 1.00     3940     2874

Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

20.5.2.1 Fit of Individuals

```r
ce_m4 <- conditional_effects(m4,
    re_formula = NULL,
    conditions = data.frame(Subject = unique(sleepstudy$Subject))
)
# Add original outcome variable
plot(ce_m4, points = TRUE, ncol = 6, plot = FALSE)[[1]] +
    geom_smooth(
        data = attr(ce_m4[[1]], "points"),
        aes(x = Days, y = resp__),
        se = FALSE, col = "red",
        linewidth = 0.8, alpha = 0.5,
        inherit.aes = FALSE
    )
```

```
`geom_smooth()` using method = 'loess' and formula = 'y ~ x'
```

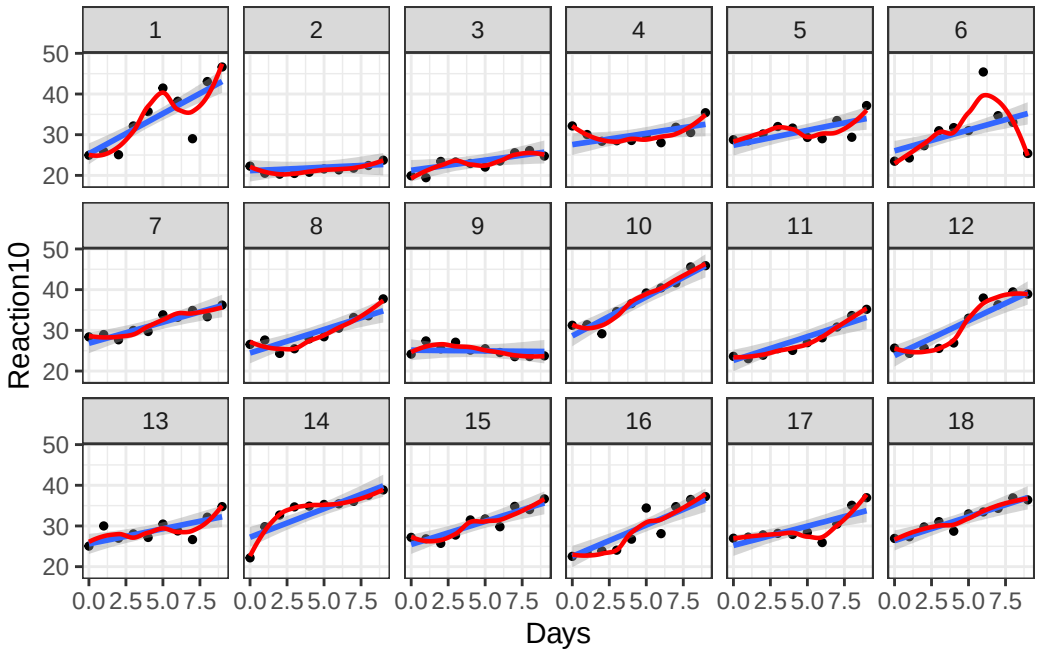


Figure 20.13: Marginal model plot by individuals, with varying slopes.

You can see that the fit is better. You can also visualize the varying regression lines:

```
plot(
    conditional_effects(m4,
        effects = "Days:Subject",
        re_formula = NULL,
        # suppress credible band
        prob = 0
    ),
    points = TRUE,
    point_args = list(size = 0.5),
)
```

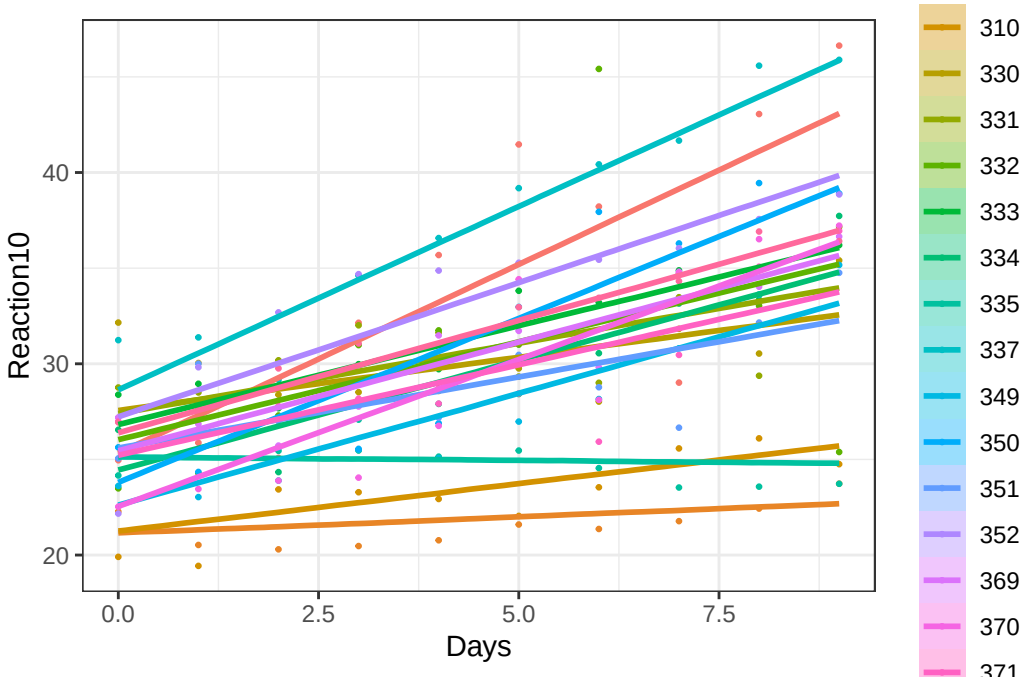


Figure 20.14: Varying regression lines on the same plot.

Interpretations

Based on the model, at Day 0, the average reaction time across individuals was 251ms, 90% CI [238ms, 264ms], and the *SD* at Day 0 was 28.3178086ms, 95% CI [18.060615ms, 40.863435ms].
The average rate of change per day in reaction time across individuals was 10ms, 90% CI [7.6ms, 13ms], and the *SD* of the rates of change at Day 0 was 6.9012462ms, 95% CI [4.6810815ms, 10.04862ms], as shown in Figure 20.14.

Fixed-Effects Model

You can compare the previous model with one that has different slopes for different persons, which can be modelled by including an interaction with the categorical `Subject` predictor. This is referred to as the *fixed-effects* model, as opposed to the *random-effects* model used to describe hierarchical models with partial pooling. Below is an example:

```
m4_fixed <- brm(Reaction10 ~ Days * I(factor(Subject)),
    data = sleepstudy,
    prior = c( # for intercept
        prior(normal(0, 50), class = "Intercept"),
        # for slope
        prior(normal(0, 10), class = "b"),
        # for sigma
        prior(student_t(4, 0, 5), class = "sigma")
```

So far, we have yet to talk about including person-level predictors. If such predictors are available, such as gender, we can use those to predict individual differences in intercepts (main effect) and slopes (i.e., interaction with `Days`). Just add those predictors to the model by:

$$\begin{aligned}
\begin{bmatrix}\beta_{0j}\\ \beta_{1j}\end{bmatrix} &\sim N_2\left(\begin{bmatrix}\mu_j^{[\beta_0]}\\ \mu_j^{[\beta_1]}\end{bmatrix}, \mathbf{T}\right)\\
\mathbf{T} &= \text{diag}(\tau)\Omega\text{diag}(\tau)\\
\mu_j^{[\beta_0]} &= \gamma_{00} + \gamma_{01}X_j\\
\mu_j^{[\beta_1]} &= \gamma_{10} + \gamma_{11}X_j
\end{aligned}$$

where X_j is a person-level predictor.

20.5.3 Varying σ

Finally, you can also allow σ to differ across individuals. This is typically used to relax the homogeneity of variance assumption, but recently, there has also been some interest in treating varying σ as an important outcome. Examples include fluctuations in mood, as two people with the same mean level of mood may fluctuate very differently, and mood swing can be an important outcome to assess. There have been some interesting applications in health research using ecological momentary assessment data. For an overview, see the paper by Hedeker et al. (2008).

Without going into the details, here is the model and the priors:

Repeated-measure level:

$$\begin{aligned}
\text{Reaction10}_{ij} &\sim N(\mu_{ij}, \sigma_j) \\
\mu_{ij} &= \beta_{0j} + \beta_{1j}\text{Days}_{ij}
\end{aligned}$$

Person level:

$$\begin{aligned}
\begin{bmatrix} \beta_{0j} \\ \beta_{1j} \\ \log(\sigma_j) \end{bmatrix} &\sim N_2 \left(\begin{bmatrix} \mu^{[\beta_0]} \\ \mu^{[\beta_1]} \\ \mu^{[s]} \end{bmatrix}, \mathbf{T} \right) \\
\mathbf{T} &= \text{diag}(\tau)\Omega\text{diag}(\tau)
\end{aligned}$$

Priors:

$$\begin{aligned}
\mu^{[\beta_0]} &\sim N(0, 50) \\
\mu^{[\beta_1]} &\sim N(0, 10) \\
\mu^{[s]} &\sim t^{+}(4, 0, 1.6) \\
\tau^{[\beta_m]} &\sim \text{Gamma}(2, 0.2),\ m = 0, 1 \\
\tau^{[s]} &\sim \text{Gamma}(2, 0.625) \\
\Omega &\sim \text{LKJ}(1)
\end{aligned}$$

```
# Use |p| to estimate the covariance between the sigma and beta random effects
m5 <- brm(
    bf(
        Reaction10 ~ Days + (Days | p | Subject),
        sigma ~ (1 | p | Subject)
    ),
    data = sleepstudy,
    prior = c( # for intercept
        prior(normal(0, 50), class = "Intercept"),
        # for slope
        prior(normal(0, 10), class = "b"),
        # for tau_beta0
        prior(gamma(2, 0.2),
            class = "sd", coef = "Intercept",
            group = "Subject"
        ),
        # for tau_beta1
        prior(gamma(2, 0.2),
            class = "sd", coef = "Days",
            group = "Subject"
        ),
        # for correlation
```

```
        prior(lkj(1), class = "cor"),
        # for sigma
        prior(student_t(4, 0, 1.6), class = "Intercept", dpar = "sigma"),
        # for tau_sigma
        prior(gamma(2, 0.625),
            class = "sd", coef = "Intercept",
            group = "Subject", dpar = "sigma"
        )
    ),
    control = list(adapt_delta = .95),
    seed = 2107,
    file = "11_m5"
)
```

```
m5
```

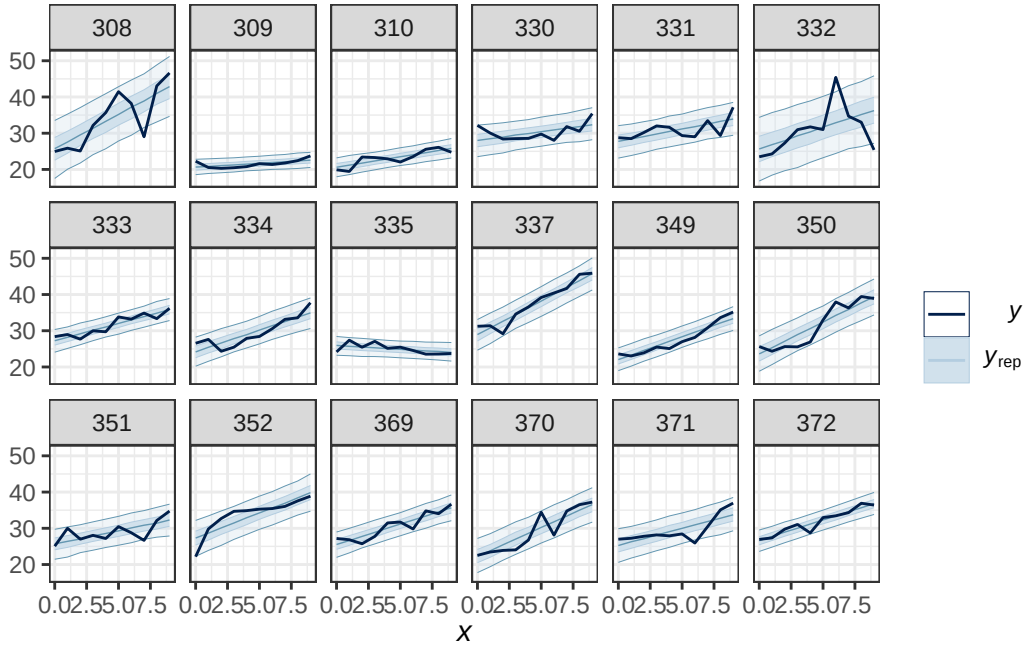
```
 Family: gaussian
  Links: mu = identity; sigma = log
Formula: Reaction10 ~ Days + (Days | p | Subject)
         sigma ~ (1 | p | Subject)
   Data: sleepstudy (Number of observations: 180)
  Draws: 4 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup draws = 4000

Multilevel Hyperparameters:
~Subject (Number of levels: 18)
                               Estimate Est.Error l-95% CI u-95% CI Rhat
sd(Intercept)                      3.16      0.71     2.06     4.87 1.00
sd(Days)                           0.70      0.16     0.46     1.07 1.00
sd(sigma_Intercept)                0.51      0.12     0.31     0.79 1.00
cor(Intercept,Days)               -0.01      0.27    -0.50     0.52 1.00
cor(Intercept,sigma_Intercept)     0.22      0.29    -0.39     0.73 1.00
cor(Days,sigma_Intercept)          0.45      0.26    -0.13     0.85 1.00
                               Bulk_ESS Tail_ESS
sd(Intercept)                      1766     2385
sd(Days)                           1574     2486
sd(sigma_Intercept)                1693     2606
cor(Intercept,Days)                1086     1634
cor(Intercept,sigma_Intercept)     1580     2292
cor(Days,sigma_Intercept)          1581     2217

Regression Coefficients:
```

```
                Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Intercept          25.11      0.83     23.52     26.77 1.00     1353     1760
sigma_Intercept     0.73      0.14      0.44      1.02 1.00     1592     1767
Days                1.05      0.18      0.70      1.40 1.00     1186     1879

Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

Here is the posterior predictive check:

```
pp_check(m5, type = "ribbon_grouped", group = "Subject", x = "Days",
         facet_args = list(ncol = 6, scales = "fixed"))
```

```
Using all posterior draws for ppc type 'ribbon_grouped' by default.
```



20.6 Model Comparisons

We can compare the previous models from `m3` to `m5`, with `m3` being the least complex and `m5` being the most complex. However, it should be noted that, because of the way how STAN computes LOOIC and WAIC,

effect		Varying Intercepts	Varying Intercepts and Slopes
fixed	b_Intercept	25.23 [23.16, 27.27]	25.12 [23.55, 26.66]
	b_Days	1.05 [0.89, 1.21]	1.04 [0.70, 1.41]
	sigma	3.11 [2.81, 3.49]	2.58 [2.29, 2.92]
	b_sigma_Intercept		
random	sd_Subject___Intercept	3.98 [2.85, 6.04]	2.75 [1.68, 4.41]
	sd_Subject___Days		0.67 [0.44, 1.09]
	cor_Subject___Intercept___Days		0.06 [−0.52, 0.67]
	sd_Subject___sigma_Intercept		
	cor_Subject___Intercept___sigma_Intercept		
	cor_Subject___Days___sigma_Intercept		
	Num.Obs.	180	180
	ELPD	−470.0	−447.0
	ELPD s.e.	14.3	22.7
	LOOIC	940.0	894.0
	LOOIC s.e.	28.6	45.5
	WAIC	939.5	891.0

> The LOOIC and WAIC computed in STAN (including `brms`) generally cannot be used to compare models with different level-2 predictors.

The problem is illustrated in this blog post: https://deepthoughtsandsilliness.blogspot.com/2007/12/focus-on-dic.html in the context of DIC.

```
msummary(
    list(
        `Varying Intercepts` = m3,
        `Varying Intercepts and Slopes` = m4,
        `Varying Intercepts, Slopes, and Variances` = m5
    ),
    metrics = c("WAIC", "LOOIC"),
    estimate = "{estimate} [{conf.low}, {conf.high}]",
    shape = effect + term ~ model,
    fmt = 2
)
```

21 Missing Data

Missing data are common in many research problems. Sometimes missing data arise from design, but more commonly, data are missing for reasons that are beyond researchers' control.

22 Missing Data Mechanisms

The treatment of missing data depends on the underlying causal structure (likely everything else), so you need some causal diagrams. The following examples are based on the ones in McElreath (2020, chapter 15.2). Let's say we have a sample of students. I want to study the association between the number of hours each student studied per day (S) and the quality of the homework (H). We have the following DAG:

```
dag1 <- dagitty("dag{ S -> H }")
coordinates(dag1) <- list(x = c(S = 0, H = 1),
                          y = c(S = 0, H = 0))
# Plot
ggdag(dag1) + theme_dag()
```

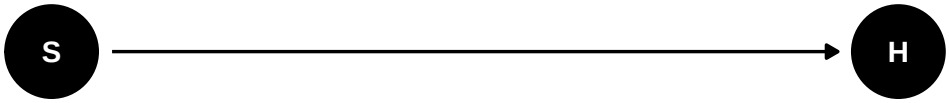


Figure 22.1: DAG for the association between study hours and homework quality.

Let's say the actual data generating model is

$$H_i \sim N(\beta_0 + \beta_1 S_i, \sigma),$$

with $\beta_0 = 5$, $\beta_1 = 1$, $\sigma = 0.7$.

```
set.seed(1551)
num_obs <- 200
full_data <- data.frame(
    S = pmin(rgamma(num_obs, shape = 10, scale = 0.2), 5)
) |>
    mutate(H = 5 + S + rnorm(S, sd = 0.7))
```

```
ggplot(full_data, aes(x = S, y = H)) +
    geom_point() +
    geom_smooth(method = "lm")
```

```
`geom_smooth()` using formula = 'y ~ x'
```

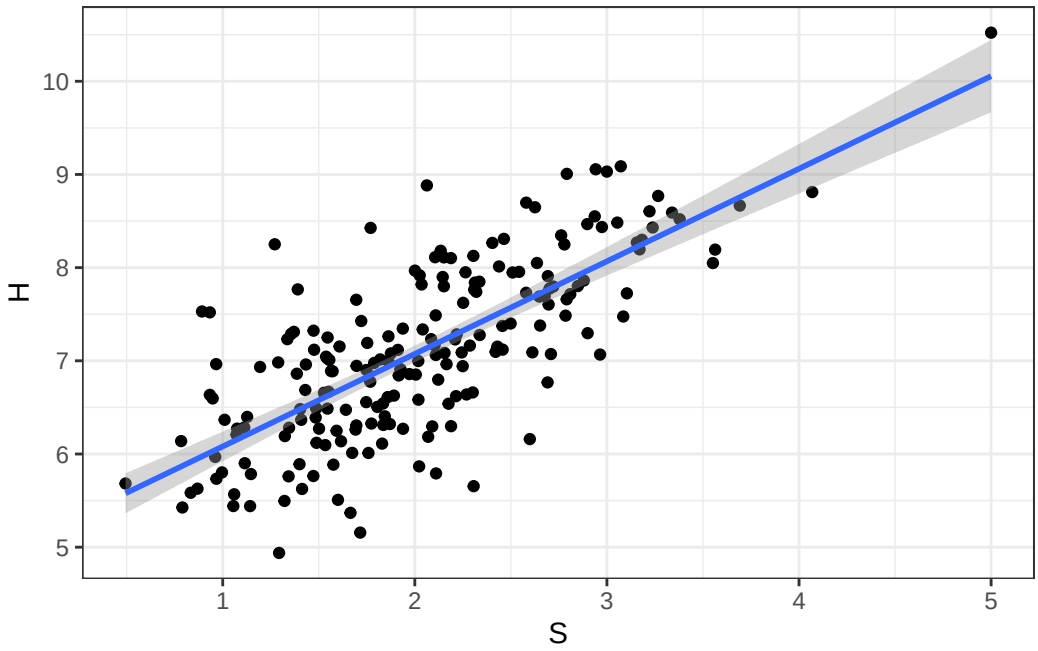


Figure 22.2: Simulated full data with the association between study hours and homework quality.

The statistical literature has generally distinguished three types of missing data mechanisms, with some confusing names: missing completely at random (MCAR), missing at random (MAR), and missing not at random (MNAR). Let's see each of them with the corresponding causal diagram.

22.1 Missing Completely At Random

Let's say all students have dogs, and somehow for some of the students, their dogs would eat their homework, producing missing data. Let D be an indicator for whether the dog ate the homework. To be consistent with the missing data literature, we set $D = 0$ to mean that the dog ate the homework, so that there is missing homework. When $D = 1$, the homework is turned in.

The impact of missing data is through two things. First, it reduces the sample size. Second, and more importantly, it can lead to a biased sample that gives non-representative estimates, compared to what you would get with the full data. Think about why polls may get election results wrong, even if they have a large sample: the sample in the pool has different characteristics from the actual voters.

The missing data mechanism that is relatively less harmful is missing completely at random (MCAR). It means that why the data are missing—or why the dog ate the homework—happens **completely** on a random basis. Let H* be the observed homework variable with missing data. We have the DAG in Figure 22.3:

```
dag2 <- dagitty('dag{ "S" -> "H" -> "H*" ; "D" -> "H*"}')
latents(dag2) <- c("H")
coordinates(dag2) <- list(x = c(S = 0, H = 1, `H*` = 1, D = 0),
                          y = c(S = 1, H = 1, `H*` = 0, D = 0))
# Plot
ggdag(dag2) + theme_dag()
```

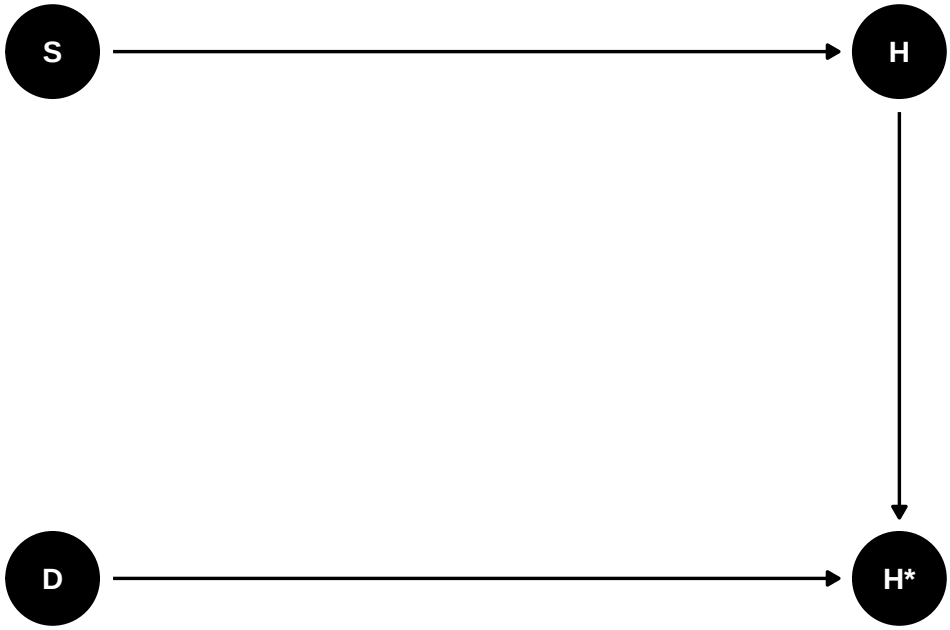


Figure 22.3: DAG for missing completely at random.

From the DAG, the association between S and H* is not confounded by D, so missing data won't bias the coefficient.

Let's simulate ~ 25% completely random missing data.

```
mcar_data <- full_data |>
    mutate(D = rbinom(num_obs, size = 1, prob = .75),
           Hs = if_else(D == 1, H, NA_real_))
```

```
ggplot(mcar_data) +
    geom_histogram(aes(x = H, fill = "full data"), alpha = 0.5) +
    geom_histogram(aes(x = Hs, fill = "observed data"), alpha = 0.5) +
    labs(fill = NULL)
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

```
Warning: Removed 59 rows containing non-finite values (`stat_bin()`).
```

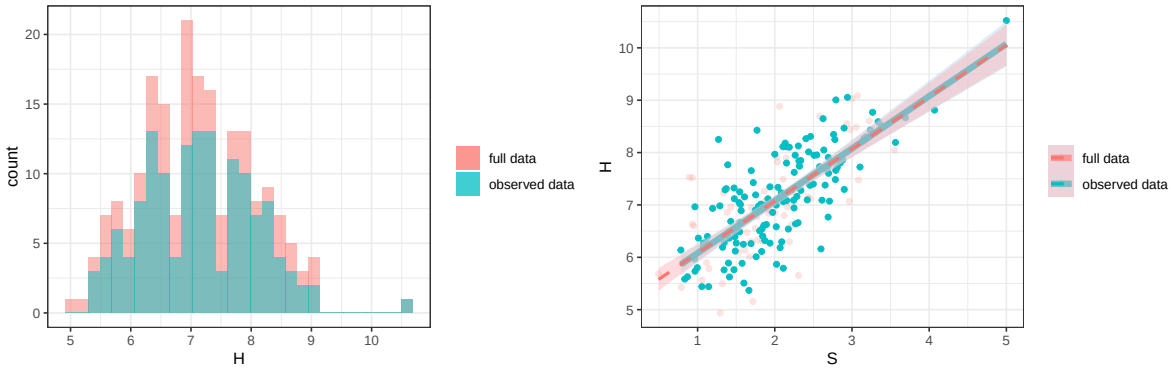
```
ggplot(full_data, aes(x = S, y = H)) +
    geom_point(aes(col = "full data"), alpha = 0.2) +
    geom_point(data = mcar_data, aes(y = Hs, col = "observed data")) +
    geom_smooth(data = mcar_data,
                aes(y = Hs, col = "observed data"),
                method = "lm", linewidth = 2, fill = "lightblue") +
    geom_smooth(aes(col = "full data"),
                method = "lm", alpha = 0.5, linetype = "dashed",
                fill = "lightpink") +
    labs(col = NULL)
```

```
`geom_smooth()` using formula = 'y ~ x'
```

```
Warning: Removed 59 rows containing non-finite values (`stat_smooth()`).
```

```
`geom_smooth()` using formula = 'y ~ x'
```

```
Warning: Removed 59 rows containing missing values (`geom_point()`).
```



(a) Histogram.

(b) Scatter plot with regression lines.

Figure 22.4: Simulated MCAR data.

The regression line is pretty much the same as what you got with the full data; just that the uncertainty bound is a bit wider.

22.2 Missing At Random

Now, let's consider the situation where dogs are more dissatisfied when the students spend more time studying, and less time with them, so they are more likely to eat the homework. The term missing at random is a very confusing terminology, but it means that observed data in the model can explain the missingness. So if we include S in the model, we account for the missing data mechanism. We can see the DAG in Figure 22.5:

```
dag3 <- dagitty('dag{ "S" -> "H" -> "H*" ; "S" -> "D" -> "H*"}')
latents(dag3) <- c("H")
coordinates(dag3) <- list(x = c(S = 0, H = 1, `H*` = 1, D = 0),
                          y = c(S = 1, H = 1, `H*` = 0, D = 0))
# Plot
ggdag(dag3) + theme_dag()
```

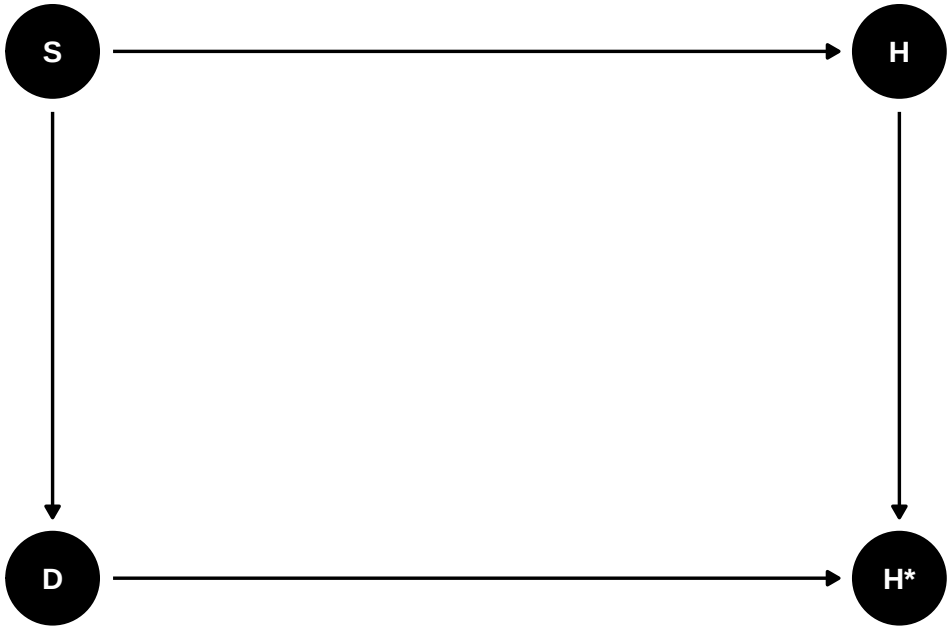


Figure 22.5: DAG for missing at random.

Another way to determine whether S is sufficient to account for the missing data mechanism is to use the d-separation criteria, which you can find in the `dagitty` package with the `dseparated()` function. The goal is to find a variable set that makes D and H conditionally independent.

```
dseparated(dag3, "D", "H", Z = c("S"))  # d-separated
```

```
[1] TRUE
```

Let's simulate some data with the dogs eating homework for the most hardworking students (or those who study too much).

```
mar_data <- full_data |>
    mutate(D = as.numeric(S < quantile(S, probs = .75)),
           Hs = if_else(D == 1, H, NA_real_))
```

As you can see in Figure 22.6, the distribution of H is now very different from that of $H*$, but it does not distort the association between S and H.

```
ggplot(mar_data) +
    geom_histogram(aes(x = H, fill = "full data"), alpha = 0.5) +
    geom_histogram(aes(x = Hs, fill = "observed data"), alpha = 0.5) +
    labs(fill = NULL)
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

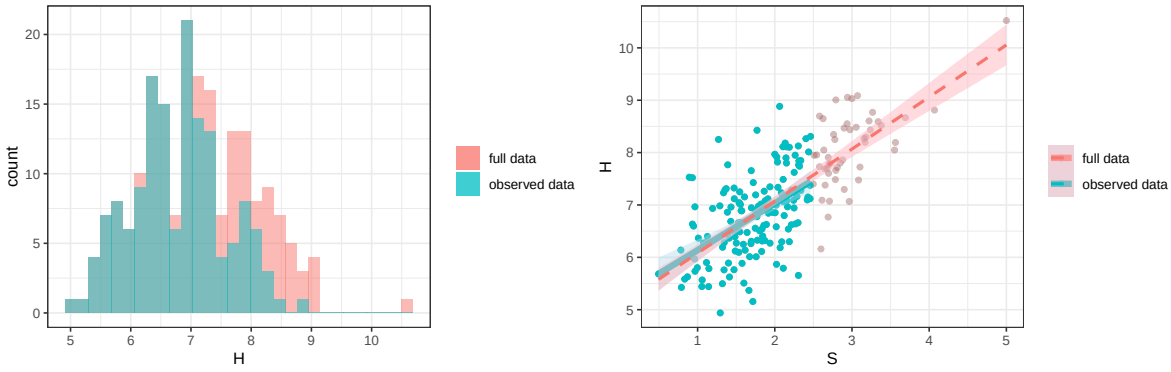
```
Warning: Removed 50 rows containing non-finite values (`stat_bin()`).
```

```
ggplot(full_data, aes(x = S, y = H)) +
    geom_point(alpha = 0.2) +
    geom_point(aes(col = "full data"), alpha = 0.2) +
    geom_point(data = mar_data, aes(y = Hs, col = "observed data")) +
    geom_smooth(data = mar_data,
                aes(y = Hs, col = "observed data"),
                method = "lm", linewidth = 2, fill = "lightblue") +
    geom_smooth(aes(col = "full data"),
                method = "lm", alpha = 0.5, linetype = "dashed",
                fill = "lightpink") +
    labs(col = NULL)
```

```
`geom_smooth()` using formula = 'y ~ x'
```

```
Warning: Removed 50 rows containing non-finite values (`stat_smooth()`).
```

```
`geom_smooth()` using formula = 'y ~ x'

Warning: Removed 50 rows containing missing values (`geom_point()`).
```



(a) Histogram.

(b) Scatter plot with regression lines.

Figure 22.6: Simulated MAR data.

22.3 Missing Not At Random

Now, let's imagine there is an additional variable, X, representing the noise level at the student's home. As you can guess, dogs are more likely to misbehave in noisier environments, and homework quality may suffer in a noisier environment. So we have Figure 22.7.

```
dag4 <- dagitty('dag{ "S" -> "H" -> "H*" ; "S" -> "D" -> "H*";
                      "D" <- "X" -> "H" }')
latents(dag4) <- c("H")
coordinates(dag4) <- list(x = c(S = 0, H = 1, `H*` = 1, D = 0, X = 0.5),
                          y = c(S = 1, H = 1, `H*` = 0, D = 0, X = 0.5))
# Plot
ggdag(dag4) + theme_dag()
```

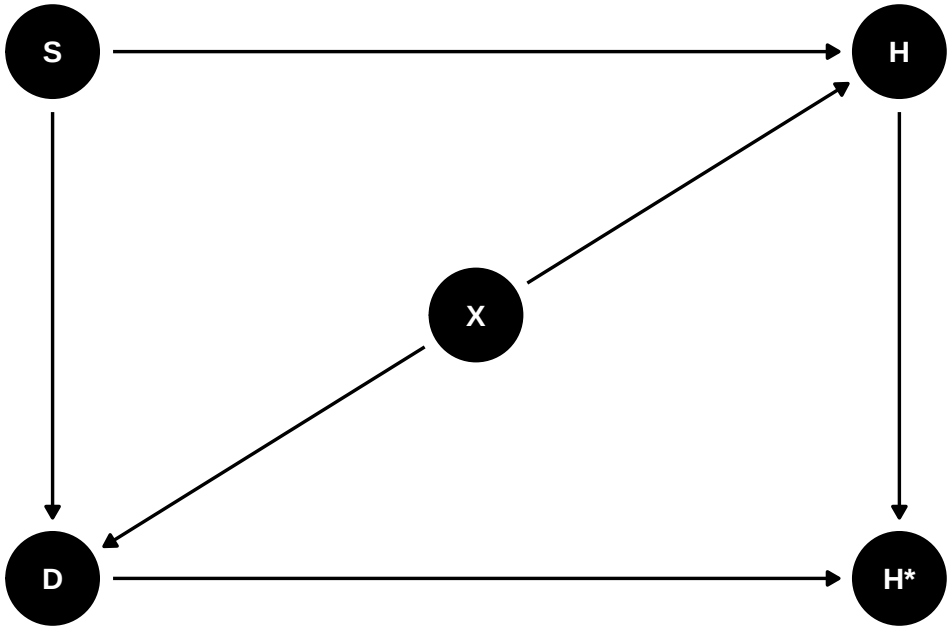


Figure 22.7: DAG for missing not at random.

If we only include $ S$ to predict $ H*$ in our model, this mechanism is called **missing not at random (MNAR)**. Here, even when we condition on S, there is still an association between D and H, due to the shared parent X. We can see this in R:

```
dseparated(dag4, "D", "H", Z = c("S"))  # not d-separated
```

```
[1] FALSE
```

So the missing data will lead to biased results. Let's simulate some data.

```
set.seed(1551)
full_data2 <- data.frame(
    S = pmin(rgamma(num_obs, shape = 10, scale = 0.2), 5),
    X = rnorm(num_obs)
) |>
    mutate(H = 5.5 + S - X + rnorm(S, sd = 0.5))
mnar_data1 <- full_data2 |>
    mutate(D = rbinom(num_obs, size = 1,
                      prob = plogis(S - 2 * X)),
           Hs = if_else(D == 1, H, NA_real_))
```

```r
ggplot(full_data2, aes(x = S, y = H)) +
    geom_point(aes(col = "full data"), alpha = 0.2) +
    geom_point(data = mnar_data1, aes(y = Hs, col = "observed data")) +
    geom_smooth(data = mnar_data1,
                aes(y = Hs, col = "observed data"),
                method = "lm", size = 2, fill = "lightblue") +
    geom_smooth(aes(col = "full data"),
                method = "lm", alpha = 0.5, linetype = "dashed",
                fill = "lightpink") +
    labs(col = NULL)
```

```
Warning: Using `size` aesthetic for lines was deprecated in ggplot2 3.4.0.
i Please use `linewidth` instead.
```

```
`geom_smooth()` using formula = 'y ~ x'
```

```
Warning: Removed 53 rows containing non-finite values (`stat_smooth()`).
```

```
`geom_smooth()` using formula = 'y ~ x'
```

```
Warning: Removed 53 rows containing missing values (`geom_point()`).
```

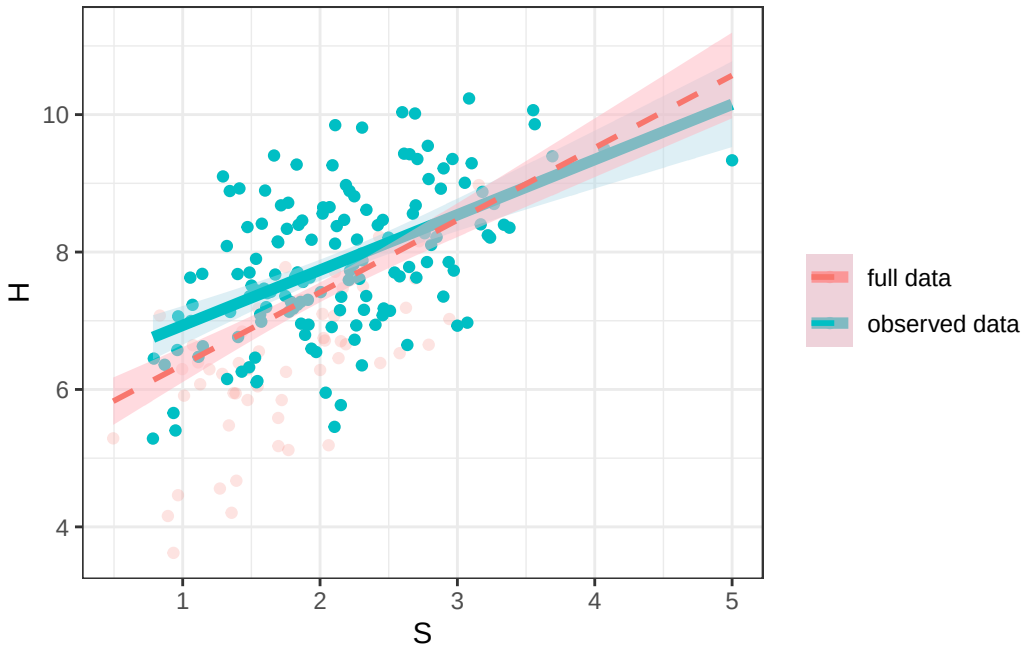


Figure 22.8: Simulated MNAR data.

As you can see in Figure 22.8, the red line gives a biased representation of the blue line.

In this case, if we have measured X, including X also in our model would give the correct result. We can check for d-separation:

```
dseparated(dag4, "D", "H", Z = c("S", "X"))  # d-separated
```

```
[1] TRUE
```

So MNAR depends on whether our model fully accounts for the missing data mechanism. Here, it is MNAR if we do not include X, but it will be MAR if we include X. The following shows the results when conditioning on X.

```
# Prediction with X added to the equation
full_data2 <- full_data2 |>
    mutate(Sres = residuals(lm(S ~ X)),
           Hres = residuals(lm(H ~ X)))
mnar_data1 <- mnar_data1 |>
    drop_na() |>
    mutate(Sres = residuals(lm(S ~ X)),
```

```
           Hres = residuals(lm(Hs ~ X)))
mnar_data1 <- cbind(
    mnar_data1,
    predict(lm(Hres ~ S, data = mnar_data1),
        newdata = mnar_data1, interval = "confidence"
    )
)
```

```
ggplot(full_data2, aes(x = Sres, y = Hres)) +
    geom_point(aes(col = "full data"), alpha = 0.2) +
    geom_point(data = mnar_data1, aes(y = Hres, col = "observed data")) +
    geom_smooth(data = mnar_data1,
                aes(col = "observed data"),
                method = "lm", size = 2, fill = "lightblue") +
    geom_smooth(aes(col = "full data"),
                method = "lm", alpha = 0.5, linetype = "dashed",
                fill = "lightpink") +
    labs(col = NULL, x = "S (conditioned on X)", y = "H (conditioned on X)")
```

```
`geom_smooth()` using formula = 'y ~ x'
`geom_smooth()` using formula = 'y ~ x'
```

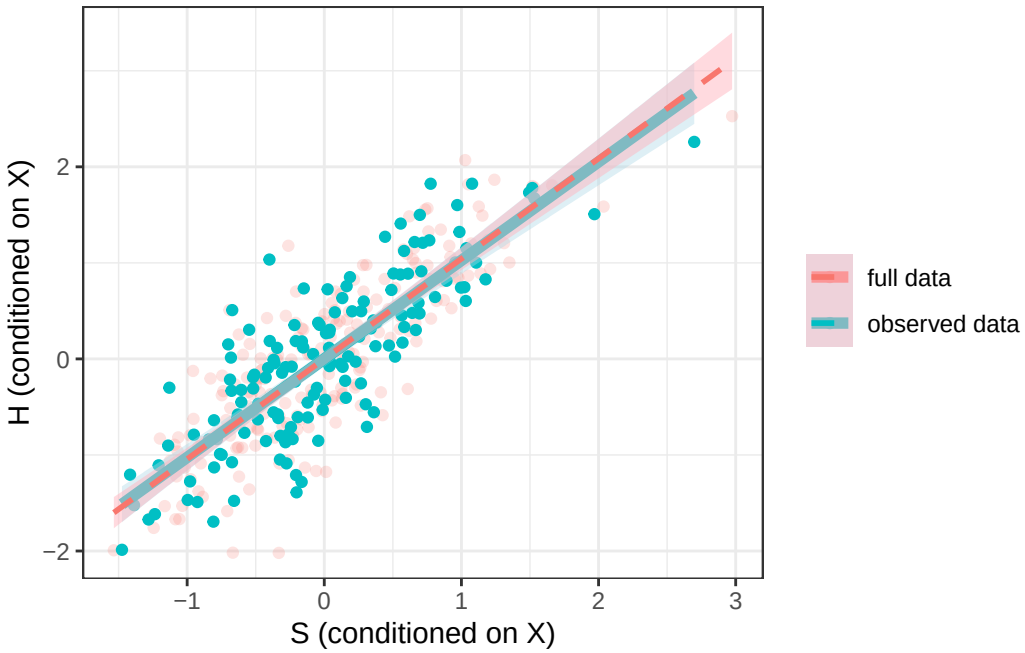


Figure 22.9: Simulated MNAR data with X included in the model.

22.4 Missing Not At Random (2)

The more prototypical situation for MNAR, which is also the most problematic, is when missingness is directly related to the outcome variable, i.e., dogs like to eat bad homework.

```
dag5 <- dagitty('dag{ "S" -> "H" -> "H*" ; "H" -> "D" -> "H*" }')
latents(dag5) <- c("H")
coordinates(dag5) <- list(x = c(S = 0, H = 1, `H*` = 1, D = 0),
                          y = c(S = 1, H = 1, `H*` = 0, D = 0))
# Plot
ggdag(dag5) + theme_dag()
```

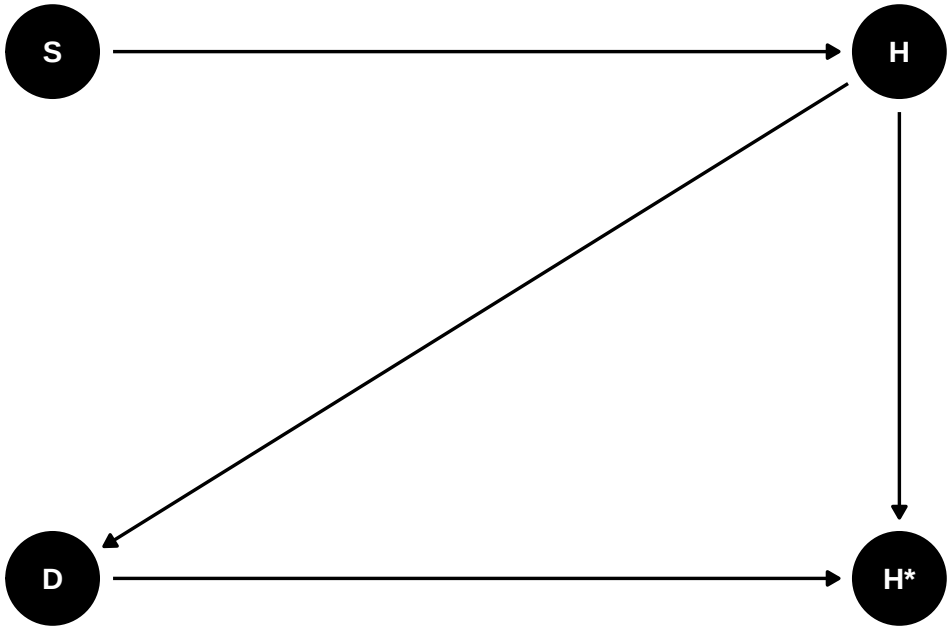


Figure 22.10: DAG for the second case of missing not at random.

```
mnar_data2 <- full_data |>
    mutate(D = as.numeric(H > quantile(H, probs = .25)),
           Hs = if_else(D == 1, H, NA_real_))
```

```
ggplot(full_data, aes(x = S, y = H)) +
    geom_point(alpha = 0.2) +
    geom_point(aes(col = "full data"), alpha = 0.2) +
    geom_point(data = mnar_data2, aes(y = Hs, col = "observed data")) +
    geom_smooth(data = mnar_data2,
                aes(y = Hs, col = "observed data"),
                method = "lm", size = 2, fill = "lightblue") +
    geom_smooth(aes(col = "full data"),
                method = "lm", alpha = 0.5, linetype = "dashed",
                fill = "lightpink") +
    labs(col = NULL)
```

```
`geom_smooth()` using formula = 'y ~ x'
```

```
Warning: Removed 50 rows containing non-finite values (`stat_smooth()`).
```

```
`geom_smooth()` using formula = 'y ~ x'

Warning: Removed 50 rows containing missing values (`geom_point()`).
```

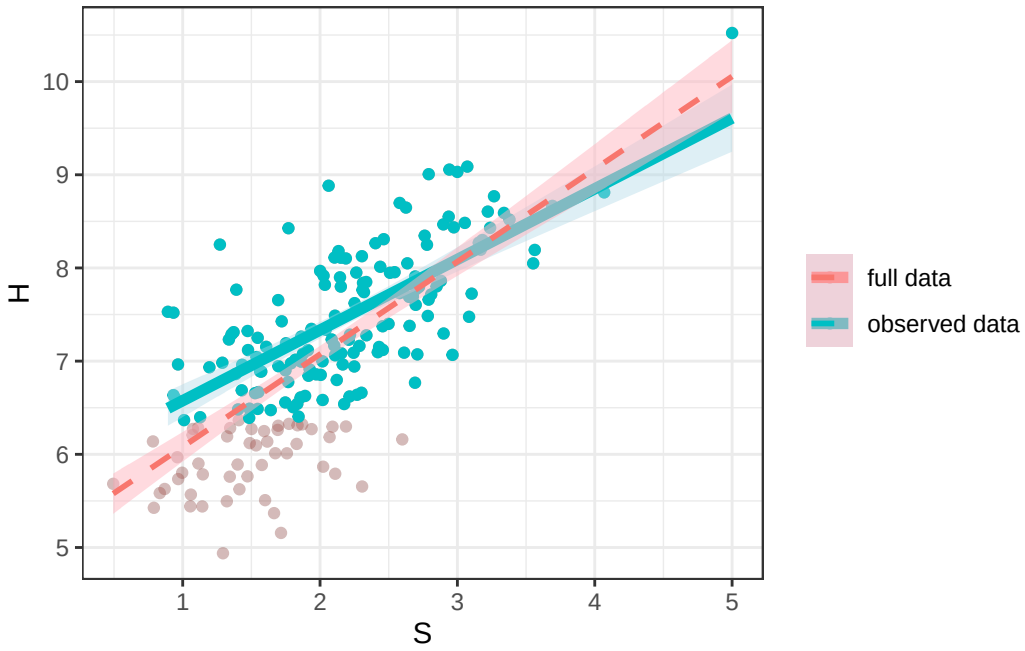


Figure 22.11: Simulated MNAR data with dogs eating bad homework.

MNAR is sometimes called *missing not at random* or *non-ignorable missingness*, and as the name suggests, it refers to conditions where MAR does not hold. If you just look at the observed data, they may look very similar to the data with MAR.

> **i** Generally speaking, there are no statistical procedures distinguishing between MAR in general and MNAR.

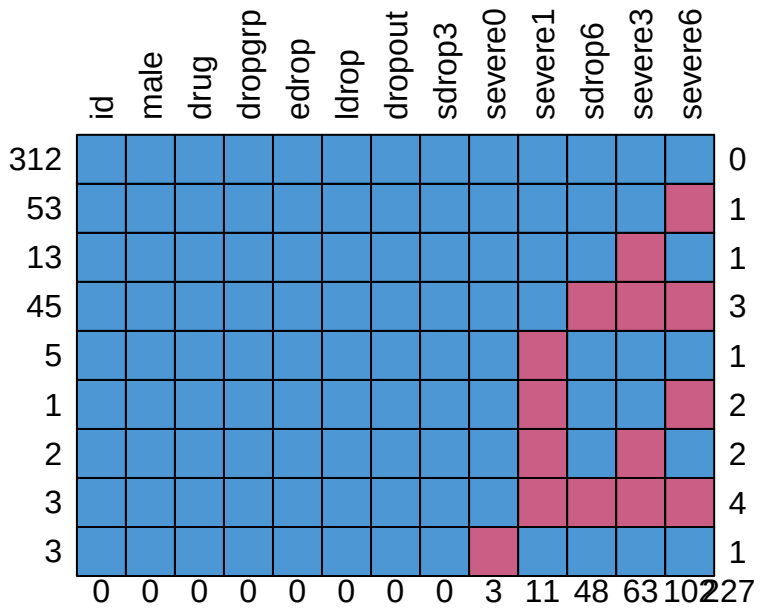
22.5 Example

The data come from the second edition of the book *Applied Missing Data Analysis*. It is from the National Institute of Mental Health Schizophrenia Collaborative Study on how treatment related to change in the severity of participants' conditions over six weeks. This paper: https://psycnet.apa.org/record/1997-07778-004 contains more descriptions of the data.

```
zip_data <- here("data", "AMDA_Chapter5.zip")
if (!file.exists(zip_data)) {
    download.file("https://dl.dropboxusercontent.com/scl/fi/isztu1ee4xxm6dm5vzngc/AMDA-Chapte
              zip_data)
}
drug_data <- read.table(
  unz(zip_data,
      "AMDA Chapter 5 - Bayesian Estimation with Missing Data/Example 5.8 - Bayes Estimation
      col.names = c("id", "male", "drug", "severe0", "severe1",
                    "severe3", "severe6", "dropgrp", "edrop",
                    "ldrop", "dropout", "sdrop3", "sdrop6"),
      na.strings = "999")
```

22.5.1 Missing Data Pattern

```
mice::md.pattern(drug_data, rotate.names = TRUE)
```




```
    id male drug dropgrp edrop ldrop dropout sdrop3 severe0 severe1 sdrop6
312  1    1    1       1     1     1       1      1       1       1       1
53   1    1    1       1     1     1       1      1       1       1       1
```

```
13    1     1     1        1      1      1        1       1        1        1       1
45    1     1     1        1      1      1        1       1        1        1       0
5     1     1     1        1      1      1        1       1        1        0       1
1     1     1     1        1      1      1        1       1        1        0       1
2     1     1     1        1      1      1        1       1        1        0       1
3     1     1     1        1      1      1        1       1        1        0       0
3     1     1     1        1      1      1        1       1        0        1       1
      0     0     0        0      0      0        0       0        3       11      48
     severe3 severe6
312        1       1   0
53         1       0   1
13         0       1   1
45         0       0   3
5          1       1   1
1          1       0   2
2          0       1   2
3          0       0   4
3          1       1   1
           63     102 227
```

22.5.2 Plausible Values of Missing Data

First, consider the missing data in `severe0`, which consists of only three cases. In practice, this is likely not going to affect the results much. However, for pedagogical purposes, we'll see how Bayesian handle these.

Let's consider this plausible DAG with `drug` and `male` predicting both `severe0` and its missingness (Ds0).

```
dag_drug1 <- dagitty(
    'dag{ drug -> s0 -> "s0*" ; male -> s0 -> "s0*";
          drug -> Ds0 -> "s0*"; male -> Ds0 -> "s0*" }'
)
latents(dag_drug1) <- c("s0")
coordinates(dag_drug1) <- list(
    x = c(drug = 0, male = 0.3, s0 = 1, `s0*` = 1, Ds0 = 0),
    y = c(drug = 0.7, male = 1, s0 = 1, `s0*` = 0, Ds0 = 0)
)
# Plot
ggdag(dag_drug1) + theme_dag()
```

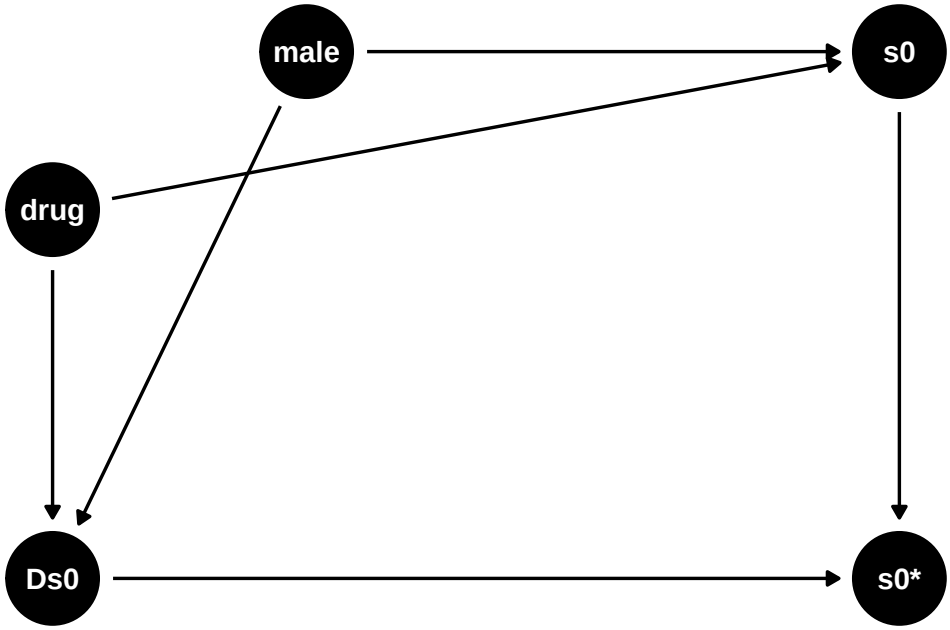


Figure 22.12: DAG for the missing data in `severe0`.

From a Bayesian perspective, any unknown can be treated as a parameter. This includes missing data. So we can treat the missing values of `severe0` as parameters, which I will call `y_mis`.

22.5.3 Using Stan

Here's the Stan code

```
data {
  int<lower=0> N_obs;  // number of observations
  int<lower=0> N_mis;  // number of observations missing Y
  int<lower=0> p;  // number of predictors
  vector[N_obs] y_obs;  // outcome observed;
  matrix[N_obs, p] x_obs;  // predictor matrix (observed);
  matrix[N_mis, p] x_mis;  // predictor matrix (missing);
}
parameters {
  real beta0;  // regression intercept
  vector[p] beta;  // regression coefficients
  real<lower=0> sigma;  // SD of prediction error
```

```
  vector[N_mis] y_mis;  // outcome missing;
}
model {
  // model
  y_obs ~ normal_id_glm(x_obs, beta0, beta, sigma);
  y_mis ~ normal_id_glm(x_mis, beta0, beta, sigma);
  // prior
  beta0 ~ normal(0, 5);
  beta ~ normal(0, 2);
  sigma ~ student_t(4, 0, 5);
}
generated quantities {
  vector[N_obs] y_rep;  // place holder
  for (n in 1:N_obs)
    y_rep[n] = normal_rng(beta0 + dot_product(beta, x_obs[n]), sigma);
}
```

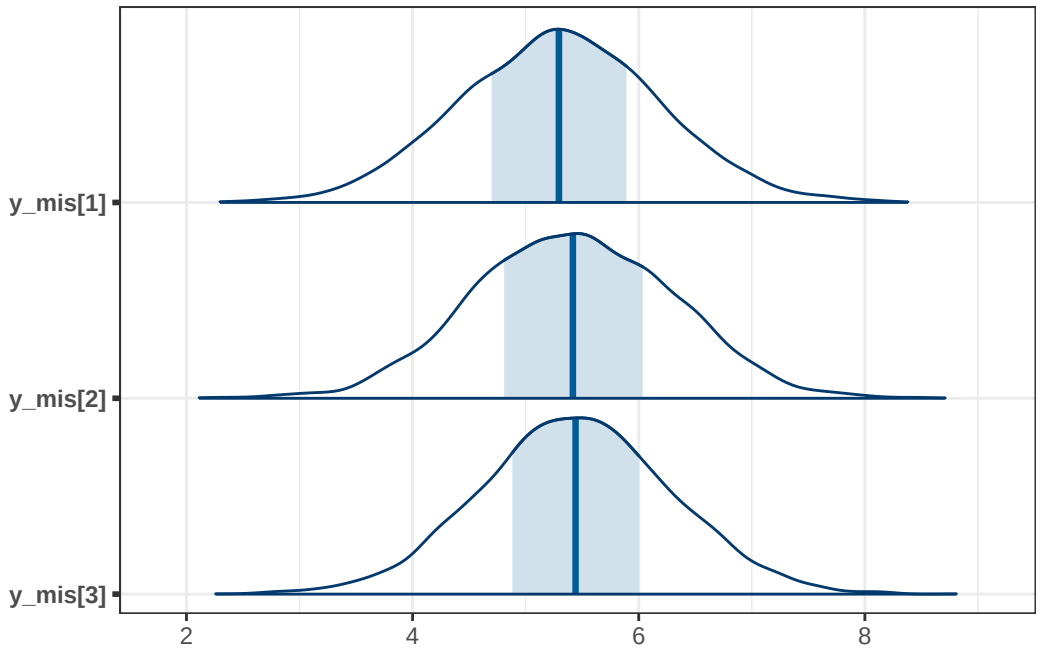
```
mr_mis <- cmdstan_model("stan_code/multiple_reg_mis.stan")
```

Notice that the data are separated into those with `severe0` observed, and those missing `severe0`.

```
# Indicator for missing `severe0`
which_mis <- which(is.na(drug_data$severe0))
which_obs <- which(!is.na(drug_data$severe0))
m1_stan <- mr_mis$sample(
    data = list(
        N_obs = length(which_obs),
        N_mis = length(which_mis),
        p = 2,
        y_obs = drug_data$severe0[which_obs],
        x_obs = drug_data[which_obs, c("drug", "male")],
        x_mis = drug_data[which_mis, c("drug", "male")]
    ),
    seed = 2222
)
```

Now, consider the posterior draws of `y_mis`

```
m1_stan$draws() |>
    mcmc_areas(regex_pars = "^y_mis")
```

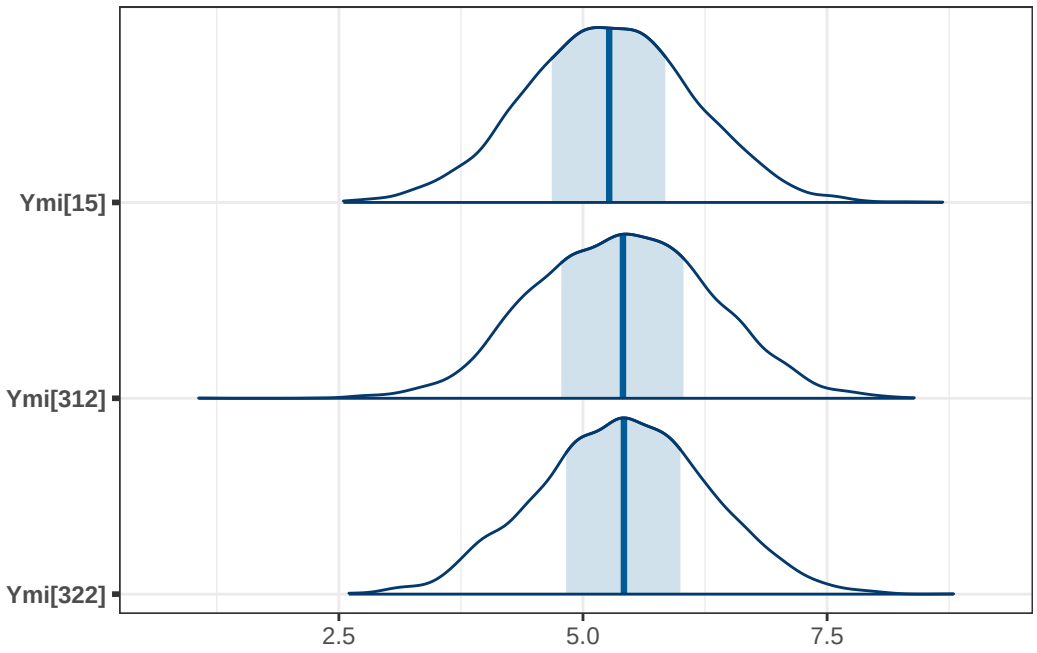


22.5.4 Using `brms`

The same can be done in `brms` with the `mi()` syntax:

```
m1_brm <- brm(severe0 | mi() ~ drug + male,
    data = drug_data,
    seed = 2234,
    file = "12_m1_brm"
)
```

```
mcmc_plot(m1_brm,
    type = "areas",
    variable = "^Ymi",
    regex = TRUE)
```



22.6 Multiple Imputations

The technique of multiple imputation is a Bayesian technique widely applied in statistics. The idea is to obtain multiple draws from the posterior distributions of the missing values. For example, we can randomly obtain five draws of the three missing values:

```
set.seed(937)
as_draws_df(m1_stan) |>
    subset_draws(variable = "y_mis",
                 draw = sample.int(4000, 5))
```

```
Merging chains in order to subset via 'draw'.
```

```
# A draws_df: 5 iterations, 1 chains, and 3 variables
  y_mis[1] y_mis[2] y_mis[3]
1      5.6      5.9      5.1
2      6.3      4.8      4.6
3      4.6      4.3      5.5
4      5.8      5.1      4.3
5      5.9      5.4      5.5
# ... hidden reserved variables {'.chain', '.iteration', '.draw'}
```

22.7 Missing Both Predictors and Outcome

```
m2_brm <- brm(
    bf(severe6 | mi() ~ drug + male + mi(severe0)) +
        bf(severe0 | mi() ~ drug + male) +
        set_rescor(FALSE),
    data = drug_data,
    seed = 2234,
    file = "12_m2_brm"
)
```

22.7.1 Analyses With Multiply-Imputed Data

There are many packages for multiple imputation with different algorithms, including popular packages like `mice` and `mdmb`. Generally speaking, these packages also used the same Bayesian logic as discussed above, but employed some assumptions and techniques that make computations faster for large data sets. One possible workflow is to use these packages to perform multiple imputations, perform Bayesian analyses in each imputed data set, and then pool the results together. Below I provide an example of doing so in `mice` and `brms`.

A word of caution is needed: the algorithms in `mice` and related packages involve a lot of choices, and there is a full manual on using `mice` that you should check out before you use the package: https://stefvanbuuren.name/fimd/. While software makes sensible defaults, in my experience, when the number of variables and the proportion of missing data is large, setting up a reasonable imputation model requires a lot of careful consideration, and still, you may run into convergence issues. One thing you should make sure to do is to check for convergence of the imputation, which is very similar to checking MCMC convergence (as imputations are kind of like MCMC draws).

Another drawback of these algorithms is that, by default, they do not take into account the causal mechanism of why data are missing. Therefore, they may introduce bias due to, for example, conditioning on a collider. So **you should carefully specify which variables you want to include when imputing missing data.**

> See this paper: https://www.tandfonline.com/doi/abs/10.1080/00273171.2014.931799 for a discussion on potential biases when including descendants of the predictors in the imputation step.

```
# First, obtain the default settings
imp <- mice(drug_data, visit = "monotone", maxit = 0)
```

```
Warning: Number of logged events: 2
```

```
# These are the default imputation method (predictive mean matching)
imp$method
```

```
     id    male    drug severe0 severe1 severe3 severe6 dropgrp   edrop   ldrop
     ""      ""      ""   "pmm"   "pmm"   "pmm"   "pmm"      ""      ""      ""
dropout  sdrop3  sdrop6
     ""      ""      ""
```

```
# We should define which variables are used to impute which variables
(pred <- imp$predictorMatrix)
```

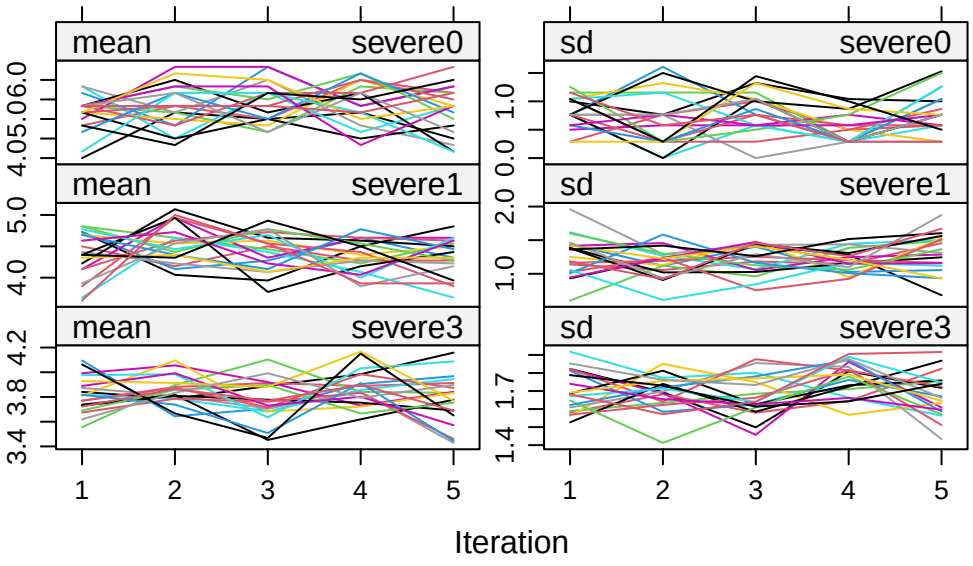
```
        id male drug severe0 severe1 severe3 severe6 dropgrp edrop ldrop
id       0    1    1       1       1       1       1       1     1     1
male     1    0    1       1       1       1       1       1     1     1
drug     1    1    0       1       1       1       1       1     1     1
severe0  1    1    1       0       1       1       1       1     1     1
severe1  1    1    1       1       0       1       1       1     1     1
severe3  1    1    1       1       1       0       1       1     1     1
severe6  1    1    1       1       1       1       0       1     1     1
dropgrp  1    1    1       1       1       1       1       0     1     1
edrop    1    1    1       1       1       1       1       1     0     1
ldrop    1    1    1       1       1       1       1       1     1     0
dropout  1    1    1       1       1       1       1       1     1     1
sdrop3   1    1    1       1       1       1       1       1     1     1
sdrop6   0    0    0       0       0       0       0       0     0     0
        dropout sdrop3 sdrop6
id            1      0      0
male          1      0      0
drug          1      0      0
severe0       1      0      0
severe1       1      0      0
severe3       1      0      0
severe6       1      0      0
dropgrp       1      0      0
edrop         1      0      0
ldrop         1      0      0
dropout       0      0      0
sdrop3        1      0      0
sdrop6        0      0      0
```

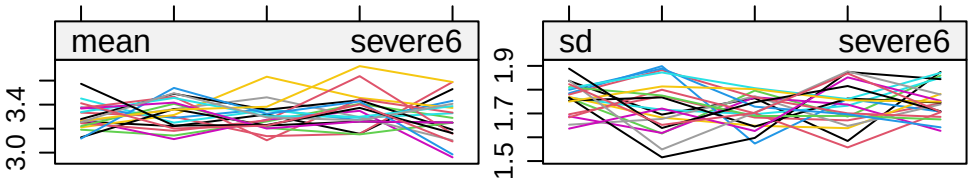
```
# Set imputation predictors to empty (0) for the four variables
# `severe0` to `severe6`
pred[c("severe0", "severe1", "severe3", "severe6"), ] <- 0
# Use male, drug, dropout to predict missing data in severe1
pred["severe0", c("male", "drug", "dropout")] <- 1
pred["severe1", c("severe0", "male", "drug", "dropout")] <- 1
pred["severe3", c("severe0", "severe1", "male", "drug", "dropout")] <- 1
pred["severe6", c("severe0", "severe1", "severe3",
                  "male", "drug", "dropout")] <- 1
# Perform imputation
imp <- mice(drug_data,
            m = 20,  # 20 imputed data sets
            predictorMatrix = pred,  # which variables to impute which
            # order of imputation
            visit = c("severe0", "severe1", "severe3", "severe6"),
            print = FALSE)
```

```
Warning: Number of logged events: 100
```

Convergence: Check the mixing of the chains.

```
plot(imp)  # the chains should mix well
```





After the imputations, we can fit a Bayesian model to *each* of the 20 imputed data sets. `brms` has a handy function `brm_multiple()` for doing it. With 20 data sets, 2 chains each, and 2,000 iterations (1,000 warm-ups) per chain, we should get a total of 20 * 2 * 1000 = 40000 draws.

```
m2_imp <- brm_multiple(severe6 ~ drug + male + severe0,
    data = imp, chains = 2,
    iter = 2000,
    file = "12_m2_imp"
)
```

Note that because we pool estimates from different data sets, the rhat statistic is unlikely to be under 1.01, unless the imputed data sets are very similar or the missing proportion is small. On the other hand, you don't want to see high rhat values within each imputed data set, which would indicate real convergence issues.

```
# Convergence with the first two chains (1st imputed data set)
as_draws_df(m2_imp) |>
    subset_draws(chain = 1:2) |>
    summarize_draws()
```

```
# A tibble: 8 x 10
```

```
  variable        mean   median     sd    mad        q5      q95  rhat ess_bulk
  <chr>          <dbl>    <dbl>  <dbl>  <dbl>     <dbl>    <dbl> <dbl>    <dbl>
1 b_Intercept    2.90     2.89  0.451  0.461     2.17      3.61   1.00    2488.
2 b_drug        -1.42    -1.42  0.151  0.150    -1.67     -1.18   1.00    2600.
3 b_male         0.284    0.285 0.132  0.128     0.0707    0.499  1.00    2368.
4 b_severe0      0.242    0.241 0.0780 0.0809    0.114     0.370  1.00    2561.
5 sigma          1.38     1.38  0.0468 0.0467    1.31      1.46   1.00    2520.
6 Intercept      3.26     3.26  0.0678 0.0682    3.15      3.37   1.00    2212.
7 lprior        -3.34    -3.34  0.0132 0.0134   -3.37     -3.32   1.00    2490.
8 lp__        -765.    -764.    1.56   1.42   -767.     -763.     1.00    1168.
# i 1 more variable: ess_tail <dbl>
```

```
# And do it for each imputed data set
```

```
m2_imp
```

```
Warning: The displayed Rhat and ESS estimates should not be trusted for
brm_multiple models. Please see ?brm_multiple for how to assess convergence of
such models.


 Family: gaussian
  Links: mu = identity; sigma = identity
Formula: severe6 ~ drug + male + severe0
   Data: imp (Number of observations: 437)
  Draws: 40 chains, each with iter = 2000; warmup = 1000; thin = 1;
         total post-warmup draws = 40000

Regression Coefficients:
          Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
Intercept     2.75      0.48     1.82     3.68 1.07      336     1844
drug         -1.45      0.19    -1.81    -1.09 1.21      129      447
male          0.23      0.15    -0.05     0.53 1.10      249     1081
severe0       0.29      0.08     0.13     0.45 1.05      442     2553

Further Distributional Parameters:
      Estimate Est.Error l-95% CI u-95% CI Rhat Bulk_ESS Tail_ESS
sigma     1.39      0.05     1.30     1.50 1.09      264      964

Draws were sampled using sample(hmc). For each parameter, Bulk_ESS
and Tail_ESS are effective sample size measures, and Rhat is the potential
scale reduction factor on split chains (at convergence, Rhat = 1).
```

```
plot(m2_imp)
```

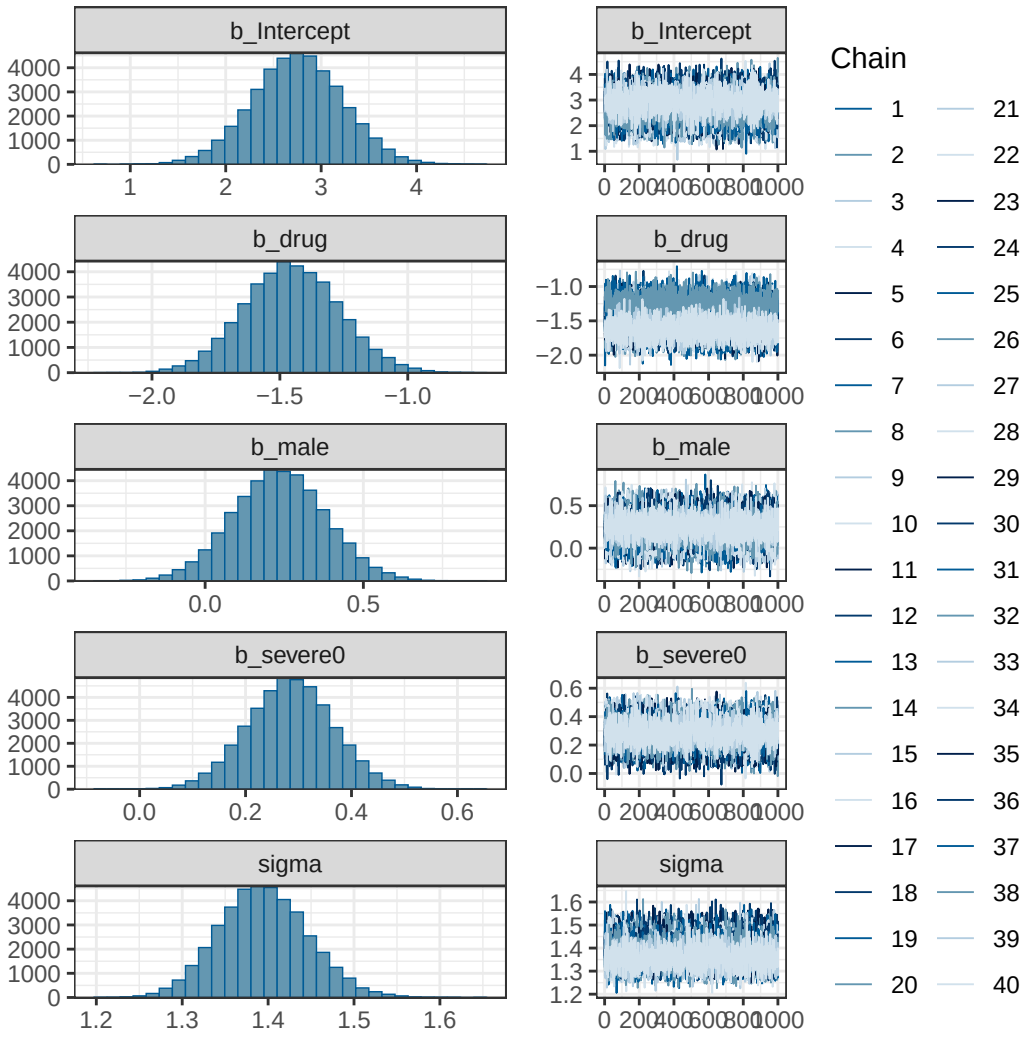


Figure 22.13: Posterior distributions of the coefficients with multiply imputed data sets.

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