Models for Binary Outcomes

Logistic regression and variations

Contents

Configuring R

Functions from these packages will be used throughout this document:

```
library(conflicted) # check for conflicting function definitions
# library(printr) # inserts help-file output into markdown output
library(rmarkdown) # Convert R Markdown documents into a variety of formats.
library(pander) # format tables for markdown
library(ggplot2) # graphics
library(ggfortify) # help with graphics
library(dplyr) # manipulate data
library(tibble) # `tibble`s extend `data.frame`s
library(magrittr) # `%>%` and other additional piping tools
library(haven) # import Stata files
library(knitr) # format R output for markdown
library(tidyr) # Tools to help to create tidy data
library(plotly) # interactive graphics
library(dobson) # datasets from Dobson and Barnett 2018
library(parameters) # format model output tables for markdown
library(haven) # import Stata files
library(latex2exp) # use LaTeX in R code (for figures and tables)
library(fs) # filesystem path manipulations
library(survival) # survival analysis
library(survminer) # survival analysis graphics
library(KMsurv) # datasets from Klein and Moeschberger
library(parameters) # format model output tables for
library(webshot2) # convert interactive content to static for pdf
library(forcats) # functions for categorical variables ("factors")
library(stringr) # functions for dealing with strings
library(lubridate) # functions for dealing with dates and times
library(broom) # Summarizes key information about statistical objects in tidy tibbles
library(broom.helpers) # Provides suite of functions to work with regression model 'broom::tidy()' t
```

Here are some R settings I use in this document:

```
rm(list = ls()) # delete any data that's already loaded into R

conflicts_prefer(dplyr::filter)
ggplot2::theme_set(
  ggplot2::theme_bw() +
        # ggplot2::labs(col = "") +
    ggplot2::theme(
      legend.position = "bottom",
      text = ggplot2::element_text(size = 12, family = "serif")))

knitr::opts_chunk$set(message = FALSE)
options('digits' = 6)

panderOptions("big.mark", ",")
pander::panderOptions("table.emphasize.rownames", FALSE)
pander::panderOptions("table.split.table", Inf)
conflicts_prefer(dplyr::filter) # use the `filter()` function from dplyr() by default
legend_text_size = 9
run_graphs = TRUE
```

```r
options(digits = 6)
```

Acknowledgements

This content is adapted from:

- Dobson and Barnett (2018), Chapter 7
- Vittinghoff et al. (2012), Chapter 5
- David Rocke[1]'s materials from the 2021 edition of Epi 204[2]
- Nahhas (2024) Chapter 6[3]

1 Introduction

Exercise 1.1. What is logistic regression?

Solution

Solution 1.1.

Def

Definition 1.1 (Logistic regression model). **Logistic regression** is a framework for modeling binary[a] outcomes, conditional on one or more *predictors* (a.k.a. *covariates*).

[a] data.qmd#def-binary

Exercise 1.2 (Examples of binary outcomes)**.** What are some examples of binary outcomes in the health sciences?

Solution

Solution 1.2. Examples of binary outcomes include:

- exposure (exposed vs unexposed)
- disease (diseased vs healthy)
- recovery (recovered vs unrecovered)
- relapse (relapse vs remission)
- return to hospital (returned vs not)
- vital status (dead vs alive)

Logistic regression uses the Bernoulli[4] distribution to model the outcome variable, conditional on one or more covariates.

Exercise 1.3. Write down a mathematical definition of the Bernoulli distribution.

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[1] https://dmrocke.ucdavis.edu/

[2] https://dmrocke.ucdavis.edu/Class/EPI204-Spring-2021/EPI204-Spring-2021.html

[3] https://www.bookdown.org/rwnahhas/RMPH/blr.html

[4] probability.qmd#def-bernoulli

Solution

Solution 1.3. The **Bernoulli distribution** family for a random variable X is defined as:

$$
\begin{aligned}
\Pr(X = x) &= 1_{x \in \{0,1\}} \pi^x (1-\pi)^{1-x} \\
&= \begin{cases} \pi, & x = 1 \\ 1 - \pi, & x = 0 \end{cases}
\end{aligned}
$$

1.0.1 Logistic regression versus linear regression

Logistic regression differs from linear regression, which uses the Gaussian ("normal") distribution to model the outcome variable, conditional on the covariates.

Exercise 1.4. Recall: what kinds of outcomes is linear regression used for?

Solution

Solution 1.4. Linear regression is typically used for numerical outcomes that aren't event counts or waiting times for an event.
Examples of outcomes that are often analyzed using linear regression include:

- weight
- height
- income
- prices

1.1 Risk estimation and prediction

In Epi 203, you have already seen methods for modeling binary outcomes using one covariate that is also binary (such as exposure/non-exposure). In this section, we review one-covariate analyses, with a special focus on risk ratios and odds ratios, which are important concepts for interpreting logistic regression.

Exm

Example 1.1 (Oral Contraceptive Use and Heart Attack)**.**

- Research question: how does oral contraceptive (OC) use affect the risk of myocardial infarction (MI; a.k.a. heart attack)?

This was an issue when oral contraceptives were first developed, because the original formulations used higher concentrations of hormones. Modern OCs don't have this issue.
Table 1 contains simulated data for an imaginary follow-up (a.k.a. *prospective*) study in which two groups are identified, one using OCs and another not using OCs, and both groups are tracked for three years to determine how many in each groups have MIs.

```r
library(dplyr)
oc_mi <-
  tribble(
    ~OC, ~MI, ~Total,
    "OC use", 13, 5000,
    "No OC use", 7, 10000
  ) |>
  mutate(`No MI` = Total - MI) |>
  relocate(`No MI`, .after = MI)

totals <-
  oc_mi |>
  summarize(across(c(MI, `No MI`, Total), sum)) |>
  mutate(OC = "Total")

tbl_oc_mi <- bind_rows(oc_mi, totals)

tbl_oc_mi |> pander::pander()
```

Table 1: Simulated data from study of oral contraceptive use and heart attack risk

OC	MI	No MI	Total
OC use	13	4,987	5,000
No OC use	7	9,993	10,000
Total	20	14,980	15,000

Exercise 1.5. Estimate the probabilities of MI for OC users and non-OC users in Example 1.1.

Solution

Solution 1.5.

$$\hat{p}(MI|OC) = \frac{13}{5000} = 0.0026$$

$$\hat{p}(MI|\neg OC) = \frac{7}{10000} = 7 \times 10^{-4}$$

Exercise 1.6. What does the term "controls" mean in the context of study design?

Solution

Solution 1.6.

Def

Definition 1.2 (Two meanings of "controls"). Depending on context, "controls" can mean either:

- individuals who don't experience an *exposure* of interest,
- or individuals who don't experience an *outcome* of interest.

Exercise 1.7. What types of studies do the two definitions of controls correspond to?

Solution

Solution 1.7.

Def

Definition 1.3 (cases and controls in retrospective studies). In *retrospective case-control studies*, participants who experience the outcome of interest are called **cases**, while participants who don't experience that outcome are called **controls**.

Def

Definition 1.4 (treatment groups and control groups in prospective studies). In *prospective studies*, the group of participants who experience the treatment or exposure of interest is called the **treatment group**, while the participants who receive the baseline or comparison treatment (for example, clinical trial participants who receive a placebo or a standard-of-care treatment rather than an experimental treatment) are called **controls**.

1.2 Comparing probabilities

1.2.1 Risk differences

The simplest comparison of two probabilities, π_1, and π_2, is the difference of their values:

Definition 1.5 (Risk difference)**.** The **risk difference** of two probabilities, π_1, and π_2, is the difference of their values:

$$\delta(\pi_1, \pi_2) \overset{\text{def}}{=} \pi_1 - \pi_2$$

Exm

Example 1.2 (Difference in MI risk)**.** In Example 1.1, the maximum likelihood estimate of the difference in MI risk between OC users and OC non-users is:

$$\begin{aligned}\hat{\delta}(\pi(OC), \pi(\neg OC)) &= \delta(\hat{\pi}(OC), \hat{\pi}(\neg OC)) \\ &= \hat{\pi}(OC) - \hat{\pi}(\neg OC) \\ &= 0.0026 - 7 \times 10^{-4} \\ &= 0.0019\end{aligned}$$

Exercise 1.8 (interpreting risk differences)**.** How can we interpret the preceding relative risk estimate in prose?

Solution (interpreting risk differences)

Solution 1.8 (interpreting risk differences). "The difference in risk of MI between OC users and non-users was 0.0019."

or

"The difference in risk of MI between OC users and non-users was 0.19 percentage points[a]."

---

[a] https://en.wikipedia.org/wiki/Percentage_point

See the note about working with percentages in the Appendix[5].

1.2.2 Risk ratios

Exercise 1.9. If π_1 and π_2 are two probabilities, what do we call the following ratio?

$$\rho(\pi_1, \pi_2) = \frac{\pi_1}{\pi_2}$$

Solution

Solution 1.9.

Def

Definition 1.6 (Relative risk ratios). The ratio of two probabilities π_1 and π_2,

$$\rho(\pi_1, \pi_2) = \frac{\pi_1}{\pi_2}$$

is called the:

- **risk ratio**,
- **relative risk ratio**,
- **probability ratio**,
- or **rate ratio**

of π_1 compared to π_2.

Exercise 1.10.

Above, we estimated that:

$$\hat{\text{p}}(MI|OC) = 0.0026$$

$$\hat{\text{p}}(MI|\neg OC) = 7 \times 10^{-4}$$

Now, estimate the *relative risk* of MI for OC versus non-OC.

Solution

Solution 1.10.

The *relative risk* of MI for OC versus non-OC is:

```
rr <- (13 / 5000) / (7 / 10000)
```

$$\begin{aligned}\hat{\rho}(OC, \neg OC) &= \frac{\hat{\text{p}}(MI|OC)}{\hat{\text{p}}(MI|\neg OC)}\\ &= \frac{0.0026}{7 \times 10^{-4}}\\ &= 3.714286\end{aligned}$$

---

[5] notation.qmd#percent-sign

Exercise 1.11. How can we interpret the preceding relative risk estimate in prose?

Solution

Solution 1.11.
We might summarize this result by saying that:

- "The estimated probability of MI among OC users was 3.714286 times as high as the estimated probability among OC non-users."

or

- "The estimated probability of MI among OC users was 2.714286 times higher than, the estimated probability among OC non-users."

see also Section 8.1.4[a] which uses similar phrasing.

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[a] https://link.springer.com/chapter/10.1007/978-1-4614-1353-0_8#Sec5_8

1.2.3 Relative risk differences

The second approach above, where we subtract 1 from the risk ratio, is actually reporting a slightly different metric:

Definition 1.7 (Relative risk difference)**.**
Sometimes, we divide the risk difference by the comparison probability; the result is called the **relative risk difference**:

$$\xi(\pi_1, \pi_2) \stackrel{\text{def}}{=} \frac{\delta(\pi_1, \pi_2)}{\pi_2}$$

Theorem 1.1 (Relative risk difference equals risk ratio minus 1)**.**

$$\xi(\pi_1, \pi_2) = \rho(\pi_1, \pi_2) - 1$$

ℹ Proof

Proof.

$$\begin{aligned}
\xi(\pi_1, \pi_2) &\stackrel{\text{def}}{=} \frac{\delta(\pi_1, \pi_2)}{\pi_2} \\
&= \frac{\pi_1 - \pi_2}{\pi_2} \\
&= \frac{\pi_1}{\pi_2} - 1 \\
&= \rho(\pi_1, \pi_2) - 1
\end{aligned}$$

□

1.2.4 Changing reference groups in risk comparisons

Risk differences, risk ratios, and relative risk differences are defined by two probabilities, plus a choice of which probability is the **baseline** or **reference** probability (i.e., which probability is the subtrahend of the risk difference or the denominator of the risk ratio).

$$\delta(\pi_2, \pi_1) = -\delta(\pi_1, \pi_2)$$

$$\rho(\pi_2, \pi_1) = (\rho(\pi_1, \pi_2))^{-1}$$
$$\xi(\pi_2, \pi_1) = (\xi(\pi_1, \pi_2) + 1)^{-1} - 1$$

Exercise 1.12. Prove the relationships above.

Exm

Example 1.3 (Switching the reference group in a risk ratio)**.** Above, we estimated that the risk ratio of OC versus non-OC is:

$$\rho(OC, \neg OC) = 3.714286$$

In comparison, the risk ratio for non-OC versus OC is:

$$\begin{aligned}\rho(\neg OC, OC) &= \frac{\hat{\text{p}}(MI|\neg OC)}{\hat{\text{p}}(MI|OC)} \\ &= \frac{7 \times 10^{-4}}{0.0026} \\ &= 0.269231 \\ &= \frac{1}{\rho(OC, \neg OC)}\end{aligned}$$

1.3 Odds and odds ratios

1.3.1 Odds and probabilities

In logistic regression, we will make use of a mathematically-convenient transformation of probability, called *odds*:

Definition 1.8 (Odds)**.**
The **odds** of an event A, is the probability that the event occurs, divided by the probability that it doesn't occur. We can represent odds with the Greek letter ω ("omega"). [6] Thus, in mathematical notation:

$$\omega \overset{\text{def}}{=} \frac{\Pr(A)}{\Pr(\neg A)} \tag{1}$$

This course is about regression models, which are conditional probability models (regression models[7]). Accordingly, we define conditional odds in terms of conditional probabilities:

---

[6] The name "omega" is a contraction of "o mega", which means "long o" in Greek, in contrast with "omicron" (o, "short o"). See https://www.etymonline.com/search?q=omega and https://en.wikipedia.org/wiki/Omega for more details.

[7] Intro-to-GLMs.qmd#def-regression-model

Definition 1.9 (Conditional odds)**.**
The **conditional odds** of an event A given a condition B, is the (conditional) probability that event A occurs (given condition B), divided by the (conditional) probability that it doesn't occur (given condition B). We can represent conditional odds using $\omega(A|B)$, $\omega(B)$ or ω_B ("omega bee"). Thus, in mathematical notation:

$$\omega(B) \stackrel{\text{def}}{=} \frac{\Pr(A|B)}{\Pr(\neg A|B)} \tag{2}$$

Exm

Example 1.4 (Computing odds from probabilities)**.** In Exercise 1.5, we estimated that the probability of MI, given OC use, is $\pi(OC) \stackrel{\text{def}}{=} \Pr(MI|OC) = 0.0026$. If this estimate is correct, then the odds of MI, given OC use, is:

$$\begin{aligned}
\omega(OC) &\stackrel{\text{def}}{=} \frac{\Pr(MI|OC)}{\Pr(\neg MI|OC)} \\
&= \frac{\Pr(MI|OC)}{1-\Pr(MI|OC)} \\
&= \frac{\pi(OC)}{1-\pi(OC)} \\
&= \frac{0.0026}{1-0.0026} \\
&\approx 0.002607
\end{aligned}$$

Exercise 1.13 (Computing odds from probabilities)**.** Estimate the odds of MI, for non-OC users.

Solution

Solution.

$$\omega(\neg OC) = 7.004903 \times 10^{-4}$$

Exercise 1.14. Find a general formula for converting probabilities into odds.

Solution

Solution 1.12. Using Definition 1.8 and the complementary probability[a]:

$$\begin{aligned}
\omega &\stackrel{\text{def}}{=} \frac{\Pr(A)}{\Pr(\neg A)} \\
&= \frac{\pi}{1-\pi}
\end{aligned}$$

---

[a] probability.qmd#cor-p-neg

Theorem 1.2 (Odds as a function of probability)**.** *If* π *is the probability of an event* A *and* ω *is the corresponding odds of* A*, then:*

$$\omega = \frac{\pi}{1-\pi} \tag{3}$$

ℹ Proof

Proof. By Solution 1.12. ☐

The mathematical relationship between odds ω and probabilities π, which is represented in Equation 3, is a core component of logistic regression models, as we will see in the rest of this chapter. Let's give the expression on the righthand side of Equation 3 its own name and symbol, so that we can refer to it concisely:

Definition 1.10 (Odds function)**.** The **odds function** is defined as:

$$\text{odds}\{\pi\} \stackrel{\text{def}}{=} \frac{\pi}{1-\pi} \tag{4}$$

We can use the odds function (Definition 1.10) to simplify Equation 3 (in Theorem 1.2) into a more concise expression, which is easier to remember and manipulate:

Corollary 1.1 (Odds via the odds function)**.** *If* π *is the probability of an outcome* A *and* ω *is the corresponding odds of* A*, then:*

$$\omega = \text{odds}\{\pi\} \tag{5}$$

In other words, the odds function rescales probabilities into odds.

ℹ Proof

Proof. By Theorem 1.2 and Definition 1.10. ☐

Exercise 1.15. Graph the odds function.

Solution

Solution 1.13.
Figure 1 graphs the odds function.

```
odds <- function(pi) pi / (1 - pi)
library(ggplot2)
ggplot() +
  geom_function(
    fun = odds,
    arrow = arrow(ends = "last"),
    mapping = aes(col = "odds function")
  ) +
  xlim(0, .99) +
  xlab("Probability") +
  ylab("Odds") +
  geom_abline(aes(
    intercept = 0,
    slope = 1,
    col = "y=x"
  )) +
  theme_bw() +
  labs(colour = "") +
  theme(legend.position = "bottom")
```

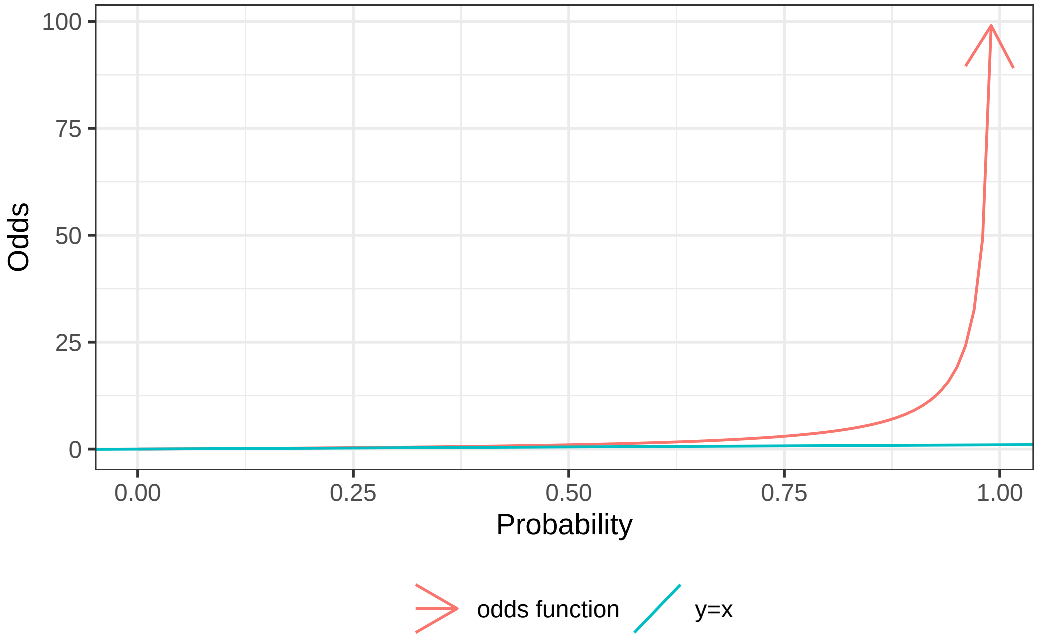


Figure 1: Odds versus probability

Theorem 1.3 (One-sample MLE for odds)**.** *Let* $X_1, ...X_n$ *be a set of* n iid *Bernoulli trials, and let* $X = \sum_{i=1}^{n} X_i$ *be their sum.*
Then the maximum likelihood estimate of the odds of $X = 1$*,* ω*, is:*

$$\hat{\omega} = \frac{x}{n - x}$$

Proof

Proof.

$$\begin{aligned} 1-\hat{\pi} &= 1-\frac{x}{n} \\ &= \frac{n}{n}-\frac{x}{n} \\ &= \frac{n-x}{n} \end{aligned}$$

Thus, the estimated odds is:

$$\begin{aligned} \frac{\hat{\pi}}{1-\hat{\pi}} &= \frac{\left(\frac{x}{n}\right)}{\left(\frac{n-x}{n}\right)} \\ &= \frac{x}{n-x} \end{aligned} \tag{6}$$

That is, the odds estimate can be computed directly as "# events" divided by "# nonevents", without needing to compute $\hat{\pi}$ and $1-\hat{\pi}$ first.

□

Exm

Example 1.5 (Calculating odds using the shortcut)**.** In Example 1.4, we calculated

$$\omega(OC) = 0.002607$$

Let's recalculate this result using our shortcut.

Solution

Solution 1.14.

$$\begin{aligned} \omega(OC) &= \frac{13}{5000-13} \\ &= 0.002607 \end{aligned}$$

Same answer as in Example 1.4!

Theorem 1.4 (Simplified expressions for odds function)**.**
Two equivalent expressions for the odds function are:

$$\begin{aligned} \text{odds}\{\pi\} &= \frac{1}{\pi^{-1}-1} \\ &= \left(\pi^{-1}-1\right)^{-1} \end{aligned} \tag{7}$$

Exercise 1.16. Prove Theorem 1.4.

Solution

Solution 1.15. Starting from Definition 1.10:

$$\begin{aligned}
\text{odds}\{\pi\} &= \frac{\pi}{1-\pi} \\
&= \frac{\pi}{1-\pi}\frac{\pi^{-1}}{\pi^{-1}} \\
&= \frac{\pi\pi^{-1}}{(1-\pi)\pi^{-1}} \\
&= \frac{1}{(\pi^{-1}-\pi\pi^{-1})} \\
&= \frac{1}{(\pi^{-1}-1)} \\
&= \left(\pi^{-1}-1\right)^{-1}
\end{aligned}$$

Corollary 1.2 (Odds of a non-event)**.** *If π is the odds of event A and ω is the corresponding odds of A, then the odds of $\neg A$ are:*

$$\begin{aligned}
\omega(\neg A) &= \frac{1-\pi}{\pi} \\
&= \pi^{-1} - 1
\end{aligned}$$

ℹ Proof

Proof. Left to the reader. ☐

Odds of rare events

Exercise 1.17. What odds value corresponds to the probability $\pi = 0.2$, and what is the numerical difference between these two values?

Solution

Solution.

$$\omega = \frac{\pi}{1-\pi} = \frac{.2}{.8} = .25$$

Exercise 1.18. Find the difference between an odds ω and its corresponding probability π, as a function of π.

Solution

Solution 1.16.

$$
\begin{aligned}
\omega - \pi &= \frac{\pi}{1-\pi} - \pi \\
&= \frac{\pi}{1-\pi} - \frac{\pi(1-\pi)}{1-\pi} \\
&= \frac{\pi}{1-\pi} - \frac{\pi-\pi^2}{1-\pi} \\
&= \frac{\pi-(\pi-\pi^2)}{1-\pi} \\
&= \frac{\pi-\pi+\pi^2}{1-\pi} \\
&= \frac{\pi^2}{1-\pi} \\
&= \frac{\pi}{1-\pi}\pi \\
&= \omega\pi
\end{aligned}
$$

Theorem 1.5 (Difference between odds and probability)**.** *Let* $\omega = \frac{\pi}{1-\pi}$. *Then:*

$$\omega - \pi = \frac{\pi^2}{1-\pi}$$

ℹ Proof

Proof. By Solution 1.16. ☐

For rare events (small π), odds and probabilities are nearly equal (see Figure 1), because $1-\pi \approx 1$ and $\pi^2 \approx 0$.

For example, in Example 1.4, the probability and odds differ by 6.777622×10^{-6}.

1.3.2 The inverse odds function

Exercise 1.19. If π is the probability of an event A and ω is the corresponding odds of A, how can we compute π from ω?
For example, if $\omega = 3/2$, what is π?

Solution

Solution 1.17. Starting from Theorem 1.2, we can solve Equation 3 for π in terms of ω:

$$
\begin{aligned}
\omega &= \frac{\pi}{1-\pi} \\
(1-\pi)\omega &= \pi \\
\omega - \pi\omega &= \pi \\
\omega &= \pi + \pi\omega \\
\omega &= (1+\omega)\pi \\
\pi &= \frac{\omega}{1+\omega}
\end{aligned}
$$

So if $\omega = 3/2$,

$$\begin{aligned}\pi &= \frac{3/2}{1+3/2}\\ &= \frac{3/2}{5/2}\\ &= \frac{3}{5}\end{aligned}$$

Theorem 1.6 (Probability as a function of odds)**.** *If π is the probability of an event and ω is the corresponding odds of that event, then:*

$$\pi = \frac{\omega}{1+\omega} \tag{8}$$

Proof

Proof. By Theorem 1.2 and Solution 1.17. ☐

Definition 1.11 (inverse odds function)**.**

$$\text{invodds}\{\omega\} \overset{\text{def}}{=} \frac{\omega}{1+\omega} \tag{9}$$

can be called the **inverse-odds function**.

Corollary 1.3 (Probability via the inverse-odds function)**.**

$$\pi = \text{invodds}\{\omega\}$$

Proof

Proof. By Definition 1.11 and Theorem 1.6. ☐

Corollary 1.4 (Inverse-odds function inverts the odds function)**.**

$$\text{invodds}\{\omega\} = \text{odds}^{-1}\{\omega\}$$

Proof

Proof. Using Corollary 1.1 and Theorem 1.6:

$$
\begin{aligned}
\text{invodds}\{\text{odds}\{\pi\}\} &= \text{invodds}\{\omega\}\\
&= \frac{\omega}{1+\omega}\\
&= \pi
\end{aligned}
$$

Likewise (not shown):

$$\text{odds}\{\text{invodds}\{\omega\}\} = \omega$$

$\square$

The inverse-odds function converts odds into their corresponding probabilities (Figure 2). Its domain of inputs is $\omega \in [0, \infty)$ and its range of outputs is $\pi \in [0, 1]$.

I haven't seen anyone give the inverse-odds function a concise name; maybe prob() or prob() or risk()?

```r
odds_inv <- function(omega) (1 + omega^-1)^-1
library(ggplot2)
ggplot() +
  geom_function(fun = odds_inv, aes(col = "inverse-odds")) +
  xlab("Odds") +
  ylab("Probability") +
  xlim(0, 5) +
  ylim(0, 1) +
  geom_abline(aes(intercept = 0, slope = 1, col = "x=y"))
```

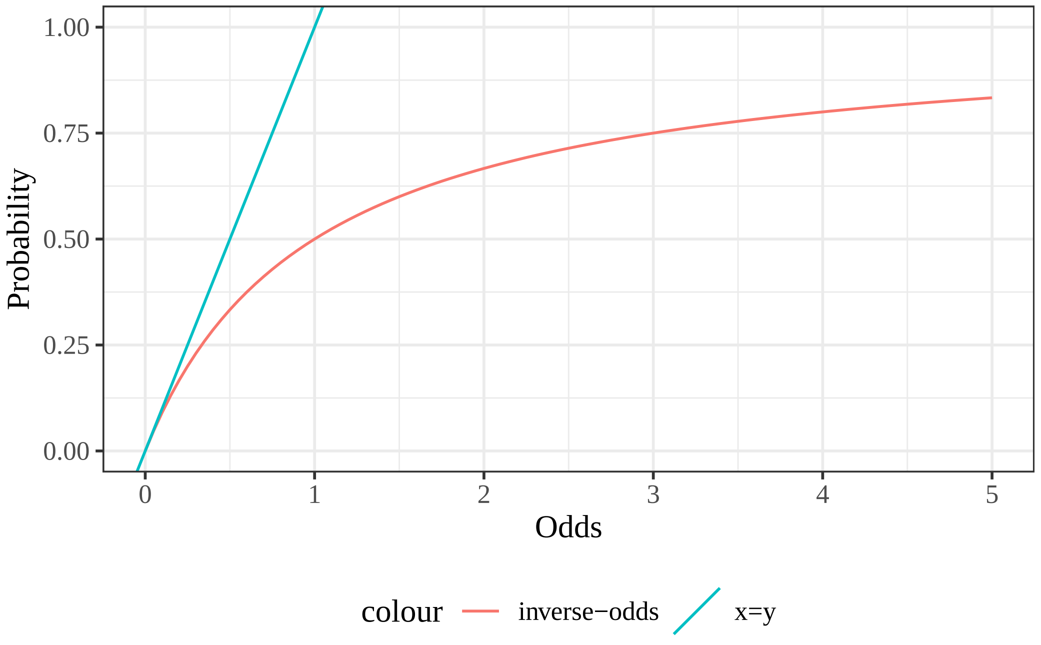


Figure 2: The inverse odds function, invodds$\{\omega\}$

Exercise 1.20. What probability corresponds to an odds of $\omega = 1$, and what is the numerical difference between these two values?

Solution

Solution.

$$\begin{aligned}\pi &= \text{invodds}\{1\}\\ &= \frac{1}{1+1}\\ &= \frac{1}{2}\\ &= .5\end{aligned}$$

$$\begin{aligned}\omega - \pi &= 1 - .5\\ &= .5\end{aligned}$$

Lemma 1.1 (Simplified expression for inverse odds function)**.**
Equivalent expressions for the inverse odds function are:

$$\begin{aligned}\text{invodds}\{\omega\} &= \frac{1}{1+\omega^{-1}}\\ &= (1+\omega^{-1})^{-1}\end{aligned} \tag{10}$$

Exercise 1.21. Prove that Equation 10 is equivalent to Definition 1.11.

Solution

Solution 1.18. Analogous to Solution 1.15.

Lemma 1.2 (One minus inverse-odds)**.**

$$1 - \pi = \frac{1}{1+\omega}$$

Proof

Proof. By Theorem 1.6:

$$\begin{aligned}1 - \pi &= 1 - \frac{\omega}{1+\omega}\\ &= \frac{1+\omega}{1+\omega} - \frac{\omega}{1+\omega}\\ &= \frac{(1+\omega) - \omega}{1+\omega}\\ &= \frac{1+\omega-\omega}{1+\omega}\\ &= \frac{1}{1+\omega}\end{aligned}$$

□

Corollary 1.5 (One plus odds in terms of non-event probability)**.**

$$1 + \omega = \frac{1}{1 - \pi}$$

1.3.3 Odds ratios

Now that we have defined odds, we can introduce another way of comparing event probabilities: odds ratios.

Definition 1.12 (Odds ratio)**.** The **odds ratio** for two conditional odds, ω_1 and ω_2, is the ratio of those odds:

$$\theta(\omega_1, \omega_2) \stackrel{\text{def}}{=} \frac{\omega_1}{\omega_2}$$

There's a 1:1 mapping between probability and odds, and according to that mapping, the odds are equal between two covariate patterns IF and ONLY IF the probabilities are also equal between those patterns. So, testing whether an odds ratio = 1 is equivalent to testing whether the corresponding risk ratio = 1, and also equivalent to testing whether the risk difference = 0. Therefore, in **hypothesis testing**, if the null hypothesis is no effect, then we can shift between RD, RR, and OR. But when we're talking about **point estimates** and **CIs**, we need to limit our conclusions to the effect measure(s) that we actually estimated, because the *sizes* of RDs, RRs, and ORs don't have a simple relationship to each other, except when pi_1=pi_2 (as shown by Figure 3).

An *odds ratio* is a *ratio of odds*. An odds is a ratio of probabilities, so odds ratios are ratios of ratios:

Theorem 1.7 (Odds ratio as a ratio of ratios)**.**

$$\begin{aligned}\theta(\omega_1, \omega_2) &= \frac{\omega_1}{\omega_2} \\ &= \frac{\left(\frac{\pi_1}{1-\pi_1}\right)}{\left(\frac{\pi_2}{1-\pi_2}\right)}\end{aligned}$$

Exm

Example 1.6 (Calculating odds ratios)**.** In Example 1.1, the odds ratio for OC users versus OC-non-users is:

$$\begin{aligned}\theta(\omega(OC), \omega(\neg OC)) &= \frac{\omega(OC)}{\omega(\neg OC)} \\ &= \frac{0.0026}{7 \times 10^{-4}} \\ &= 3.714286\end{aligned}$$

A shortcut for calculating odds ratio estimates

The general form of a two-by-two table is shown in Table 2.

Table 2: A generic 2x2 table

	Event	Non-Event	Total
Exposed	a	b	a+b
Non-exposed	c	d	c+d
Total	a+c	b+d	a+b+c+d

From this table, we have:

- $\hat{\pi}(Event|Exposed) = a/(a+b)$
- $\hat{\pi}(\neg Event|Exposed) = b/(a+b)$
- $\hat{\omega}(Event|Exposed) = \frac{\frac{a}{a+b}}{\frac{b}{a+b}} = \frac{a}{b}$
- $\hat{\omega}(Event|\neg Exposed) = \frac{c}{d}$ (see Exercise 1.22)
- $\theta_{\omega}(Exposed, \neg Exposed) = \frac{\frac{a}{b}}{\frac{c}{d}} = \frac{ad}{bc}$

Exercise 1.22. Given Table 2, show that $\hat{\omega}(Event|\neg Exposed) = \frac{c}{d}$.

Properties of odds ratios

Odds ratios have a special property: we can swap a covariate with the outcome, and the odds ratio remains the same.

Theorem 1.8 (Odds ratios are reversible)**.** *For any two events A, B:*

$$\theta_{\omega}(A|B) = \theta_{\omega}(B|A)$$

Proof

Proof.

$$
\begin{aligned}
\theta_\omega(A|B) &\overset{\text{def}}{=} \frac{\omega(A|B)}{\omega(A|\neg B)} \\
&= \frac{\left(\frac{\mathrm{p}(A|B)}{\mathrm{p}(\neg A|B)}\right)}{\left(\frac{\mathrm{p}(A|\neg B)}{\mathrm{p}(\neg A|\neg B)}\right)} \\
&= \left(\frac{\mathrm{p}(A|B)}{\mathrm{p}(\neg A|B)}\right)\left(\frac{\mathrm{p}(A|\neg B)}{\mathrm{p}(\neg A|\neg B)}\right)^{-1} \\
&= \left(\frac{\mathrm{p}(A|B)}{\mathrm{p}(\neg A|B)}\right)\left(\frac{\mathrm{p}(\neg A|\neg B)}{\mathrm{p}(A|\neg B)}\right) \\
&= \left(\frac{\mathrm{p}(A|B)}{\mathrm{p}(\neg A|B)} \cdot \frac{\mathrm{p}(B)}{\mathrm{p}(B)}\right)\left(\frac{\mathrm{p}(\neg A|\neg B)}{\mathrm{p}(A|\neg B)} \cdot \frac{\mathrm{p}(\neg B)}{\mathrm{p}(\neg B)}\right) \\
&= \left(\frac{\mathrm{p}(A,B)}{\mathrm{p}(\neg A,B)}\right)\left(\frac{\mathrm{p}(\neg A,\neg B)}{\mathrm{p}(A,\neg B)}\right) \\
&= \left(\frac{\mathrm{p}(B,A)}{\mathrm{p}(B,\neg A)}\right)\left(\frac{\mathrm{p}(\neg B,\neg A)}{\mathrm{p}(\neg B,A)}\right) \\
&= \left(\frac{\mathrm{p}(B,A)}{\mathrm{p}(\neg B,A)}\right)\left(\frac{\mathrm{p}(\neg B,\neg A)}{\mathrm{p}(B,\neg A)}\right) \\
&= [\text{reverse the preceding steps}] \\
&= \theta_\omega(B|A)
\end{aligned}
$$

□

Exm

Example 1.7. In Example 1.1, we have:

$$
\begin{aligned}
\theta_\omega(MI;OC) &\overset{\text{def}}{=} \frac{\omega(MI|OC)}{\omega(MI|\neg OC)} \\
&\overset{\text{def}}{=} \frac{\left(\frac{\Pr(MI|OC)}{\Pr(\neg MI|OC)}\right)}{\left(\frac{\Pr(MI|\neg OC)}{\Pr(\neg MI|\neg OC)}\right)} \\
&= \frac{\left(\frac{\Pr(MI,OC)}{\Pr(\neg MI,OC)}\right)}{\left(\frac{\Pr(MI,\neg OC)}{\Pr(\neg MI,\neg OC)}\right)} \\
&= \left(\frac{\Pr(MI,OC)}{\Pr(\neg MI,OC)}\right)\left(\frac{\Pr(\neg MI,\neg OC)}{\Pr(MI,\neg OC)}\right) \\
&= \left(\frac{\Pr(MI,OC)}{\Pr(MI,\neg OC)}\right)\left(\frac{\Pr(\neg MI,\neg OC)}{\Pr(\neg MI,OC)}\right) \\
&= \left(\frac{\Pr(OC,MI)}{\Pr(\neg OC,MI)}\right)\left(\frac{\Pr(\neg OC,\neg MI)}{\Pr(OC,\neg MI)}\right) \\
&= \left(\frac{\Pr(OC|MI)}{\Pr(\neg OC|MI)}\right)\left(\frac{\Pr(\neg OC|\neg MI)}{\Pr(OC|\neg MI)}\right) \\
&= \frac{\left(\frac{\Pr(OC|MI)}{\Pr(\neg OC|MI)}\right)}{\left(\frac{\Pr(OC|\neg MI)}{\Pr(\neg OC|\neg MI)}\right)} \\
&\overset{\text{def}}{=} \frac{\omega(OC|MI)}{\omega(OC|\neg MI)} \\
&\overset{\text{def}}{=} \theta_\omega(OC;MI)
\end{aligned}
$$

Exercise 1.23. For Table 2, show that $\hat{\theta}_\omega(Exposed, Unexposed) = \hat{\theta}_\omega(Event, \neg Event)$.

Conditional odds ratios have the same reversibility property:

Theorem 1.9 (Conditional odds ratios are reversible)**.** *For any three events A, B, C:*

$$\theta_\omega(A|B,C) = \theta_\omega(B|A,C)$$

ℹ Proof

Proof. Apply the same steps as for Theorem 1.8, inserting C into the conditions (RHS of $|$) of every expression. ☐

Odds Ratios vs Probability (Risk) Ratios

When the outcome is rare (i.e., its probability is small) for both groups being compared in an odds ratio, the odds of the outcome will be similar to the probability of the outcome, and thus the risk ratio will be similar to the odds ratio.

Case 1: rare events

For rare events, odds ratios and probability (a.k.a. risk, a.k.a. prevalence) ratios will be close:

$$\pi_1 = .01$$

$$\pi_2 = .02$$

```
pi1 <- .01
pi2 <- .02
pi2 / pi1
#> [1] 2
odds(pi2) / odds(pi1)
#> [1] 2.02041
```

Exm

Example 1.8. In Example 1.1, the outcome is rare for both OC and non-OC participants, so the odds for both groups are similar to the corresponding probabilities, and the odds ratio is similar the risk ratio.

Case 2: frequent events

$$\pi_1 = .4$$

$$\pi_2 = .5$$

For more frequently-occurring outcomes, this won't be the case:

```
pi1 <- .4
pi2 <- .5
pi2 / pi1
#> [1] 1.25
odds(pi2) / odds(pi1)
#> [1] 1.5
```

Figure 3 compares risk differences, risk ratios, and odds ratios as functions of the underlying probabilities being compared.

```r
if (run_graphs) {
  RD <- function(p1, p2) p2 - p1
  RR <- function(p1, p2) p2 / p1
  odds <- function(p) p / (1 - p)
  OR <- function(p1, p2) odds(p2) / odds(p1)
  OR_minus_RR <- function(p1, p2) OR(p2, p1) - RR(p2, p1)

  n_ticks <- 201
  probs <- seq(.001, .99, length.out = n_ticks)
  RD_mat <- outer(probs, probs, RD)
  RR_mat <- outer(probs, probs, RR)
  OR_mat <- outer(probs, probs, OR)

  opacity <- .3
  z_min <- -1
  z_max <- 5
  plotly::plot_ly(
    x = ~probs,
    y = ~probs
  ) |>
    plotly::add_surface(
      z = ~ t(RD_mat),
      contours = list(
        z = list(
          show = TRUE,
          start = -1,
          end = 1,
          size = .1
        )
      ),
      name = "Risk Difference",
      showscale = FALSE,
      opacity = opacity,
      colorscale = list(c(0, 1), c("green", "green"))
    ) |>
    plotly::add_surface(
      opacity = opacity,
      colorscale = list(c(0, 1), c("red", "red")),
      z = ~ t(RR_mat),
      contours = list(
        z = list(
          show = TRUE,
          start = z_min,
          end = z_max,
          size = .2
        )
      ),
      showscale = FALSE,
      name = "Risk Ratio"
    ) |>
    plotly::add_surface(
      opacity = opacity,
      colorscale = list(c(0, 1), c("blue", "blue")),
      z = ~ t(OR_mat),
      contours = list(
        z = list(
          show = TRUE,
          start = z_min,
          end = z_max,
          size = .2
        )
      ),
      showscale = FALSE
```

Odds Ratios in Case-Control Studies

Table 1 simulates a follow-up study in which two populations were followed and the number of MI's was observed. The risks are $P(MI|OC)$ and $P(MI|\neg OC)$ and we can estimate these risks from the data.

But suppose we had a case-control study in which we had 100 women with MI and selected a comparison group of 100 women without MI (matched as groups on age, etc.). Then MI is not random, and we cannot compute P(MI|OC) and we cannot compute the risk ratio. However, the odds ratio however can be computed.

The disease odds ratio is the odds for the disease in the exposed group divided by the odds for the disease in the unexposed group, and we cannot validly compute and use these separate parts.

We can still validly compute and use the exposure odds ratio, which is the odds for exposure in the disease group divided by the odds for exposure in the non-diseased group (because exposure can be treated as random):

$$\hat{\theta}(OC|MI) = \frac{\hat{\omega}(OC|MI)}{\hat{\omega}(OC|\neg MI)}$$

And these two odds ratios, $\hat{\theta}(MI|OC)$ and $\hat{\theta}(OC|MI)$, are mathematically equivalent, as we saw in Section 1.3.3:

$$\hat{\theta}(MI|OC) = \hat{\theta}(OC|MI)$$

Exercise 1.24. Calculate the odds ratio of MI with respect to OC use, assuming that Table 1 comes from a case-control study. Confirm that the result is the same as in Example 1.6.

Solution

Solution.

```r
tbl_oc_mi |> pander::pander()
```

Table 3: Simulated data from study of oral contraceptive use and heart attack risk

OC	MI	No MI	Total
OC use	13	4,987	5,000
No OC use	7	9,993	10,000
Total	20	14,980	15,000

- $\omega(OC|MI) = P(OC|MI)/(1–P(OC|MI) = \frac{13}{7} = 1.857143$
- $\omega(OC|\neg MI) = P(OC|\neg MI)/(1–P(OC|\neg MI) = \frac{4987}{9993} = 0.499049$
- $\theta_{\omega}(OC, MI) = \frac{\omega(OC|MI)}{\omega(OC|\neg MI)} = \frac{13/7}{4987/9993} = 3.721361$

This is the same estimate we calculated in Example 1.6.

Odds Ratios in Cross-Sectional Studies

- If a cross-sectional study is a uniform probability sample of a population (which it rarely is), then we can estimate prevalence (sometimes called "prevalence risk" or just "risk") using standard methods (Lee 1994), and we can thus also estimate prevalence differences, prevalence ratios, and prevalence odds ratios comparing sub-populations.
- If the cross-sectional study is a stratified probability sample, then we can estimate prevalence, prevalence differences, prevalence ratios, and prevalence odds ratios using specialized methods for complex surveys (Lumley 2010).
- If the study has sampling biases that we cannot adjust for with survey weights, such as in a convenience sample, then we need to treat it in the same way as a case-control study, and we cannot validly estimate prevalence, prevalence differences, or prevalence ratios; we can only validly estimate prevalence *odds* ratios.

1.4 The logit and expit functions

1.4.1 The logit function

Definition 1.13 (log-odds)**.**
If ω is the odds of an event A, then the **log-odds** of A, which we will represent by η ("eta"), is the natural logarithm of the odds of A:

$$\eta \stackrel{\text{def}}{=} \log\{\omega\} \tag{11}$$

Theorem 1.10 (Log-odds as a function of probability)**.** *If π is the probability of an event A, ω is the corresponding odds of A, and η is the corresponding log-odds of A, then:*

$$\eta = \log\left\{\frac{\pi}{1-\pi}\right\} \tag{12}$$

Proof

Proof. Apply Definition 1.13 and then Theorem 1.2. ☐

Definition 1.14 (logit function)**.**
The **logit function** of a probability π is the natural logarithm of the odds function of π:

$$\text{logit}(\pi) \stackrel{\text{def}}{=} \log\{\text{odds}\{\pi\}\}$$

The **logit function** is a composite function[a].

---

[a] https://en.wikipedia.org/wiki/Function_composition

Exercise 1.25 (Compose the logit function)**.** Mathematically expand the definition of the logit function.

Solution (Compose the logit function)

Solution 1.19 (Compose the logit function).

Lem

Theorem 1.11 (Expanded expression for logit).

$$\text{logit}(\pi) = \log\left\{\frac{\pi}{1-\pi}\right\} \tag{13}$$

Proof

Proof. Apply Definition 1.14 and then Definition 1.8 (details left to the reader). ☐

Corollary 1.6 (Log-odds via the logit function)**.** *If π is the probability of an event A and η is the corresponding log-odds of A, then:*

$$\eta = \text{logit}\{\pi\}$$

Proof

Proof. Apply Theorem 1.10 and Theorem 1.11. ☐

Figure 4 shows the shape of the logit() function.

```
odds <- function(pi) pi / (1 - pi)

logit <- function(p) log(odds(p))

library(ggplot2)
logit_plot <-
  ggplot() +
  geom_function(
    fun = logit,
    arrow = arrow(ends = "both")
  ) +
  xlim(.001, .999) +
  ylab("logit(p)") +
  xlab("p") +
  theme_bw()
print(logit_plot)
```

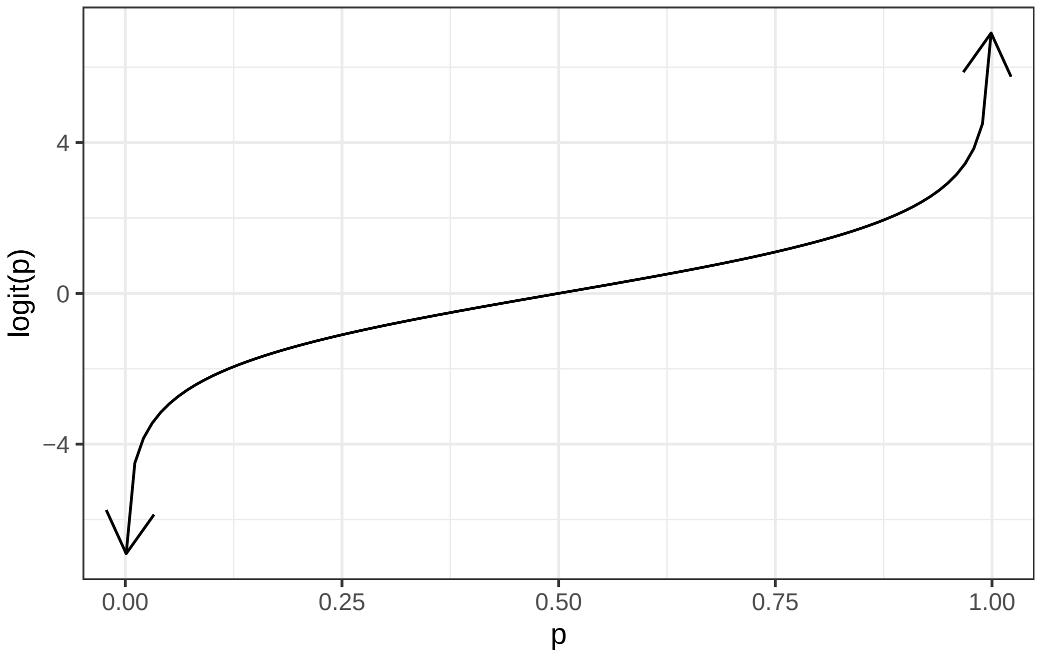


Figure 4: The logit function

1.4.2 The expit function

Lemma 1.3 (Odds from log-odds)**.**
If ω is the odds of an event A and η is the corresponding log-odds of A, then:

$$\omega = \exp\{\eta\}$$

ℹ Proof

Proof. Start from Definition 1.13 and solve for ω. ☐

Theorem 1.12 (Probability as a function of log-odds)**.**
If π is the probability of an event A, ω is the corresponding odds of A, and η is the corresponding log-odds of A, then:

$$\pi = \frac{\exp\{\eta\}}{1 + \exp\{\eta\}}$$

ℹ Proof

Proof. Apply Theorem 1.6 and then Lemma 1.3. ☐

Definition 1.15 (expit, logistic, inverse-logit)**.** The **expit function** of a log-odds η, also known as the **inverse-logit function** or **logistic function**, is the inverse-odds of the exponential of η:

$$\text{expit}(\eta) \overset{\text{def}}{=} \text{invodds}\{\exp\{\eta\}\}$$

Theorem 1.13 (Expressions for expit function)**.**

$$\begin{aligned}\text{expit}(\eta) &= \frac{\exp\{\eta\}}{1+\exp\{\eta\}} \\ &= \frac{1}{1+\exp\{-\eta\})} \\ &= (1+\exp\{-\eta\})^{-1}\end{aligned}$$

Proof

Proof. Apply definitions and Lemma 1.1. Details left to the reader. $\square$

Theorem 1.14 (Probability via the expit function)**.** *If π is the probability of an event A, ω is the corresponding odds of A, and η is the corresponding log-odds of A, then:*

$$\pi = \text{expit}\{\eta\}$$

Proof

Proof. Apply Theorem 1.12 and Theorem 1.13. $\square$

Figure 5 graphs the expit function.

```r
expit <- function(eta) {
  exp(eta) / (1 + exp(eta))
}
library(ggplot2)
expit_plot <-
  ggplot() +
  geom_function(
    fun = expit,
    arrow = arrow(ends = "both")
  ) +
  xlim(-8, 8) +
  ylim(0, 1) +
  ylab(expression(expit(eta))) +
  xlab(expression(eta)) +
  theme_bw()
print(expit_plot)
```

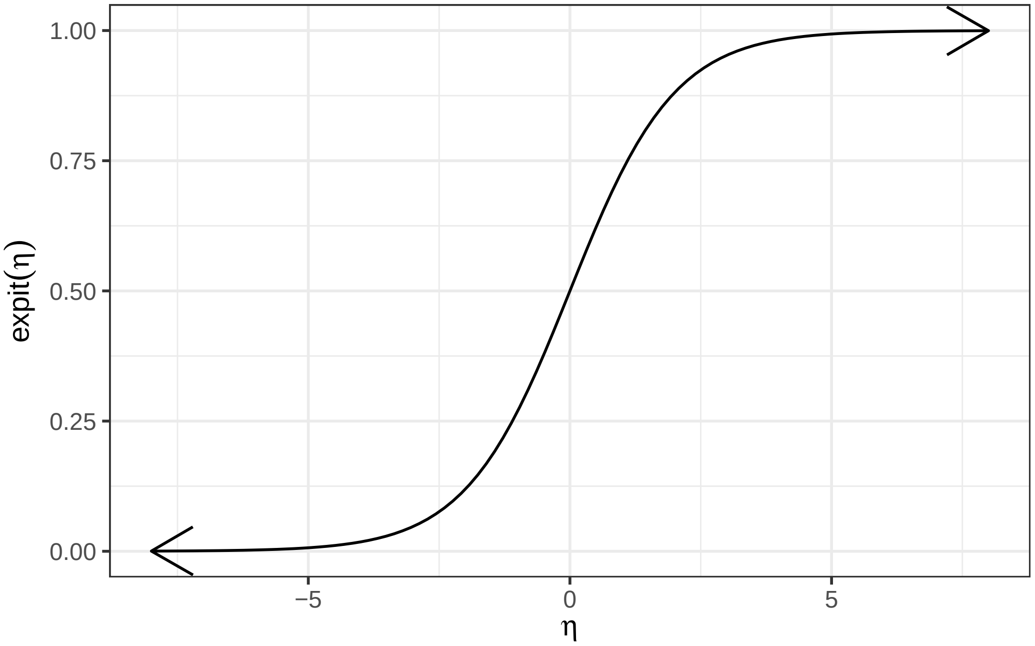


Figure 5: The expit function

Theorem 1.15 (logit and expit are each others' inverses)**.**

$$\text{logit}\{\text{expit}\{\eta\}\} = \eta$$

$$\text{expit}\{\text{logit}\{\pi\}\} = \pi$$

Proof

Proof. Left to the reader. □

1.4.3 Diagram of expit and logit

$$\left[\pi \overset{\text{def}}{=} \Pr(Y=1|\tilde{X}=\tilde{x})\right] \overbrace{\underbrace{\underset{\frac{\omega}{1+\omega}}{\overset{\frac{\pi}{1-\pi}}{\rightleftarrows}} \left[\omega \overset{\text{def}}{=} \text{odds}(Y=1|\tilde{X}=\tilde{x})\right] \underset{\exp\{\eta\}}{\overset{\log\{\omega\}}{\rightleftarrows}}}_{\text{expit}(\eta)}}^{\text{logit}(\pi)} \left[\eta(\tilde{x}) \overset{\text{def}}{=} \text{log-odds}(Y=1|\tilde{X}=\tilde{x})\right]$$

Figure 6: Diagram of logistic regression link and inverse link functions

2 Introduction to logistic regression

- In Example 1.1, we estimated the risk and the odds of MI for two groups, defined by oral contraceptive use.

- If the predictor is quantitative (dose) or there is more than one predictor, the task becomes more difficult.
- In this case, we will use logistic regression, which is a generalization of the linear regression models you have been using that can account for a binary response instead of a continuous one.

2.0.1 Independent binary outcomes - general

Exercise 2.1. Let $\tilde{y}$ represent a data set of mutually independent binary outcomes, each with a potentially different event probability π_i:

$$\begin{aligned} \tilde{y} &= (y_1, ..., y_n) \\ y_i &\sim_{\perp\!\!\!\perp} \text{Ber}(\pi_i) \end{aligned}$$

Write the likelihood of $\tilde{y}$.

Solution

Solution 2.1.

$$\begin{aligned} \pi_i &\overset{\text{def}}{=} \text{P}(Y_i = 1) \\ \text{P}(Y_i = 0) &= 1 - \pi_i \\ \text{P}(Y_i = y_i) &= \text{P}(Y_i = 1)^{y_i}\,\text{P}(Y_i = 0)^{1-y_i} \\ &= (\pi_i)^{y_i}(1-\pi_i)^{1-y_i} \\ \mathcal{L}_i(\pi_i) &\overset{\text{def}}{=} \text{P}(Y_i = y_i) \\ \mathcal{L}(\tilde{\pi}) &\overset{\text{def}}{=} \text{P}(Y_1 = y_1, \ldots, Y_n = y_n) \\ &= \prod_{i=1}^{n} \text{P}(Y_i = y_i) \\ &= \prod_{i=1}^{n} \mathcal{L}_i(\pi_i) \\ &= \prod_{i=1}^{n} (\pi_i)^{y_i}(1-\pi_i)^{1-y_i} \end{aligned}$$

Exercise 2.2. Write the log-likelihood of $\tilde{y}$.

Solution

Solution 2.2.

$$
\begin{aligned}
\ell(\tilde{\pi}) &\overset{\text{def}}{=} \log\{\mathcal{L}(\tilde{\pi})\} \\
&= \log\left\{\prod_{i=1}^{n} \mathcal{L}_i(\pi_i)\right\} \\
&= \sum_{i=1}^{n} \log\{\mathcal{L}_i(\pi_i)\} \\
&= \sum_{i=1}^{n} \ell_i(\pi_i) \\
\ell_i(\pi_i) &\overset{\text{def}}{=} \log\{\mathcal{L}_i(\pi_i)\} \\
&= y_i \log\{\pi_i\} + (1 - y_i) \log\{1 - \pi_i\}
\end{aligned}
$$

2.0.2 Modeling π_i as a function of X_i

If there are only a few distinct X_i values, we can model π_i separately for each value of X_i.

Otherwise, we need regression.

$$
\begin{aligned}
\pi(x) &\equiv \text{E}(Y = 1 | X = x) \\
&= f(x^\top \beta)
\end{aligned}
$$

Typically, we use the expit inverse-link:

$$\pi(\tilde{x}) = \text{expit}(\tilde{x}' \beta) \tag{14}$$

2.0.3 Meet the beetles

Table 4: Mortality rates of adult flour beetles after five hours' exposure to gaseous carbon disulphide (Bliss 1935)

```r
library(glmx)
library(dplyr)
data(BeetleMortality, package = "glmx")
beetles <- BeetleMortality |>
  mutate(
    pct = died / n,
    survived = n - died,
    dose_c = dose - mean(dose)
  )
beetles
#> # A tibble: 8 x 6
#>    dose  died     n   pct survived   dose_c
#>   <dbl> <int> <int> <dbl>    <int>    <dbl>
#> 1  1.69     6    59 0.102       53 -0.103
#> 2  1.72    13    60 0.217       47 -0.0692
#> 3  1.76    18    62 0.290       44 -0.0382
#> 4  1.78    28    56 0.5         28 -0.00923
#> 5  1.81    52    63 0.825       11  0.0179
#> 6  1.84    53    59 0.898        6  0.0435
#> 7  1.86    61    62 0.984        1  0.0676
#> 8  1.88    60    60 1            0  0.0905
```

```r
library(ggplot2)
plot1 <-
  beetles |>
  ggplot(aes(x = dose, y = pct)) +
  geom_point(aes(size = n)) +
  xlab("Dose (log mg/L)") +
  ylab("Mortality rate (%)") +
  scale_y_continuous(labels = scales::percent) +
  scale_size(range = c(1, 2)) +
  theme_bw(base_size = 18)

print(plot1)
```

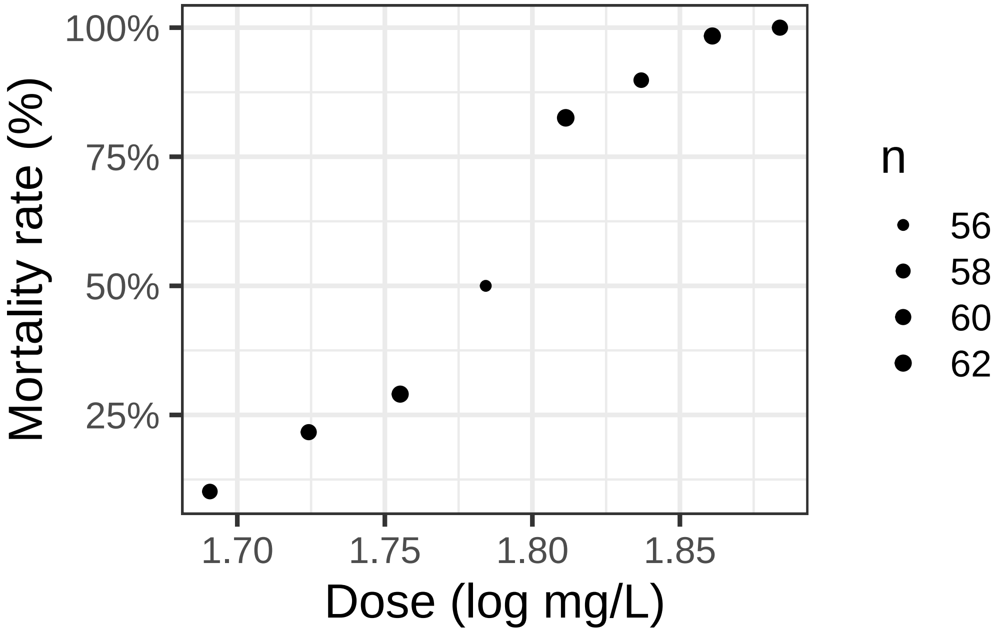


Figure 7: Mortality rates of adult flour beetles after five hours' exposure to gaseous carbon disulphide (Bliss 1935)

2.0.4 Why don't we use linear regression?

```
beetles_long <- beetles |>
  reframe(
    .by = everything(),
    outcome = c(
      rep(1, times = died),
      rep(0, times = survived)
    )
  ) |>
  as_tibble()

lm1 <- beetles_long |> lm(formula = outcome ~ dose)
f_linear <- function(x) predict(lm1, newdata = data.frame(dose = x))

range1 <- range(beetles$dose) + c(-.2, .2)

plot2 <-
  plot1 +
  geom_function(
    fun = f_linear,
    aes(col = "Straight line")
  ) +
  labs(colour = "Model", size = "")

plot2 |> print()
```

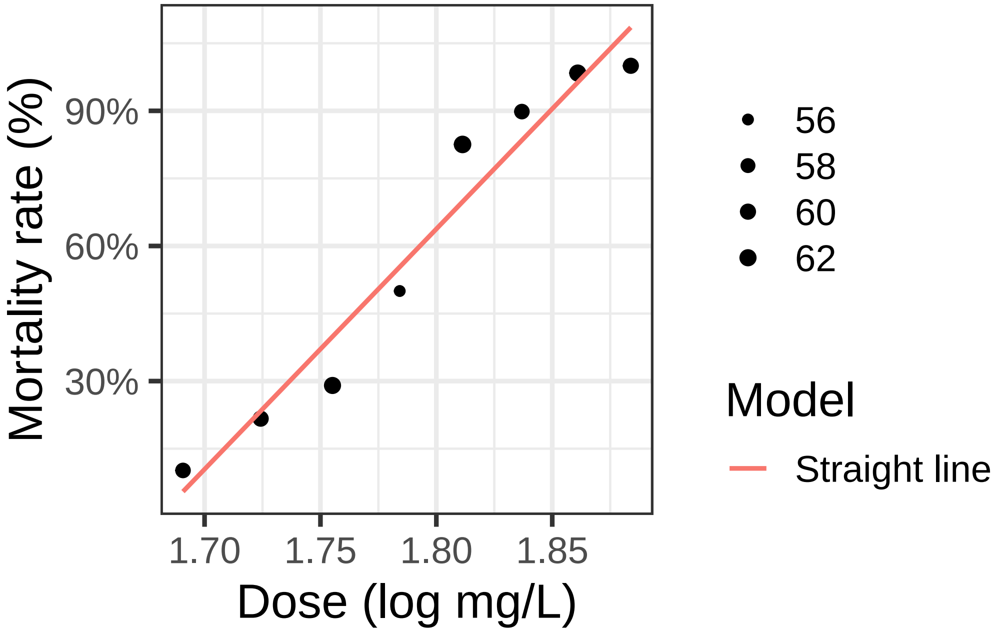


Figure 8: Mortality rates of adult flour beetles after five hours' exposure to gaseous carbon disulphide (Bliss 1935)

2.0.5 Zoom out

```
(plot2 + expand_limits(x = c(1.6, 2))) |> print()
```

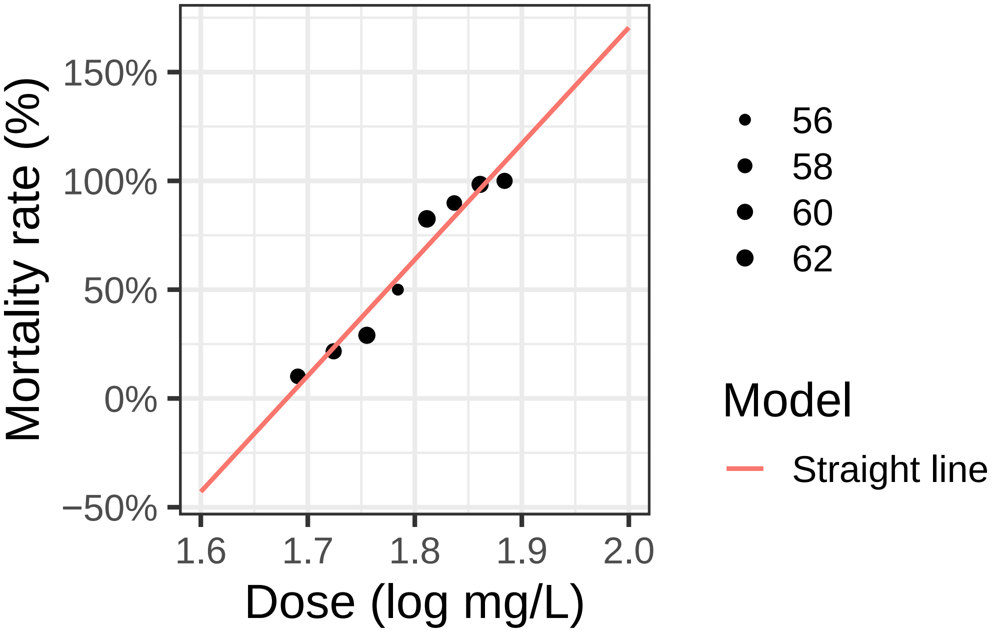


Figure 9: Mortality rates of adult flour beetles after five hours’ exposure to gaseous carbon disulphide (Bliss 1935)

2.0.6 log transformation of dose?

```
lm2 <- beetles_long |> lm(formula = outcome ~ log(dose))
f_linearlog <- function(x) predict(lm2, newdata = data.frame(dose = x))

plot3 <- plot2 +
  expand_limits(x = c(1.6, 2)) +
  geom_function(fun = f_linearlog, aes(col = "Log-transform dose"))
(plot3 + expand_limits(x = c(1.6, 2))) |> print()
```

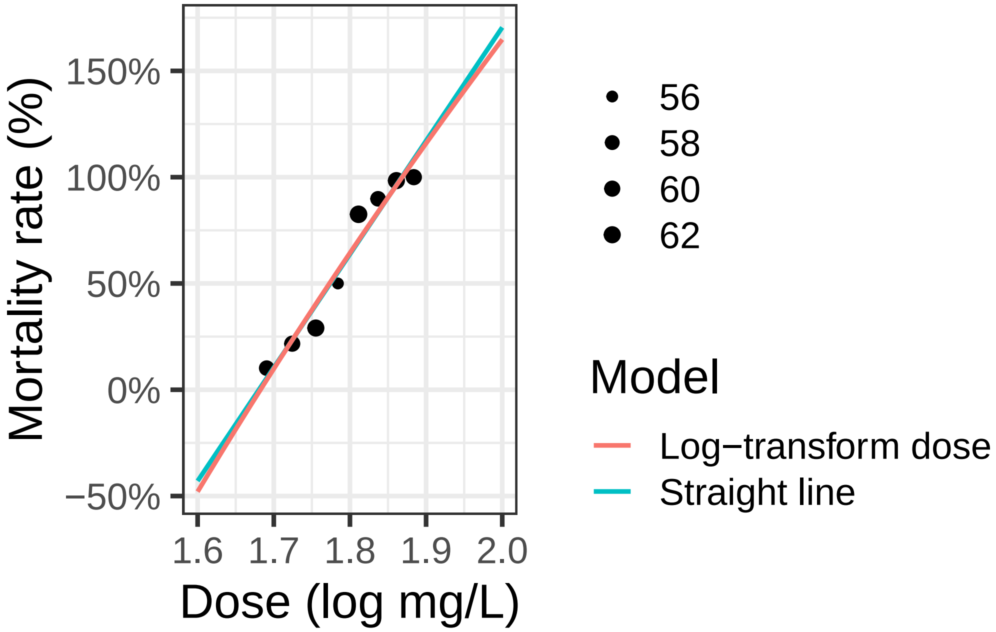


Figure 10: Mortality rates of adult flour beetles after five hours' exposure to gaseous carbon disulphide (Bliss 1935)

2.0.7 Logistic regression

```
beetles_glm_grouped <- beetles |>
  glm(formula = cbind(died, survived) ~ dose, family = "binomial")
f <- function(x) {
  beetles_glm_grouped |>
    predict(newdata = data.frame(dose = x), type = "response")
}

plot4 <- plot3 + geom_function(fun = f, aes(col = "Logistic regression"))
plot4 |> print()
```

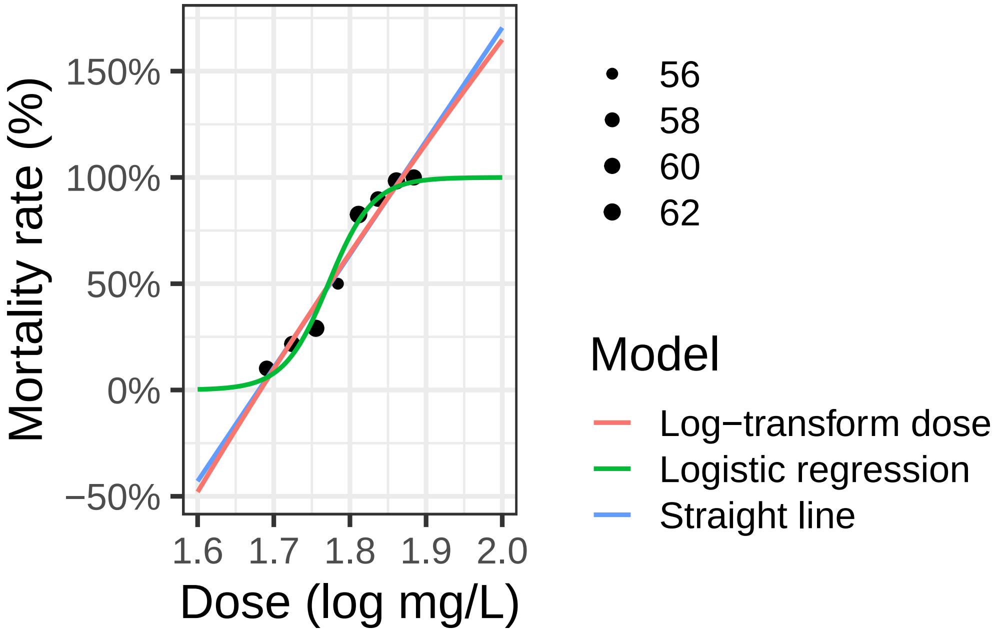


Figure 11: Mortality rates of adult flour beetles after five hours' exposure to gaseous carbon disulphide (Bliss 1935).

2.0.8 Three parts to regression models

- What distribution does the outcome have for a specific subpopulation defined by covariates? (outcome model)
- How does the combination of covariates relate to the mean? (link function)
- How do the covariates combine? (linear predictor, interactions)

2.0.9 Fitting and manipulating logistic regression models in R

```
library(glmx)
library(dplyr)
data(BeetleMortality)
beetles <- BeetleMortality |>
  mutate(
    pct = died / n,
    survived = n - died
  )
```

Table 6

```
fitted(beetles_glm_grouped)
#>        1        2        3        4        5        6        7        8
#> 0.058601 0.164028 0.362119 0.605315 0.795172 0.903236 0.955196 0.979049
predict(beetles_glm_grouped, type = "response")
#>        1        2        3        4        5        6        7        8
#> 0.058601 0.164028 0.362119 0.605315 0.795172 0.903236 0.955196 0.979049
```

```
beetles_glm_grouped <-
  beetles |>
  glm(
    formula = cbind(died, survived) ~ dose,
    family = "binomial"
  )

library(parameters)
beetles_glm_grouped |>
  parameters() |>
  print_md()
```

Table 5: logistic regression model for beetles data with grouped (binomial) data

Parameter	Log-Odds	SE	95% CI	z	p
(Intercept)	-60.72	5.18	(-71.44, -51.08)	-11.72	< .001
dose	34.27	2.91	(28.85, 40.30)	11.77	< .001

Fitted values

Fitted values are provided on the probability scale (Table 6)

Count scale

For grouped data, we can convert to the count scale by multiplying by the group size:

```
beetles$n * fitted(beetles_glm_grouped)
#>        1        2        3        4        5        6        7        8
#>  3.45746  9.84167 22.45138 33.89763 50.09582 53.29091 59.22216 58.74296
```

Logit scale

```
predict(beetles_glm_grouped, type = "link")
#>         1         2         3         4         5         6         7         8
#> -2.776615 -1.628559 -0.566179  0.427661  1.356386  2.233707  3.059622  3.844412
```

Converting between logit and probability scales works as expected:

```
predict(beetles_glm_grouped, type = "link") |> arm::invlogit()
#>        1        2        3        4        5        6        7        8
#> 0.058601 0.164028 0.362119 0.605315 0.795172 0.903236 0.955196 0.979049
predict(beetles_glm_grouped, type = "response")
#>        1        2        3        4        5        6        7        8
```

```
#> 0.058601 0.164028 0.362119 0.605315 0.795172 0.903236 0.955196 0.979049

predict(beetles_glm_grouped, type = "response") |> arm::logit()
#>         1         2         3         4         5         6         7         8
#> -2.776615 -1.628559 -0.566179  0.427661  1.356386  2.233707  3.059622  3.844412
predict(beetles_glm_grouped, type = "link")
#>         1         2         3         4         5         6         7         8
#> -2.776615 -1.628559 -0.566179  0.427661  1.356386  2.233707  3.059622  3.844412
```

`type = "terms"` is confusing, because the variables get centered:

```
predict(beetles_glm_grouped, type = "terms")
#>        dose
#> 1 -3.520419
#> 2 -2.372363
#> 3 -1.309983
#> 4 -0.316144
#> 5  0.612582
#> 6  1.489902
#> 7  2.315817
#> 8  3.100608
#> attr(,"constant")
#> [1] 0.743804
coef(beetles_glm_grouped)["dose"] * beetles$dose
#> [1] 57.9408 59.0889 60.1513 61.1451 62.0738 62.9512 63.7771 64.5619
```

We can construct the link-scale predictions from the terms:

```
terms_pred <- predict(beetles_glm_grouped, type = "terms")
terms_pred + attr(terms_pred, "constant")
#>        dose
#> 1 -2.776615
#> 2 -1.628559
#> 3 -0.566179
#> 4  0.427661
#> 5  1.356386
#> 6  2.233707
#> 7  3.059622
#> 8  3.844412
#> attr(,"constant")
#> [1] 0.743804
predict(beetles_glm_grouped, type = "link")
#>         1         2         3         4         5         6         7         8
#> -2.776615 -1.628559 -0.566179  0.427661  1.356386  2.233707  3.059622  3.844412
```

Individual observations

```
beetles_glm_ungrouped <-
  beetles_long |>
  glm(
    formula = outcome ~ dose,
    family = "binomial"
  )
```

Table 7: `beetles` data in long format

```
beetles_long
#> # A tibble: 481 x 7
#>     dose  died     n   pct survived dose_c outcome
#>    <dbl> <int> <int> <dbl>    <int>  <dbl>   <dbl>
#>  1  1.69     6    59 0.102       53 -0.103       1
#>  2  1.69     6    59 0.102       53 -0.103       1
#>  3  1.69     6    59 0.102       53 -0.103       1
#>  4  1.69     6    59 0.102       53 -0.103       1
#>  5  1.69     6    59 0.102       53 -0.103       1
#>  6  1.69     6    59 0.102       53 -0.103       1
#>  7  1.69     6    59 0.102       53 -0.103       0
#>  8  1.69     6    59 0.102       53 -0.103       0
#>  9  1.69     6    59 0.102       53 -0.103       0
#> 10  1.69     6    59 0.102       53 -0.103       0
#> # i 471 more rows
```

```
beetles_glm_ungrouped |>
  parameters() |>
  print_md()
```

Table 8: logistic regression model for beetles data with individual Bernoulli data

Parameter	Log-Odds	SE	95% CI	z	p
(Intercept)	-60.72	5.18	(-71.44, -51.08)	-11.72	$<$ .001
dose	34.27	2.91	(28.85, 40.30)	11.77	$<$ .001

Exercise 2.3. Compare this model with the grouped-observations model (Table 5).

Solution

Solution 2.3.
They seem the same! But not quite:

```
logLik(beetles_glm_grouped)
#> 'log Lik.' -18.7151 (df=2)
logLik(beetles_glm_ungrouped)
#> 'log Lik.' -186.235 (df=2)
```

The difference is due to the binomial coefficient $\binom{n}{x}$ which isn't included in the individual-observations (Bernoulli) version of the model.

3 Derivatives of logistic regression functions

In order to interpret logistic regression models and find their MLEs, we will need to compute various derivatives. This section compiles some useful results.

3.0.1 Derivatives of odds function

Theorem 3.1 (Derivative of odds function)**.**

$$\text{odds}'\{\pi\} = \frac{\partial\omega}{\partial\pi} = \frac{1}{(1-\pi)^2}$$

Proof

Proof. We can use Theorem 1.2 and the quotient rule[a]:

$$\begin{aligned}
\frac{\partial\omega}{\partial\pi} &= \frac{\partial}{\partial\pi}\left(\frac{\pi}{1-\pi}\right) \\
&= \frac{\frac{\partial}{\partial\pi}\pi}{1-\pi} - \left(\frac{\pi}{(1-\pi)^2} \cdot \frac{\partial}{\partial\pi}(1-\pi)\right) \\
&= \frac{1}{1-\pi} - \frac{\pi}{(1-\pi)^2} \cdot (-1) \\
&= \frac{1}{1-\pi} + \frac{\pi}{(1-\pi)^2} \\
&= \frac{1-\pi}{(1-\pi)^2} + \frac{\pi}{(1-\pi)^2} \\
&= \frac{1-\pi+\pi}{(1-\pi)^2} \\
&= \frac{1}{(1-\pi)^2}
\end{aligned}$$

□

---

[a] math-prereqs.qmd#thm-quotient-rule

Corollary 3.1 (Derivative of odds function in terms of odds)**.**

$$\frac{\partial\omega}{\partial\pi} = (1+\omega)^2$$

Proof

Proof. By Theorem 3.1 and Corollary 1.5. □

3.0.2 Derivatives of inverse-odds function

Theorem 3.2 (Derivative of inverse odds function)**.**

$$\text{invodds}'\{\omega\} = \frac{\partial\pi}{\partial\omega} = (1-\pi)^2 = \frac{1}{(1+\omega)^2} \tag{15}$$

Proof

Proof. By Theorem 3.1 and Corollary 3.1.
Or for a direct approach, use the quotient rule[a] again:

$$
\begin{aligned}
\frac{\partial \pi}{\partial \omega} &= \frac{\partial}{\partial \omega}\frac{\omega}{1+\omega} \\
&= \frac{\frac{\partial}{\partial \omega}\omega}{1+\omega} - \frac{\omega}{(1+\omega)^2} \cdot \frac{\partial}{\partial \omega}(1+\omega) \\
&= \frac{1}{1+\omega} - \frac{\omega}{(1+\omega)^2} \cdot 1 \\
&= \frac{1}{1+\omega} - \frac{\omega}{(1+\omega)^2} \\
&= \frac{1+\omega}{(1+\omega)^2} - \frac{\omega}{(1+\omega)^2} \\
&= \frac{1+\omega-\omega}{(1+\omega)^2} \\
&= \frac{1}{(1+\omega)^2}
\end{aligned}
$$

□

---

[a] math-prereqs.qmd#thm-quotient-rule

3.0.3 Derivatives of logit function

Lemma 3.1 (Derivative of log-odds by odds)**.**

$$\frac{\partial \eta}{\partial \omega} = \omega^{-1}$$

Proof

Proof. Using Definition 1.13:

$$
\begin{aligned}
\frac{\partial \eta}{\partial \omega} &= \frac{\partial}{\partial \omega}\log \omega \\
&= \omega^{-1}
\end{aligned}
$$

□

Theorem 3.3 (Derivative of log-odds by odds)**.**

$$\frac{\partial \eta}{\partial \omega} = \frac{1-\pi}{\pi}$$

Proof

Proof. Using Theorem 1.2 and Lemma 3.1:

$$\begin{aligned}\frac{\partial \eta}{\partial \omega} &= \omega^{-1} \\ &= \frac{1-\pi}{\pi}\end{aligned}$$

$\square$

Theorem 3.4 (Derivative of log-odds by probability)**.**

$$\frac{\partial \eta}{\partial \pi} = \frac{1}{(\pi)(1-\pi)}$$

Proof

Proof. Using Theorem 3.3, Theorem 3.1, and the chain rule[a]:

$$\begin{aligned}\frac{\partial \eta}{\partial \pi} &= \frac{\partial \eta}{\partial \omega}\frac{\partial \omega}{\partial \pi} \\ &= \frac{1-\pi}{\pi}\frac{1}{(1-\pi)^2} \\ &= \frac{1}{(\pi)(1-\pi)}\end{aligned}$$

$\square$

---

[a] math-prereqs.qmd#thm-chain-rule

Corollary 3.2 (Derivative of logit function)**.**

$$\text{logit}'(\pi) = \frac{1}{(\pi)(1-\pi)}$$

Proof

Proof. By Theorem 3.4 and Corollary 1.6. $\square$

3.0.4 Derivatives of expit function

Lemma 3.2 (Derivative of odds w.r.t. log-odds)**.**

$$\frac{\partial \omega}{\partial \eta} = \omega$$

Proof

Proof. Using Lemma 1.3 and the derivative of the exponential function[a]:

$$\begin{aligned}\frac{\partial \omega}{\partial \eta} &= \frac{\partial}{\partial \eta} \exp\{\eta\} \\ &= \exp\{\eta\} \\ &= \omega\end{aligned}$$

□

---

[a] math-prereqs.qmd#thm-deriv-exp

Theorem 3.5 (Derivative of odds in terms of probability)**.**

$$\frac{\partial \omega}{\partial \eta} = \frac{\pi}{1-\pi} \tag{16}$$

Proof

Proof. Use Lemma 3.2 and Theorem 1.2. □

Theorem 3.6 (Derivative of probability w.r.t. log-odds)**.**

$$\frac{\partial \pi}{\partial \eta} = \pi(1-\pi)$$

Proof

Proof. By the chain rule[a], Theorem 3.5, and Theorem 3.2:

$$\begin{aligned}\frac{\partial \pi}{\partial \eta} &= \frac{\partial \omega}{\partial \eta}\frac{\partial \pi}{\partial \omega} \\ &= \frac{\pi}{1-\pi}(1-\pi)^2 \\ &= \pi(1-\pi)\end{aligned}$$

Alternatively, by Theorem 3.4:

$$\begin{aligned}\frac{\partial \pi}{\partial \eta} &= \left(\frac{\partial \eta}{\partial \pi}\right)^{-1} \\ &= \left(\frac{1}{(\pi)(1-\pi)}\right)^{-1} \\ &= \pi(1-\pi)\end{aligned}$$

□

---

[a] math-prereqs.qmd#thm-chain-rule

Table 9: Matrix of logistic regression derivatives (p = number of predictors, $\eta = \tilde{x} \cdot \tilde{\beta}$, $\omega = \exp\{\eta\}$, $\pi = \omega/(1+\omega)$). Each entry is the derivative of the **column quantity** with respect to the **row quantity**. Entries marked "undef" are not defined because the column quantity is a model input, not a function of the row quantity.

	π	ω	η	$\tilde{x}$	$\tilde{\beta}$
π	1	$(1+\omega)^2$	$\frac{(1+\omega)^2}{\omega}$	undef	undef
ω	$(1-\pi)^2$	1	$\frac{1}{\omega}$	undef	undef
η	$\pi(1-\pi)$	ω	1	undef	undef
$\tilde{x}$	$\tilde{\beta}\pi(1-\pi)$	$\tilde{\beta}\omega$	$\tilde{\beta}$	▯	$\mathbf{0}$
$\tilde{\beta}$	$\tilde{x}\pi(1-\pi)$	$\tilde{x}\omega$	$\tilde{x}$	$\mathbf{0}$	▯

Corollary 3.3 (Derivative of probability w.r.t. linear predictor as a variance)**.** *If* $\pi = \Pr(Y = 1|\tilde{X} = \tilde{x})$*, then:*

$$\frac{\partial \pi}{\partial \eta} = \text{Var}(Y|X = x)$$

3.0.5 Summary matrix of derivatives

Each entry gives the derivative of the **column quantity** with respect to the **row quantity**; that is, the entry in row i and column j is $\frac{\partial(\text{col } j)}{\partial(\text{row } i)}$.

Dimensions of each entry depend on the types of the row and column quantities:

- **Scalar/scalar** (upper-left 3×3 block): row and column are both scalars (π, ω, or η); derivative is a scalar.
- **Gradient** (lower-left 2×3 block): row is a p-vector ($\tilde{x}$ or $\tilde{\beta}$), column is a scalar; derivative is a p-vector (gradient).
- **Jacobian** (lower-right 2×2 block): both row and column are p-vectors; derivative is a $p \times p$ matrix.
- **Undefined** (upper-right 3×2 block): row is a scalar, column is $\tilde{x}$ or $\tilde{\beta}$. Since $\tilde{x}$ and $\tilde{\beta}$ are model inputs rather than functions of π, ω, or η, these derivatives are not defined.

4 Understanding logistic regression models

Lemma 4.1 (Derivative of log-odds w.r.t. predictor)**.** *By the derivative of a linear combination*[a]*:*

$$\begin{aligned}\frac{\partial \eta}{\partial \tilde{x}} &= \frac{\partial}{\partial \tilde{x}} \tilde{x} \cdot \tilde{\beta} \\ &= \tilde{\beta}\end{aligned}$$

---

[a] math-prereqs.qmd#thm-deriv-lincom

Exercise 4.1. Consider a logistic regression model with a single predictor, X:

$$\begin{aligned} Y_i|X_i \ &\sim_{\perp\!\!\!\perp} \ \text{Ber}(\pi(X_i)) \\ \pi(x) &= \text{expit}\{\eta(x)\} = \pi(\omega(\eta(x))) \\ \eta(x) &= \alpha + \beta x \end{aligned} \tag{17}$$

Find the derivative of $\pi(x) = \text{E}[Y|X = x]$ with respect to x:

$$\frac{\partial \pi}{\partial x} = ?$$

Solution

Solution 4.1. By Theorem 3.6, Lemma 4.1, and the chain rule[a]:

$$\begin{aligned} \frac{\partial \pi}{\partial x} &= \frac{\partial \pi}{\partial \eta} \frac{\partial \eta}{\partial x} \\ &= \pi(1-\pi)\beta \\ &= \text{Var}(Y|X = x) \cdot \beta \end{aligned}$$

The slope is steepest at $\pi = 0.5$, i.e., at $\eta = 0$, which for a unipredictor model occurs at $x = -\alpha/\beta$. The slope goes to 0 as x goes to $-\infty$ or $+\infty$ (compare with Figure 5).

---

[a] math-prereqs.qmd#thm-chain-rule

Note

In order to interpret β_j: differentiate or difference $\eta(\tilde{x})$ with respect to x_j (depending on whether x_j is continuous or discrete, respectively):

$$\frac{\partial}{\partial x_j} \eta(\tilde{x})$$

In order to find the MLE $\hat{\tilde{\beta}}$: differentiate the log-likelihood function $\ell(\tilde{\beta})$ with respect to $\tilde{\beta}$:

$$\frac{\partial}{\partial \tilde{\beta}} \ell(\tilde{\beta})$$

Exercise 4.2 (General formula for odds ratios in logistic regression)**.** Consider the generic logistic regression model:

- $Y_i|\tilde{X}_i \ \sim_{\perp\!\!\!\perp} \ \text{Ber}(\pi(\tilde{X}_i))$
- $\text{logit}\{\pi(\tilde{x})\} = \eta(\tilde{x})$
- $\eta(\tilde{x}) = \tilde{x}'\tilde{\beta}$

Let $\tilde{x}$ and $\tilde{x}^*$ be two covariate patterns, representing two individuals or two subpopulations. Find a concise formula to compute the odds ratio comparing covariate patterns $\tilde{x}$ and $\tilde{x}^*$:

$$\theta_\omega(\tilde{x}, \tilde{x}^*) \overset{\text{def}}{=} \frac{\omega(\tilde{x})}{\omega(\tilde{x}^*)} \tag{18}$$

Solution (General formula for odds ratios in logistic regression)

Solution 4.2 (General formula for odds ratios in logistic regression).

$$\begin{aligned}\theta_\omega(\tilde{x}, \tilde{x}^*) &\stackrel{\text{def}}{=} \frac{\omega(\tilde{x})}{\omega(\tilde{x}^*)} \\ &= \frac{\exp\{\eta(\tilde{x})\}}{\exp\{\eta(\tilde{x}^*)\}} \\ &= \exp\{\eta(\tilde{x}) - \eta(\tilde{x}^*)\}\end{aligned}$$

Solution 4.2 is more concrete than Equation 18, but it doesn't yet completely explain how to compute $\theta_\omega(\tilde{x}, \tilde{x}^*)$, so let's mark it as a lemma:

Lemma 4.2 (General formula for odds ratios in logistic regression)**.**

$$\theta_\omega(\tilde{x}, \tilde{x}^*) = \exp\{\eta(\tilde{x}) - \eta(\tilde{x}^*)\} \tag{19}$$

ℹ Proof

Proof. By Solution 4.2. ☐

Definition 4.1 (Difference in log-odds)**.**
Let $\tilde{x}$ and $\tilde{x}^*$ be two covariate patterns, representing two individuals or two subpopulations. Then we can define the difference in log-odds between $\tilde{x}$ and $\tilde{x}^*$, denoted $\Delta\eta(\tilde{x}, \tilde{x}^*)$ or $\Delta\eta$ for short, as:

$$\Delta\eta \stackrel{\text{def}}{=} \eta(\tilde{x}) - \eta(\tilde{x}^*)$$

Corollary 4.1 (Shorthand general formula for odds ratios in logistic regression)**.**

$$\theta_\omega(\tilde{x}, \tilde{x}^*) = \exp\{\Delta\eta\} \tag{20}$$

ℹ Proof

Proof. By Lemma 4.2 and Definition 4.1. ☐

Exercise 4.3 (Difference in log-odds)**.** Find a concise expression for the difference in log-odds:

$$\Delta\eta \stackrel{\text{def}}{=} \eta(\tilde{x}) - \eta(\tilde{x}^*)$$

Solution (Difference in log-odds)

Solution 4.3 (Difference in log-odds).

$$\begin{aligned}
\Delta\eta &\stackrel{\text{def}}{=} \eta(\tilde{x}) - \eta(\tilde{x}^*) \\
&= (\tilde{x} \cdot \tilde{\beta}) - (\tilde{x}^* \cdot \tilde{\beta}) \\
&= (\tilde{x}^\top \tilde{\beta}) - ((\tilde{x}^*)^\top \tilde{\beta}) \\
&= (\tilde{x}^\top - (\tilde{x}^*)^\top)\tilde{\beta} \\
&= (\tilde{x} - \tilde{x}^*)^\top \tilde{\beta} \\
&= (\tilde{x} - \tilde{x}^*) \cdot \tilde{\beta}
\end{aligned}$$

Lemma 4.3 (Difference in log-odds)**.**

$$\Delta\eta = (\tilde{x} - \tilde{x}^*) \cdot \tilde{\beta}$$

Proof

Proof. By Solution 4.3. ☐

Definition 4.2 (Difference in covariate patterns)**.**
Let $\tilde{x}$ and $\tilde{x}^*$ be two covariate patterns, representing two individuals or two subpopulations. The difference in covariate patterns, denoted $\Delta\tilde{x}$, is defined as:

$$\Delta\tilde{x} \stackrel{\text{def}}{=} \tilde{x} - \tilde{x}^*$$

Corollary 4.2 (Difference in log-odds)**.**

$$\Delta\eta = (\Delta\tilde{x}) \cdot \tilde{\beta}$$

Proof

Proof. By Lemma 4.3 and Definition 4.2. ☐

Exercise 4.4. Find an expression for the odds ratio $\theta_\omega(\tilde{x}, \tilde{x}^*)$ in terms of $\Delta\tilde{x}$ and $\tilde{\beta}$.

Solution

Solution 4.4. Combine Corollary 4.1 and Corollary 4.2:

$$\begin{aligned}\theta_\omega(\tilde{x}, \tilde{x}^*) &= \exp\{\Delta \eta\} \\ &= \exp\left\{\Delta \tilde{x} \cdot \tilde{\beta}\right\}\end{aligned}$$

Theorem 4.1 (Odds ratio from difference in covariate patterns)**.** *The odds ratio comparing covariate patterns $\tilde{x}$ and $\tilde{x}^*$ is:*

$$\theta_\omega(\tilde{x}, \tilde{x}^*) = \exp\left\{(\Delta \tilde{x}) \cdot \tilde{\beta}\right\} \tag{21}$$

ℹ Proof

Proof. By Solution 4.4. ☐

Corollary 4.3 (Log odds ratio equals the difference in log-odds)**.**

$$\log\{\theta_\omega(\tilde{x}, \tilde{x}^*)\} = \Delta \eta$$

5 Estimating logistic regression models

5.0.1 Model

Assume:

- $Y_i | \tilde{X}_i \ \sim_{\perp\!\!\perp} \ \text{Ber}(\pi(X_i))$
- $\pi(\tilde{x}) = \text{expit}\{\eta(\tilde{x})\}$
- $\eta(\tilde{x}) = \tilde{x} \cdot \tilde{\beta}$

5.0.2 Likelihood function

Exercise 5.1. Compute and graph the likelihood for the `beetles` data model:

Table 10: Mortality rates of adult flour beetles after five hours' exposure to gaseous carbon disulphide (Bliss 1935)

```
library(glmx)
library(dplyr)
data(BeetleMortality)
beetles <- BeetleMortality |>
  mutate(
    pct = died / n,
    survived = n - died,
    dose_c = dose - mean(dose)
  )
beetles_long <-
  beetles |>
  reframe(
    .by = everything(),
    outcome = c(
      rep(1, times = died),
      rep(0, times = survived)
    )
  )
beetles
#> # A tibble: 8 x 6
#>    dose  died     n   pct survived   dose_c
#>   <dbl> <int> <int> <dbl>    <int>    <dbl>
#> 1  1.69     6    59 0.102       53 -0.103
#> 2  1.72    13    60 0.217       47 -0.0692
#> 3  1.76    18    62 0.290       44 -0.0382
#> 4  1.78    28    56 0.5         28 -0.00923
#> 5  1.81    52    63 0.825       11  0.0179
#> 6  1.84    53    59 0.898        6  0.0435
#> 7  1.86    61    62 0.984        1  0.0676
#> 8  1.88    60    60 1            0  0.0905
```

```
beetles_glm <-
  beetles |>
  glm(
    formula = cbind(died, survived) ~ dose,
    family = "binomial"
  )
equatiomatic::extract_eq(beetles_glm)
```

$$\log\left[\frac{P(\text{died} = 60)}{1 - P(\text{died} = 60)}\right] = \alpha + \beta_1(\text{dose}) \tag{22}$$

```
beetles_glm |>
  parameters::parameters() |>
  parameters::print_md()
```

Table 11: Fitted logistic regression model for `beetles` data

Parameter	Log-Odds	SE	95% CI	z	p
(Intercept)	-60.72	5.18	(-71.44, -51.08)	-11.72	$<$ .001
dose	34.27	2.91	(28.85, 40.30)	11.77	$<$ .001

Solution

Solution 5.1.

```
odds_inv <- function(omega) (1 + omega^-1)^-1
lik_beetles0 <- function(beta_0, beta_1) {
  beetles |>
    mutate(
      eta = beta_0 + beta_1 * dose,
      omega = exp(eta),
      pi = odds_inv(omega),
      Lik = pi^died * (1 - pi)^survived,
      # llik = died*eta + n*log(1 - pi)
    ) |>
    pull(Lik) |>
    prod()
}

lik_beetles <- Vectorize(lik_beetles0)
```

5.0.3 Log-likelihood function

Exercise 5.2. Find the log-likelihood function for the general logistic regression model.

Solution

Solution 5.2.

$$\begin{aligned}\ell(\tilde{\beta}, \tilde{y}) &= \log\left\{\mathcal{L}(\tilde{\beta}, \tilde{y})\right\} \\ &= \sum_{i=1}^{n} \ell_i(\pi(\tilde{x}_i))\end{aligned} \tag{23}$$

Using Theorem 1.10 and Corollary 1.5:

$$\begin{aligned}\ell_i(\pi_i) &= y_i \log\{\pi_i\} + (1 - y_i)\log\{1 - \pi_i\} \\ &= y_i \log\{\pi_i\} + (1 \cdot \log\{1 - \pi_i\} - y_i \cdot \log\{1 - \pi_i\}) \\ &= y_i \log\{\pi_i\} + (\log\{1 - \pi_i\} - y_i \log\{1 - \pi_i\}) \\ &= y_i \log\{\pi_i\} + \log\{1 - \pi_i\} - y_i \log\{1 - \pi_i\} \\ &= y_i \log\{\pi_i\} - y_i \log\{1 - \pi_i\} + \log\{1 - \pi_i\} \\ &= (y_i \log\{\pi_i\} - y_i \log\{1 - \pi_i\}) + \log\{1 - \pi_i\} \\ &= y_i(\log\{\pi_i\} - \log\{1 - \pi_i\}) + \log\{1 - \pi_i\} \\ &= y_i\left(\log\left\{\frac{\pi_i}{1 - \pi_i}\right\}\right) + \log\{1 - \pi_i\} \\ &= y_i \operatorname{logit}(\pi_i) + \log\{1 - \pi_i\} \\ &= y_i\eta_i + \log\{1 - \pi_i\} \\ &= y_i\eta_i + \log\left\{(1 + \omega_i)^{-1}\right\} \\ &= y_i\eta_i - \log\{1 + \omega_i\}\end{aligned}$$

Lemma 5.1 (Per-observation log-likelihood component)**.**

$$\ell_i(\pi_i) = y_i \eta_i - \log\{1 + \omega_i\}$$

Exercise 5.3. Compute and graph the log-likelihood for the `beetles` data.

Solution

Solution 5.3.

```
odds_inv <- function(omega) (1 + omega^-1)^-1
llik_beetles0 <- function(beta_0, beta_1) {
  beetles |>
    mutate(
      eta = beta_0 + beta_1 * dose,
      omega = exp(eta),
      pi = odds_inv(omega), # need for next line:
      llik = died*eta + n*log(1 - pi)
    ) |>
    pull(llik) |>
    sum()
}

llik_beetles <- Vectorize(llik_beetles0)

# to check that we implemented it correctly:
# ests = coef(beetles_glm_ungrouped)
# logLik(beetles_glm_ungrouped)
# llik_beetles(ests[1], ests[2])
```

Let's center dose:

```
beetles_glm_grouped_centered <- beetles |>
  glm(
    formula = cbind(died, survived) ~ dose_c,
    family = "binomial"
  )

beetles_glm_ungrouped_centered <- beetles_long |>
  mutate(died = outcome) |>
  glm(
    formula = died ~ dose_c,
    family = "binomial"
  )

equatiomatic::extract_eq(beetles_glm_ungrouped_centered)
```

$$\log\left[\frac{P(\text{died} = 1)}{1 - P(\text{died} = 1)}\right] = \alpha + \beta_1(\text{dose\_c}) \tag{24}$$

```
beetles_glm_grouped_centered |>
  parameters::parameters() |>
```

```
  parameters::print_md()
```

Table 12: Fitted logistic regression model for `beetles` data, with `dose` centered

Parameter	Log-Odds	SE	95% CI	z	p
(Intercept)	0.74	0.14	(0.48, 1.02)	5.40	$< .001$
dose c	34.27	2.91	(28.85, 40.30)	11.77	$< .001$

```
odds_inv <- function(omega) (1 + omega^-1)^-1
lik_beetles0 <- function(beta_0, beta_1) {
  beetles |>
    mutate(
      eta = beta_0 + beta_1 * dose_c,
      omega = exp(eta),
      pi = odds_inv(omega),
      Lik = (pi^died) * (1 - pi)^(survived)
    ) |>
    pull(Lik) |>
    prod()
}

lik_beetles <- Vectorize(lik_beetles0)
```

```
odds_inv <- function(omega) (1 + omega^-1)^-1
llik_beetles0 <- function(beta_0, beta_1) {
  beetles |>
    mutate(
      eta = beta_0 + beta_1 * dose_c,
      omega = exp(eta),
      pi = odds_inv(omega),
      llik = died * eta + n*log(1 - pi)
    ) |>
    pull(llik) |>
    sum()
}

llik_beetles <- Vectorize(llik_beetles0)
```

5.0.4 Score function

As usual, by independence, we have:

Lemma 5.2 (Score function decomposes over observations)**.**

$$\begin{aligned}
\tilde{\ell}'(\tilde{\beta}) &\overset{def}{=} \frac{\partial}{\partial\tilde{\beta}}\ell(\tilde{\beta}) \\
&= \frac{\partial}{\partial\tilde{\beta}}\sum_{i=1}^{n}\ell_i(\tilde{\beta}) \\
&= \sum_{i=1}^{n}\frac{\partial}{\partial\tilde{\beta}}\ell_i(\tilde{\beta}) \\
&= \sum_{i=1}^{n}\tilde{\ell}_i'(\tilde{\beta})
\end{aligned}$$

Starting from Lemma 5.1, we can apply the vector chain rule[8]:

Lemma 5.3 (Chain rule applied to the score component)**.**

$$\begin{aligned}
\tilde{\ell}_i'(\tilde{\beta}) &= \frac{\partial}{\partial\tilde{\beta}}\ell_i(\tilde{\beta}) \\
&= \frac{\partial}{\partial\tilde{\beta}}(y_i\eta_i - \log\{1+\omega_i\}) \\
&= \frac{\partial}{\partial\tilde{\beta}}y_i\eta_i - \frac{\partial}{\partial\tilde{\beta}}\log\{1+\omega_i\} \\
&= \frac{\partial\eta_i}{\partial\tilde{\beta}}y_i - \frac{\partial\omega_i}{\partial\tilde{\beta}}\frac{1}{1+\omega_i}
\end{aligned}$$

Lemma 5.4 (Derivative of log-odds with respect to coefficients)**.** *By the derivative of a linear combination*[a]*:*

$$\begin{aligned}
\frac{\partial\eta}{\partial\tilde{\beta}} &= \frac{\partial}{\partial\tilde{\beta}}(\tilde{x}\cdot\tilde{\beta}) \\
&= \tilde{x}
\end{aligned} \tag{25}$$

---

[a] math-prereqs.qmd#thm-deriv-lincom

Lemma 5.4 is very similar to Lemma 4.1, but not quite the same; Lemma 4.1 differentiates by $\tilde{x}$, whereas Lemma 5.4 differentiates by $\tilde{\beta}$.

Theorem 5.1 (Gradient of odds w.r.t. coefficients)**.**
To derive $\frac{\partial\omega}{\partial\tilde{\beta}}$*, we can apply the vector chain rule*[a] *again along with Lemma 3.2 and Lemma 5.4:*

$$\begin{aligned}
\frac{\partial\omega}{\partial\tilde{\beta}} &= \frac{\partial\eta}{\partial\tilde{\beta}}\frac{\partial\omega}{\partial\eta} \\
&= \tilde{x}\omega
\end{aligned}$$

---

[a] math-prereqs.qmd#thm-chain-vec

---

[8] math-prereqs.qmd#thm-chain-vec

Corollary 5.1 (Gradient of odds w.r.t. coefficients in terms of probability)**.**

$$\frac{\partial \omega}{\partial \tilde{\beta}} = \tilde{x}\frac{\pi}{1-\pi}$$

Now we can combine Lemma 5.3, Lemma 5.4, and Theorem 5.1:

$$\begin{aligned}
\ell_i'(\tilde{\beta}) &= \frac{\partial \eta_i}{\partial \tilde{\beta}} y_i - \frac{\partial \omega_i}{\partial \tilde{\beta}} \frac{1}{1+\omega_i} \\
&= \tilde{x}_i y_i - \tilde{x}\omega_i \frac{1}{1+\omega_i} \\
&= \tilde{x}_i y_i - \tilde{x}\frac{\omega_i}{1+\omega_i} \\
&= \tilde{x}_i y_i - \tilde{x}_i \pi_i \\
&= \tilde{x}_i (y_i - \pi_i) \\
&= \tilde{x}_i (y_i - \mu_i) \\
&= \tilde{x}_i (y_i - \mathrm{E}[Y_i|\tilde{X}_i = \tilde{x}_i]) \\
&= \tilde{x}_i \ \varepsilon(y_i|\tilde{X}_i = \tilde{x}_i) \\
&= \tilde{x}_i \varepsilon_i
\end{aligned}$$

Theorem 5.2 (Score component for one observation)**.**

$$\ell_i'(\tilde{\beta}) = \tilde{x}_i \varepsilon_i \tag{26}$$

This last expression is essentially the same as we found in linear regression[9].

Finally, combining Lemma 5.2 and Theorem 5.2, we have:

Theorem 5.3 (Logistic-model score function)**.**

$$\begin{aligned}
\tilde{\ell}'(\tilde{\beta}) &= \sum_{i=1}^{n} \ell_i'(\tilde{\beta}) \\
&= \sum_{i=1}^{n} \tilde{x}_i \varepsilon_i \\
&= \mathbf{X}^\top \tilde{\varepsilon}
\end{aligned} \tag{27}$$

The score function is vector-valued; its components are:

$$\frac{\partial \ell}{\partial \tilde{\beta}} = \begin{pmatrix} \frac{\partial \ell}{\partial \beta_0} \\ \frac{\partial \ell}{\partial \beta_1} \\ \vdots \\ \frac{\partial \ell}{\partial \beta_p} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n 1 \varepsilon_i \\ \sum_{i=1}^n x_{i,1} \varepsilon_i \\ \vdots \\ \sum_{i=1}^n x_{i,p} \varepsilon_i \end{pmatrix} = \begin{pmatrix} \tilde{1} \cdot \tilde{\varepsilon} \\ \tilde{x}_1 \cdot \tilde{\varepsilon} \\ \vdots \\ \tilde{x}_p \cdot \tilde{\varepsilon} \end{pmatrix}$$

Thus, the score equation $\tilde{\ell}' = 0$ means that for the MLE $\hat{\tilde{\beta}}$:

1. the sum of the errors (aka deviations) equals 0:

---

[9] Linear-models-overview.qmd#eq-scorefun-linreg

$$\sum_{i=1}^{n} \varepsilon_i = 0$$

2. the sums of the errors times each covariate also equal 0:

$$\tilde{x}_j \cdot \tilde{\varepsilon} = \sum_{i=1}^{n} x_{ij}\varepsilon_i = 0, \forall j \in \{1:p\}$$

Exm

Example 5.1. In our model for the `beetles` data, we only have an intercept plus one covariate, gas concentration (c):

$$\tilde{x} = (1, c)$$

If c_i is the gas concentration for the beetle in observation i, and $\tilde{c} = (c_1, c_2, ...c_n)$, then the score equation $\tilde{\ell}' = 0$ means that for the MLE $\hat{\tilde{\beta}}$:

1. the sum of the errors (aka deviations) equals 0:

$$\sum_{i=1}^{n} \varepsilon_i = 0$$

2. the weighted sum of the error times the gas concentrations equals 0:

$$\sum_{i=1}^{n} c_i \varepsilon_i = 0$$

Exercise 5.4. Implement and graph the score function for the beetles data

---

Solution

Solution 5.4.

```r
odds_inv <- function(omega) (1 + omega^-1)^-1

score_fn_beetles_beta0_0 <- function(beta_0, beta_1) {
  beetles |>
    mutate(
      eta = beta_0 + beta_1 * dose_c,
      omega = exp(eta),
      pi = odds_inv(omega),
      mu = pi * n,
      epsilon = died - mu,
      score = epsilon
    ) |>
    pull(score) |>
    sum()
}
score_fn_beetles_beta_0 <- Vectorize(score_fn_beetles_beta0_0)

score_fn_beetles_beta1_0 <- function(beta_0, beta_1) {
  beetles |>
    mutate(
      eta = beta_0 + beta_1 * dose_c,
      omega = exp(eta),
      pi = odds_inv(omega),
      mu = pi * n,
      epsilon = died - mu,
      score = dose_c * epsilon
    ) |>
    pull(score) |>
    sum()
}
score_fn_beetles_beta_1 <- Vectorize(score_fn_beetles_beta1_0)
```

5.0.5 Hessian function

$$\ell''(\tilde{\beta}) = \sum_{i=1}^{n} \ell_i''(\tilde{\beta}) \tag{28}$$

$$\begin{aligned} \ell_i''(\tilde{\beta}) &= \frac{\partial}{\partial \tilde{\beta}^\top} \tilde{\ell}_i' \\ &= \frac{\partial}{\partial \tilde{\beta}^\top} \tilde{x}_i \varepsilon_i \\ &= \tilde{x}_i \frac{\partial}{\partial \tilde{\beta}^\top} \varepsilon_i \\ &= \tilde{x}_i \varepsilon_i' \end{aligned} \tag{29}$$

Theorem 5.4 (Gradient of fitted probability w.r.t. coefficients)**.** *Using Lemma 5.4 and Theorem 3.6:*

$$\begin{aligned} \frac{\partial \pi}{\partial \tilde{\beta}} &= \frac{\partial \eta}{\partial \tilde{\beta}} \frac{\partial \pi}{\partial \eta} \\ &= \tilde{x} \pi (1 - \pi) \end{aligned}$$

Using Theorem 5.4:

$$
\begin{aligned}
\varepsilon_i' &= \frac{\partial \varepsilon_i}{\partial \tilde{\beta}^\top} \\
&= \frac{\partial}{\partial \tilde{\beta}^\top} \varepsilon_i \\
&= \frac{\partial}{\partial \tilde{\beta}^\top} (y_i - \mu_i) \\
&= \frac{\partial}{\partial \tilde{\beta}^\top} y_i - \frac{\partial}{\partial \tilde{\beta}^\top} \mu_i \\
&= 0 - \frac{\partial}{\partial \tilde{\beta}^\top} \mu_i \\
&= -\frac{\partial \mu_i}{\partial \tilde{\beta}^\top} \\
&= -\frac{\partial \pi_i}{\partial \tilde{\beta}^\top} \\
&= -\pi_i (1 - \pi_i) \tilde{x}_i^\top \\
&= -\operatorname{Var}(Y_i | X_i = x_i) \tilde{x}_i^\top
\end{aligned}
$$

Returning to Equation 29:

$$
\begin{aligned}
\ell_i''(\tilde{\beta}) &= \tilde{x}_i \varepsilon_i' \\
&= -\tilde{x}_i \operatorname{Var}(Y_i | X_i = x_i) \tilde{x}_i^\top
\end{aligned}
\tag{30}
$$

Returning to Equation 28:

$$
\begin{aligned}
\ell''(\tilde{\beta}) &= \sum_{i=1}^{n} \ell_i''(\tilde{\beta}) \\
&= -\sum_{i=1}^{n} \tilde{x}_i \operatorname{Var}(Y_i | X_i = x_i) \tilde{x}_i' \\
&= -\mathbf{X}^\top \mathbf{D} \mathbf{X}
\end{aligned}
\tag{31}
$$

where $\mathbf{D} \overset{\text{def}}{=} \operatorname{diag}(\operatorname{Var}(Y_i | X_i = x_i))$ is the diagonal matrix whose i^{th} diagonal element is $\operatorname{Var}(Y_i | X_i = x_i)$.

Compare with the linear regression Hessian[10]:

$$
\begin{aligned}
\ell''(\tilde{\beta}) &= -\frac{1}{\sigma^2} \sum_{i=1}^{n} \tilde{x}_i \tilde{x}_i' \\
&= -\mathbf{X}^\top \mathbf{D}^{-1} \mathbf{X}
\end{aligned}
\tag{32}
$$

Exercise 5.5. Determine the elements of the Hessian matrix for logistic regression.

---

[10] Linear-models-overview.qmd#eq-lm-hess

Solution

Solution 5.5. The components of the Hessian are:

$$
\begin{aligned}
\ell''(\beta) &= \frac{\partial^2}{\partial \beta^\top \partial \beta} \ell \\
&= \frac{\partial}{\partial \beta^\top} \ell' \\
&= \begin{bmatrix} \frac{\partial \ell'}{\partial \beta_0} & \frac{\partial \ell'}{\partial \beta_1} & \cdots & \frac{\partial \ell'}{\partial \beta_p} \end{bmatrix} \\
&= \begin{bmatrix}
\frac{\partial^2 \ell}{\partial \beta_0^2} & \frac{\partial^2 \ell}{\partial \beta_0 \partial \beta_1} & \cdots & \frac{\partial^2 \ell}{\partial \beta_0 \partial \beta_p} \\
\frac{\partial^2 \ell}{\partial \beta_1 \partial \beta_0} & \frac{\partial^2 \ell}{\partial \beta_1^2} & \cdots & \frac{\partial^2 \ell}{\partial \beta_0 \partial \beta_p} \\
\vdots & \ddots & \ddots & \vdots \\
\frac{\partial^2 \ell}{\partial \beta_p \partial \beta_0} & \frac{\partial^2 \ell}{\partial \beta_p \partial \beta_1} & \cdots & \frac{\partial^2 \ell}{\partial \beta_p^2}
\end{bmatrix}
\end{aligned}
$$

Exercise 5.6. Determine the Hessian for the `beetles` model.

Solution

Solution 5.6. In the `beetles` model, the Hessian is:

$$
\begin{aligned}
\ell''(\beta) &= \begin{bmatrix} \frac{\partial \ell'}{\partial \beta_0} & \frac{\partial \ell'}{\partial \beta_1} \end{bmatrix} \\
&= \begin{bmatrix}
\frac{\partial^2 \ell}{\partial \beta_0^2} & \frac{\partial^2 \ell}{\partial \beta_0 \partial \beta_1} \\
\frac{\partial^2 \ell}{\partial \beta_1 \partial \beta_0} & \frac{\partial^2 \ell}{\partial \beta_1^2}
\end{bmatrix} \\
&= \begin{bmatrix}
-\sum_{i=1}^n \pi_i(1-\pi_i) & -\sum_{i=1}^n c_i \pi_i(1-\pi_i) \\
-\sum_{i=1}^n c_i \pi_i(1-\pi_i) & -\sum_{i=1}^n c_i^2 \pi_i(1-\pi_i)
\end{bmatrix}
\end{aligned}
$$

Setting $\ell'(\tilde{\beta};\tilde{y}) = 0$ gives us:

$$
\sum_{i=1}^n \{\tilde{x}_i(y_i - \text{expit}\{\tilde{x}_i'\beta\})\} = 0 \tag{33}
$$

In general, the estimating equation $\ell'(\tilde{\beta};\tilde{y}) = 0$ cannot be solved analytically.

Instead, we can use the Newton-Raphson method[11]:

$$
\hat{\theta}^* \leftarrow \hat{\theta}^* - \left(\ell''\left(\tilde{y};\hat{\theta}^*\right)\right)^{-1} \ell'\left(\tilde{y};\hat{\theta}^*\right)
$$

We make an iterative series of guesses, and each guess helps us make the next guess better (i.e., higher log-likelihood). You can see some information about this process like so:

```r
beetles_glm_ungrouped <-
  beetles_long |>
  glm(
    control = glm.control(trace = TRUE),
    formula = outcome ~ dose,
```

---

[11] intro-MLEs.qmd#sec-newton-raphson

Table 13: Fitted model for `beetles` data

```
beetles_glm_ungrouped |> summary()
#> 
#> Call:
#> glm(formula = outcome ~ dose, family = "binomial", data = beetles_long, 
#>     control = glm.control(trace = TRUE))
#> 
#> Coefficients:
#>             Estimate Std. Error z value Pr(>|z|)    
#> (Intercept)   -60.72       5.18   -11.7   <2e-16 ***
#> dose           34.27       2.91    11.8   <2e-16 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#> 
#> (Dispersion parameter for binomial family taken to be 1)
#> 
#>     Null deviance: 645.44  on 480  degrees of freedom
#> Residual deviance: 372.47  on 479  degrees of freedom
#> AIC: 376.5
#> 
#> Number of Fisher Scoring iterations: 5
```

Table 14: Parameter estimate covariance matrix for `beetles` data

```
beetles_glm_ungrouped |> vcov()
#>             (Intercept)      dose
#> (Intercept)     26.8393 -15.08189
#> dose           -15.0819   8.48041
```

```
    family = "binomial"
  )
#> Deviance = 383.249 Iterations - 1
#> Deviance = 372.921 Iterations - 2
#> Deviance = 372.472 Iterations - 3
#> Deviance = 372.471 Iterations - 4
#> Deviance = 372.471 Iterations - 5
```

After each iteration of the fitting procedure, the deviance $(2(\ell_{\text{full}} - \ell(\hat{\beta}))$) is printed. You can see that the algorithm took 5 iterations to converge to a solution where the likelihood wasn't changing much anymore.

Table 13 and Table 14 show the fitted model and the covariance matrix of the estimates, respectively.

6 Inference for logistic regression models

6.1 Inference for individual predictor coefficients

6.1.1 Wald tests and confidence intervals

By the central limit theorem for MLEs[12], the maximum likelihood estimates $\hat{\beta}_k$ are approximately Gaussian for large sample sizes; see also the table of Gaussian vs. MLE-based tests[13].

Wald test statistic

---

[12] intro-MLEs.qmd#thm-dist-mle

[13] intro-MLEs.qmd#tbl-gaussian-vs-mle-tests

To test $H_0 : \beta_k = \beta_{k,0}$ (typically $\beta_{k,0} = 0$):

$$z_k = \frac{\hat{\beta}_k - \beta_{k,0}}{\widehat{SE}(\hat{\beta}_k)}$$

Under H_0, $z_k \dot{\sim} N(0, 1)$ for large n.

Confidence intervals for regression coefficients

A 95% confidence interval for β_k is:

$$\hat{\beta}_k \pm 1.96 \cdot \widehat{SE}(\hat{\beta}_k)$$

Confidence intervals for exponentiated coefficients

By the invariance property of MLEs, the MLE of e^{β_k} is $e^{\hat{\beta}_k}$.

A 95% confidence interval for e^{β_k} is obtained by exponentiating the endpoints of the CI for β_k:

$$e^{\beta_k} \in \left(e^{\hat{\beta}_k - 1.96 \cdot \widehat{SE}(\hat{\beta}_k)},\ e^{\hat{\beta}_k + 1.96 \cdot \widehat{SE}(\hat{\beta}_k)}\right)$$

For covariate coefficients ($k \neq 0$), e^{β_k} is an odds ratio (the multiplicative change in odds per 1-unit increase in x_k, holding all other covariates fixed). For the intercept ($k = 0$), e^{β_0} is the baseline odds (the odds when all covariates equal zero), not an odds ratio.

In R

In R, `parameters()` from the `parameters` package automatically computes Wald tests and confidence intervals for logistic regression model coefficients:

```
beetles_glm_ungrouped |>
  parameters() |>
  print_md()
#> Deviance = 372.714 Iterations - 1
#> Deviance = 372.714 Iterations - 2
#> Deviance = 373.417 Iterations - 1
#> Deviance = 373.417 Iterations - 2
#> Deviance = 374.544 Iterations - 1
#> Deviance = 374.544 Iterations - 2
#> Deviance = 376.063 Iterations - 1
#> Deviance = 376.063 Iterations - 2
#> Deviance = 377.943 Iterations - 1
#> Deviance = 377.943 Iterations - 2
#> Deviance = 380.156 Iterations - 1
#> Deviance = 380.156 Iterations - 2
#> Deviance = 372.727 Iterations - 1
#> Deviance = 372.727 Iterations - 2
#> Deviance = 373.526 Iterations - 1
#> Deviance = 373.526 Iterations - 2
#> Deviance = 374.912 Iterations - 1
#> Deviance = 374.912 Iterations - 2
#> Deviance = 376.937 Iterations - 1
#> Deviance = 376.937 Iterations - 2
#> Deviance = 376.937 Iterations - 3
#> Deviance = 379.654 Iterations - 1
#> Deviance = 379.654 Iterations - 2
#> Deviance = 379.654 Iterations - 3
```

```
#> Deviance = 372.727 Iterations - 1
#> Deviance = 372.727 Iterations - 2
#> Deviance = 373.526 Iterations - 1
#> Deviance = 373.526 Iterations - 2
#> Deviance = 374.913 Iterations - 1
#> Deviance = 374.913 Iterations - 2
#> Deviance = 376.94 Iterations - 1
#> Deviance = 376.94 Iterations - 2
#> Deviance = 379.66 Iterations - 1
#> Deviance = 379.66 Iterations - 2
#> Deviance = 379.66 Iterations - 3
#> Deviance = 372.714 Iterations - 1
#> Deviance = 372.714 Iterations - 2
#> Deviance = 373.417 Iterations - 1
#> Deviance = 373.417 Iterations - 2
#> Deviance = 374.543 Iterations - 1
#> Deviance = 374.543 Iterations - 2
#> Deviance = 376.061 Iterations - 1
#> Deviance = 376.061 Iterations - 2
#> Deviance = 377.939 Iterations - 1
#> Deviance = 377.939 Iterations - 2
#> Deviance = 380.151 Iterations - 1
#> Deviance = 380.151 Iterations - 2
```

Table 15: Wald tests and 95% CIs for `beetles` logistic regression

Parameter	Log-Odds	SE	95% CI	z	p
(Intercept)	-60.72	5.18	(-71.44, -51.08)	-11.72	< .001
dose	34.27	2.91	(28.85, 40.30)	11.77	< .001

Pass `exponentiate = TRUE` to `parameters()` to report exponentiated coefficients. The intercept is then interpreted as baseline odds, while the non-intercept coefficients are odds ratios:

```
beetles_glm_ungrouped |>
  parameters(exponentiate = TRUE) |>
  print_md()
#> Deviance = 372.714 Iterations - 1
#> Deviance = 372.714 Iterations - 2
#> Deviance = 373.417 Iterations - 1
#> Deviance = 373.417 Iterations - 2
#> Deviance = 374.544 Iterations - 1
#> Deviance = 374.544 Iterations - 2
#> Deviance = 376.063 Iterations - 1
#> Deviance = 376.063 Iterations - 2
#> Deviance = 377.943 Iterations - 1
#> Deviance = 377.943 Iterations - 2
#> Deviance = 380.156 Iterations - 1
#> Deviance = 380.156 Iterations - 2
#> Deviance = 372.727 Iterations - 1
#> Deviance = 372.727 Iterations - 2
#> Deviance = 373.526 Iterations - 1
#> Deviance = 373.526 Iterations - 2
#> Deviance = 374.912 Iterations - 1
#> Deviance = 374.912 Iterations - 2
#> Deviance = 376.937 Iterations - 1
#> Deviance = 376.937 Iterations - 2
#> Deviance = 376.937 Iterations - 3
```

```
#> Deviance = 379.654 Iterations - 1
#> Deviance = 379.654 Iterations - 2
#> Deviance = 379.654 Iterations - 3
#> Deviance = 372.727 Iterations - 1
#> Deviance = 372.727 Iterations - 2
#> Deviance = 373.526 Iterations - 1
#> Deviance = 373.526 Iterations - 2
#> Deviance = 374.913 Iterations - 1
#> Deviance = 374.913 Iterations - 2
#> Deviance = 376.94 Iterations - 1
#> Deviance = 376.94 Iterations - 2
#> Deviance = 379.66 Iterations - 1
#> Deviance = 379.66 Iterations - 2
#> Deviance = 379.66 Iterations - 3
#> Deviance = 372.714 Iterations - 1
#> Deviance = 372.714 Iterations - 2
#> Deviance = 373.417 Iterations - 1
#> Deviance = 373.417 Iterations - 2
#> Deviance = 374.543 Iterations - 1
#> Deviance = 374.543 Iterations - 2
#> Deviance = 376.061 Iterations - 1
#> Deviance = 376.061 Iterations - 2
#> Deviance = 377.939 Iterations - 1
#> Deviance = 377.939 Iterations - 2
#> Deviance = 380.151 Iterations - 1
#> Deviance = 380.151 Iterations - 2
```

Table 16: Exponentiated coefficients and 95% CIs for `beetles`

Parameter	Odds Ratio	SE	95% CI	z	p
(Intercept)	4.27e-27	2.21e-26	(9.39e-32, 6.56e-23)	-11.72	< .001
dose	7.65e+14	2.23e+15	(3.40e+12, 3.18e+17)	11.77	< .001

6.2 Inference for predicted probabilities

Exercise 6.1. Given a maximum likelihood estimate $\hat{\beta}$ and a corresponding estimated covariance matrix $\hat{\Sigma} \overset{\text{def}}{=} \widehat{\text{Cov}}(\hat{\beta})$, calculate a 95% confidence interval for the predicted probability $\pi(\tilde{x}) = \Pr(Y = 1|\tilde{X} = \tilde{x})$.

Solution

Solution 6.1.
By the central limit theorem for MLEs[a], a 95% confidence interval for $\pi(\tilde{x})$ can be constructed as:

$$\hat{\pi}(\tilde{x}) \pm 1.96 * \widehat{\text{SE}}(\hat{\pi}(\tilde{x}))$$

However, $\widehat{\text{SE}}(\hat{\pi}(\tilde{x}))$ seems difficult to compute; doing so would require using the delta method[b]. Instead, using the invariance property of MLEs, we can first calculate a confidence interval for the log-odds,

$$\eta(\tilde{x}) = \tilde{x}'\tilde{\beta} \in (L, R)$$

and then apply expit to the endpoints of that log-odds-scale confidence interval:

$$\pi(\tilde{x}) \in (\text{expit}(L), \text{expit}(R)) \tag{34}$$

---

[a] intro-MLEs.qmd#thm-dist-mle
[b] https://en.wikipedia.org/wiki/Delta_method

Exercise 6.2. Find a 95% confidence interval for the log-odds $\eta(\tilde{x}) = \tilde{x}'\tilde{\beta}$.

Solution

Solution 6.2. By the central limit theorem for MLEs[a], a 95% confidence interval for $\eta(\tilde{x})$ can be constructed as:

$$\hat{\eta}(\tilde{x}) \pm 1.96 * \widehat{\text{SE}}(\hat{\eta}(\tilde{x}))$$

where $\hat{\eta}(\tilde{x}) = \tilde{x}'\hat{\beta}$.

---

[a] intro-MLEs.qmd#thm-dist-mle

Exercise 6.3.
How can we estimate the standard error of $\hat{\eta}(\tilde{x})$?

$$\widehat{\text{SE}}(\hat{\eta}(\tilde{x})) = ?$$

Solution

Solution 6.3.

$$\text{SE}(\hat{\eta}(\tilde{x})) = \sqrt{\text{Var}(\hat{\eta}(\tilde{x}))} \tag{35}$$

By the definition $\hat{\eta}(\tilde{x}) = \tilde{x}'\hat{\beta}$ and the variance of a linear combination[a]:

$$\begin{aligned} \text{Var}(\hat{\eta}(\tilde{x})) &= \text{Var}\left(\tilde{x}'\hat{\beta}\right) \\ &= \tilde{x}' \,\text{Cov}\left(\hat{\beta}\right)\tilde{x} \\ &= \tilde{x}^{\top}\Sigma\tilde{x} \end{aligned} \tag{36}$$

where $\Sigma \stackrel{\text{def}}{=} \text{Cov}(\hat{\beta})$.

Expanding Equation 36 out of matrix-vector notation, we have:

$$\begin{aligned} \tilde{x}^{\top}\Sigma\tilde{x} &= \sum_{i=1}^{p}\sum_{j=1}^{p} x_i \Sigma_{ij} x_j \\ &= \sum_{i=1}^{p}\sum_{j=1}^{p} x_i \,\text{Cov}(\hat{\beta}_i, \hat{\beta}_j) x_j \end{aligned}$$

Combining Equation 36 and MLE invariance:

Lem

Theorem 6.1 (Estimated variance and standard error of log-odds).

$$\widehat{\text{Var}}(\hat{\eta}(\tilde{x})) = \tilde{x}^{\top}\hat{\Sigma}\tilde{x} \tag{37}$$

$$\widehat{\text{SE}}(\hat{\eta}(\tilde{x})) = \sqrt{\tilde{x}^{\top}\hat{\Sigma}\tilde{x}} \tag{38}$$

Note: on the RHS, we have plugged in $\hat{\Sigma}$, our estimate of Σ.

---

[a] probability.qmd#thm-var-lincom

In R

In R, `predict()` with `type = "link"` and `se.fit = TRUE` computes the estimated log-odds $\hat{\eta}(\tilde{x}) = \tilde{x}'\hat{\beta}$ and its estimated standard error for each covariate pattern:

```r
library(dplyr)
new_doses <- tibble(dose = c(1.7, 1.8, 1.9))

pred_logodds <-
  beetles_glm_ungrouped |>
  predict(
    newdata = new_doses,
    type = "link",
    se.fit = TRUE
  )

new_doses |>
  mutate(
    logodds_hat = pred_logodds$fit,
    se = pred_logodds$se.fit,
    ci_lower_logodds = logodds_hat - 1.96 * se,
    ci_upper_logodds = logodds_hat + 1.96 * se,
    pi_hat = plogis(logodds_hat),
    ci_lower_prob = plogis(ci_lower_logodds),
    ci_upper_prob = plogis(ci_upper_logodds)
  ) |>
  knitr::kable(digits = 3)
```

Table 17: Predicted log-odds and 95% CI for `beetles` logistic regression

dose	logodds_hat	se	ci_lower_logodds	ci_upper_logodds	pi_hat	ci_lower_prob	ci_upper_prob
1.7	-2.458	0.263	-2.974	-1.942	0.079	0.049	0.125
1.8	0.969	0.145	0.685	1.253	0.725	0.665	0.778
1.9	4.396	0.377	3.656	5.136	0.988	0.975	0.994

6.3 Inference for odds ratios

Exercise 6.4. Given a maximum likelihood estimate $\hat{\beta}$ and a corresponding estimated covariance matrix $\hat{\Sigma} \overset{\text{def}}{=} \widehat{\text{Cov}}(\hat{\beta})$, calculate a 95% confidence interval for the odds ratio comparing covariate patterns $\tilde{x}$ and $\tilde{x}^*$, $\theta_{\omega}(\tilde{x}, \tilde{x}^*)$.

Solution

Solution 6.4.
By the central limit theorem for MLEs[a], a 95% confidence interval for $\theta_{\omega}(\tilde{x}, \tilde{x}^*)$ can be

constructed as:

$$\hat{\theta}_{\omega} \pm 1.96 * \widehat{\text{SE}}\left(\hat{\theta}_{\omega}\right) \tag{39}$$

However, $\widehat{\text{SE}}\left(\hat{\theta}_{\omega}\right)$ seems difficult to compute; doing so would require using the delta method[b]. Instead, using the invariance property of MLEs, we can first calculate a confidence interval for the logarithm of the odds ratio,

$$\log\{\theta_{\omega}(\tilde{x}, \tilde{x}^*)\} \in (L, R) \tag{40}$$

and then exponentiate the endpoints of that log-odds-scale confidence interval:

$$\theta_{\omega}(\tilde{x}, \tilde{x}^*) \in (e^L, e^R) \tag{41}$$

---

[a] intro-MLEs.qmd#thm-dist-mle

[b] https://en.wikipedia.org/wiki/Delta_method

Exercise 6.5. Find a 95% confidence interval for the natural logarithm of the odds ratio, $\log\{\theta_{\omega}(\tilde{x}, \tilde{x}^*)\}$

Solution

Solution 6.5. From Corollary 4.3, we know:

$$\log\{\theta_{\omega}(\tilde{x}, \tilde{x}^*)\} = \Delta\eta$$

By the central limit theorem for MLEs[a], a 95% confidence interval for $\Delta\eta$ can be constructed as:

$$\widehat{\Delta\eta} \pm 1.96 * \widehat{\text{SE}}\left(\widehat{\Delta\eta}\right)$$

---

[a] intro-MLEs.qmd#thm-dist-mle

Exercise 6.6.
How can we estimate the standard error of $\widehat{\Delta\eta}$?

$$\widehat{\text{SE}}\left(\widehat{\Delta\eta}\right) = ?$$

Solution

Solution 6.6.

$$\text{SE}\left(\widehat{\Delta\eta}\right) = \sqrt{\text{Var}\left(\widehat{\Delta\eta}\right)} \tag{42}$$

By Lemma 4.3 and the variance of a linear combination[a]:

$$\begin{aligned} \text{Var}\left(\widehat{\Delta\eta}\right) &= \text{Var}\left((\Delta\tilde{x}) \cdot \hat{\beta}\right) \\ &= (\Delta\tilde{x})^{\top} \text{Cov}\left(\hat{\beta}\right)(\Delta\tilde{x}) \\ &= (\Delta\tilde{x})^{\top}\Sigma(\Delta\tilde{x}) \end{aligned} \tag{43}$$

where $\Sigma \overset{\text{def}}{=} \text{Cov}(\hat{\beta})$.

Expanding Equation 43 out of matrix-vector notation, we have:

$$
\begin{aligned}
(\Delta\tilde{x})^{\top}\Sigma(\Delta\tilde{x}) &= \sum_{i=1}^{p}\sum_{j=1}^{p}(\Delta\tilde{x})_i\Sigma_{ij}(\Delta\tilde{x})_j \\
&= \sum_{i=1}^{p}\sum_{j=1}^{p}(\Delta x_i)\Sigma_{ij}(\Delta x_j) \\
&= \sum_{i=1}^{p}\sum_{j=1}^{p}(x_i - x_i^*)\,\text{Cov}(\hat{\beta}_i, \hat{\beta}_j)(x_j - x_j^*)
\end{aligned}
$$

Combining Equation 43 and MLE invariance:

Lem

Theorem 6.2 (Estimated variance and standard error of difference in log-odds).

$$\widehat{\text{Var}}(\Delta\hat{\eta}) = \Delta\tilde{x}^{\top}\hat{\Sigma}(\Delta\tilde{x}) \tag{44}$$

$$\widehat{\text{SE}}(\Delta\hat{\eta}) = \sqrt{\Delta\tilde{x}^{\top}\hat{\Sigma}(\Delta\tilde{x})} \tag{45}$$

Note: on the RHS, we have plugged in $\hat{\Sigma}$, our estimate of Σ.
Compare this result with confidence intervals[b].

---

[a] probability.qmd#thm-var-lincom
[b] Linear-models-overview.qmd#sec-se-fitted

7 Multiple logistic regression

7.0.1 Coronary heart disease (WCGS) study data

Let's use the data from the Western Collaborative Group Study (WCGS) (Rosenman et al. (1975)) to explore multiple logistic regression:

From Vittinghoff et al. (2012):

"The **Western Collaborative Group Study (WCGS)** was a large epidemiological study designed to investigate the association between the"type A" behavior pattern and coronary heart disease (CHD)".

Exercise 7.1. What is "type A" behavior?

Solution

Solution 7.1. *From Wikipedia, "Type A and Type B personality theory":*
"The hypothesis describes Type A individuals as outgoing, ambitious, rigidly organized, highly status-conscious, impatient, anxious, proactive, and concerned with time management….
The hypothesis describes Type B individuals as a contrast to those of Type A. Type B personalities, by definition, are noted to live at lower stress levels. They typically work steadily and may enjoy achievement, although they have a greater tendency to disregard physical or mental stress when they do not achieve."

Study design

from `?faraway::wcgs`:

3154 healthy young men aged 39-59 from the San Francisco area were assessed for their personality type. All were free from coronary heart disease at the start of the research. Eight and a half years later change in CHD status was recorded.

Details (from `faraway::wcgs`)

The WCGS began in 1960 with 3,524 male volunteers who were employed by 11 California companies. Subjects were 39 to 59 years old and free of heart disease as determined by electrocardiogram. After the initial screening, the study population dropped to 3,154 and the number of companies to 10 because of various exclusions. The cohort comprised both blue- and white-collar employees.

7.0.2 Baseline data collection

socio-demographic characteristics:

- age
- education
- marital status
- income
- occupation
- physical and physiological including:
- height
- weight
- blood pressure
- electrocardiogram
- corneal arcus

---

biochemical measurements:

- cholesterol and lipoprotein fractions;
- medical and family history and use of medications;

---

behavioral data:

- Type A interview,
- smoking,
- exercise
- alcohol use.

Later surveys added data on:

- anthropometry
- triglycerides
- Jenkins Activity Survey
- caffeine use

Average follow-up continued for 8.5 years with repeat examinations.

7.0.3 Load the data

Here, I load the data:

```r
### load the data directly from a UCSF website:
library(haven)
url <- paste0(
```

Table 18: `wcgs` data

```
wcgs
#> # A tibble: 3,154 x 22
#>      age arcus behpat   bmi chd69  chol   dbp dibpat height    id lnsbp lnwght
#>    <dbl> <lgl> <fct>  <dbl> <fct> <dbl> <dbl> <fct>   <dbl> <dbl> <dbl>  <dbl>
#>  1    50 TRUE  A1      31.3 No      249    90 Type A     67  2343  4.88   5.30
#>  2    51 FALSE A1      25.3 No      194    74 Type A     73  3656  4.79   5.26
#>  3    59 TRUE  A1      28.7 No      258    94 Type A     70  3526  5.06   5.30
#>  4    51 TRUE  A1      22.1 No      173    80 Type A     69 22057  4.84   5.01
#>  5    44 FALSE A1      22.3 No      214    80 Type A     71 12927  4.84   5.08
#>  6    47 FALSE A1      27.1 No      206    76 Type A     64 16029  4.75   5.06
#>  7    40 FALSE A1      23.2 No      190    78 Type A     70  3894  4.80   5.09
#>  8    41 FALSE A1      23.0 No      212    84 Type A     70 11389  4.87   5.08
#>  9    50 TRUE  A1      27.2 No      130    70 Type A     71 12681  4.72   5.27
#> 10    43 FALSE A1      28.4 No      233    80 Type A     68 10005  4.79   5.23
#> # i 3,144 more rows
#> # i 10 more variables: ncigs <dbl>, sbp <dbl>, smoke <fct>, t1 <dbl>,
#> #   time169 <dbl>, typchd69 <fct>, uni <dbl>, weight <dbl>, wghtcat <fct>,
#> #   agec <fct>
```

```
  # I'm breaking up the url into two chunks for readability
  "https://regression.ucsf.edu/sites/g/files/",
  "tkssra6706/f/wysiwyg/home/data/wcgs.dta"
)
wcgs <- haven::read_dta(url)
```

A copy is also available on Kaggle[14].

7.0.4 Data cleaning

Now let's do some data cleaning

```
library(arsenal) # provides `set_labels()`
library(forcats) # provides `as_factor()`
library(haven)
library(plotly)
wcgs <- wcgs |>
  mutate(
    age = age |>
      arsenal::set_labels("Age (years)"),
    arcus = arcus |>
      as.logical() |>
      arsenal::set_labels("Arcus Senilis"),
    time169 = time169 |>
      as.numeric() |>
      arsenal::set_labels("Observation (follow up) time (days)"),
    dibpat = dibpat |>
      as_factor() |>
      relevel(ref = "Type B") |>
      arsenal::set_labels("Behavioral Pattern"),
    typchd69 = typchd69 |>
      labelled(
        label = "Type of CHD Event",
        labels =
```

---

[14] https://www.kaggle.com/datasets/nmd2104/wcgs-data

```
          c(
            "None" = 0,
            "infdeath" = 1,
            "silent" = 2,
            "angina" = 3
          )
      ),

    # turn stata-style labelled variables in to R-style factors:
    across(
      where(is.labelled),
      haven::as_factor
    )
  )
```

7.0.5 What's in the data

Table 19 summarizes the data.

7.0.6 Data by age and personality type

For now, we will look at the interaction between age and personality type (`dibpat`). To make it easier to visualize the data, we summarize the event rates for each combination of age:

```
library(dplyr)
odds <- function(pi) pi / (1 - pi)
chd_grouped_data <-
  wcgs |>
  summarize(
    .by = c(age, dibpat),
    n = sum(chd69 %in% c("Yes", "No")),
    x = sum(chd69 == "Yes")
  ) |>
  mutate(
    `n - x` = n - x,
    `p(chd)` = (x / n) |>
      labelled(label = "CHD Event by 1969"),
    `odds(chd)` = `p(chd)` / (1 - `p(chd)`),
    `logit(chd)` = log(`odds(chd)`)
  )

chd_grouped_data
#> # A tibble: 42 x 8
#>      age dibpat     n     x `n - x` `p(chd)`   `odds(chd)` `logit(chd)`
#>    <dbl> <fct>  <int> <int>   <int> <dbl+lbl>        <dbl>        <dbl>
#>  1    50 Type A    76     8      68 0.105           0.118         -2.14
#>  2    51 Type A    67    11      56 0.164           0.196         -1.63
#>  3    59 Type A    30     7      23 0.233           0.304         -1.19
#>  4    44 Type A   113     9     104 0.0796          0.0865        -2.45
#>  5    47 Type A    72     7      65 0.0972          0.108         -2.23
#>  6    40 Type A   133     9     124 0.0677          0.0726        -2.62
#>  7    41 Type A   108     7     101 0.0648          0.0693        -2.67
#>  8    43 Type A    97     7      90 0.0722          0.0778        -2.55
#>  9    54 Type A    53     7      46 0.132           0.152         -1.88
#> 10    48 Type A    80    12      68 0.15            0.176         -1.73
#> # i 32 more rows
```

Table 19: Baseline characteristics by CHD status at end of follow-up

```r
library(gtsummary)
wcgs |>
  dplyr::select(
    -dplyr::all_of(c("id", "uni", "t1"))
  ) |>
  gtsummary::tbl_summary(
    by = "chd69",
    missing_text = "Missing"
  ) |>
  gtsummary::add_p() |>
  gtsummary::add_overall() |>
  gtsummary::bold_labels() |>
  gtsummary::separate_p_footnotes()
```

Characteristic	**Overall** N = 3,154[1]	**No** N = 2,897[1]	**Yes** N = 2
Age (years)	45.0 (42.0, 50.0)	45.0 (41.0, 50.0)	49.0 (44.0, 5
Arcus Senilis	941 (30%)	839 (29%)	102 (40%
Missing	2	0	2
Behavioral Pattern			
A1	264 (8.4%)	234 (8.1%)	30 (12%
A2	1,325 (42%)	1,177 (41%)	148 (58%
B3	1,216 (39%)	1,155 (40%)	61 (24%
B4	349 (11%)	331 (11%)	18 (7.0%
Body Mass Index (kg/m2)	24.39 (22.96, 25.84)	24.39 (22.89, 25.84)	24.82 (23.63,
Total Cholesterol	223 (197, 253)	221 (195, 250)	245 (222, 2
Missing	12	12	0
Diastolic Blood Pressure	80 (76, 86)	80 (76, 86)	84 (80, 9
Behavioral Pattern			
Type B	1,565 (50%)	1,486 (51%)	79 (31%
Type A	1,589 (50%)	1,411 (49%)	178 (69%
Height (inches)	70.00 (68.00, 72.00)	70.00 (68.00, 72.00)	70.00 (68.00,
Ln of Systolic Blood Pressure	4.84 (4.79, 4.91)	4.84 (4.77, 4.91)	4.87 (4.82,
Ln of Weight	5.14 (5.04, 5.20)	5.13 (5.04, 5.20)	5.16 (5.09,
Cigarettes per day	0 (0, 20)	0 (0, 20)	20 (0, 30
Systolic Blood Pressure	126 (120, 136)	126 (118, 136)	130 (124, 1
Current smoking	1,502 (48%)	1,343 (46%)	159 (62%
Observation (follow up) time (days)	2,942 (2,842, 3,037)	2,952 (2,864, 3,048)	1,666 (934, 2
Type of CHD Event			
None	0 (0%)	0 (0%)	0 (0%)
infdeath	2,897 (92%)	2,897 (100%)	0 (0%)
silent	135 (4.3%)	0 (0%)	135 (53%
angina	71 (2.3%)	0 (0%)	71 (28%
4	51 (1.6%)	0 (0%)	51 (20%
Weight (lbs)	170 (155, 182)	169 (155, 182)	175 (162, 1
Weight Category			
< 140	232 (7.4%)	217 (7.5%)	15 (5.8%
140-170	1,538 (49%)	1,440 (50%)	98 (38%
170-200	1,171 (37%)	1,049 (36%)	122 (47%
> 200	213 (6.8%)	191 (6.6%)	22 (8.6%
RECODE of age (Age)			
35-40	543 (17%)	512 (18%)	31 (12%
41-45	1,091 (35%)	1,036 (36%)	55 (21%
46-50	750 (24%)	680 (23%)	70 (27%
51-55	528 (17%)	463 (16%)	65 (25%

7.0.7 Graphical exploration

```
library(ggplot2)
library(scales)
chd_plot_probs <-
  chd_grouped_data |>
  ggplot() +
  aes(
    x = age,
    y = `p(chd)`,
    col = dibpat
  ) +
  geom_point(aes(size = n), alpha = .7) +
  scale_size(range = c(1, 4)) +
  geom_line() +
  theme_bw() +
  ylab("P(CHD Event by 1969)") +
  scale_y_continuous(
    labels = scales::label_percent(),
    sec.axis = sec_axis(
      ~ odds(.),
      name = "odds(CHD Event by 1969)"
    )
  ) +
  theme(legend.position = "bottom")

print(chd_plot_probs)
```

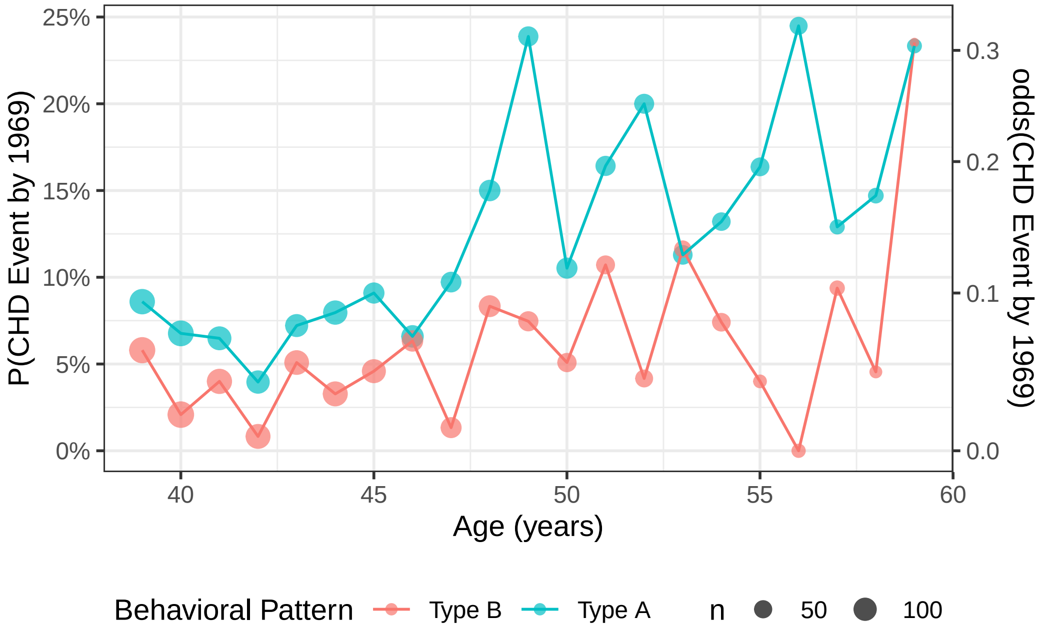


Figure 12: CHD rates by age group, probability scale

7.1 Odds scale

```r
odds_inv <- function(omega) omega / (1 + omega)
trans_odds <- trans_new(
  name = "odds",
  transform = odds,
  inverse = odds_inv
)

chd_plot_odds <- chd_plot_probs +
  scale_y_continuous(
    trans = trans_odds, # this line changes the vertical spacing
    name = chd_plot_probs$labels$y,
    sec.axis = sec_axis(
      ~ odds(.),
      name = "odds(CHD Event by 1969)"
    )
  )

print(chd_plot_odds)
```

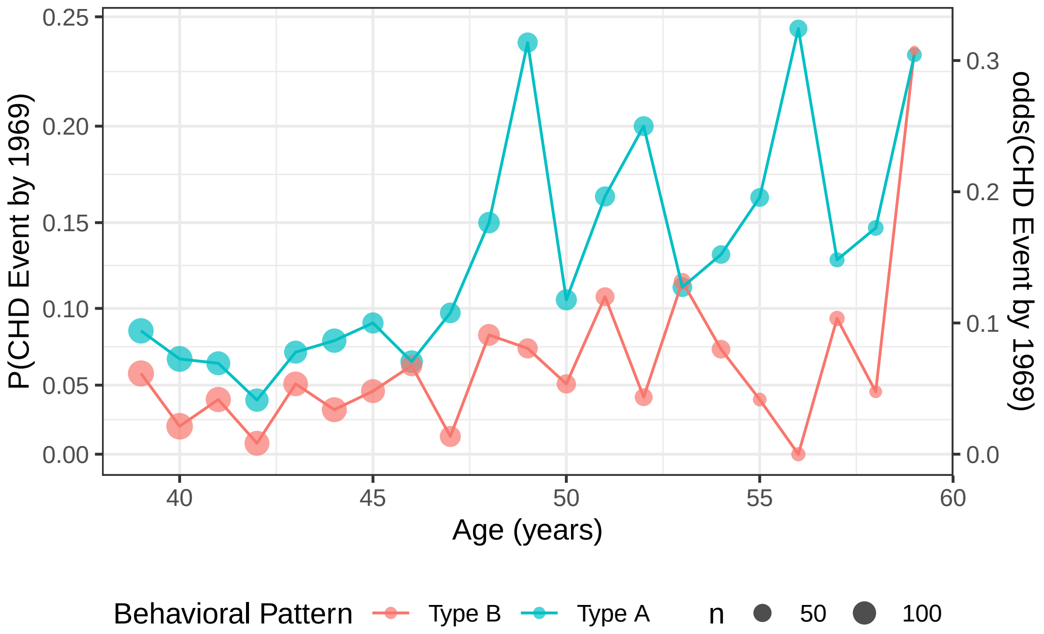


Figure 13: CHD rates by age group, odds spacing

7.2 Log-odds (logit) scale

```r
logit <- function(pi) log(odds(pi))
expit <- function(eta) odds_inv(exp(eta))
trans_logit <- trans_new(
  name = "logit",
  transform = logit,
  inverse = expit
)

chd_plot_logit <-
```

```
  chd_plot_probs +
  scale_y_continuous(
    trans = trans_logit, # this line changes the vertical spacing
    name = chd_plot_probs$labels$y,
    breaks = c(seq(.01, .1, by = .01), .15, .2),
    minor_breaks = NULL,
    sec.axis = sec_axis(
      ~ logit(.),
      name = "log(odds(CHD Event by 1969))"
    )
  )

print(chd_plot_logit)
```

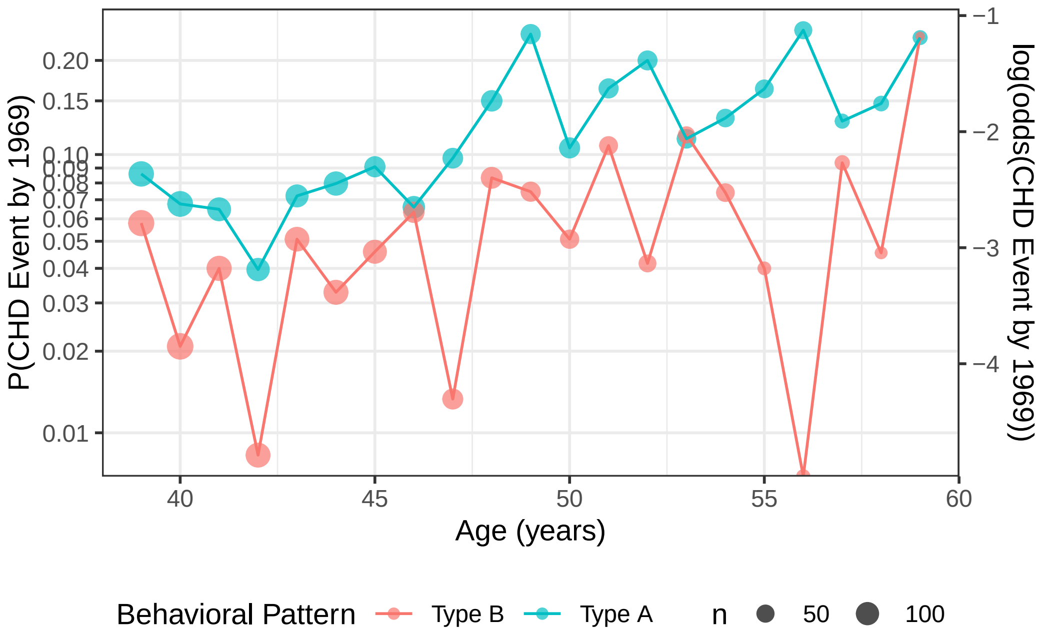


Figure 14: CHD data (logit-scale)

7.2.1 Logistic regression models for CHD data

For the `wgcs` dataset, let's consider a **logistic regression model** for the outcome of Coronary Heart Disease (Y; `chd` in computer output):

- $Y = 1$ if an individual developed CHD by the end of the study;
- $Y = 0$ if they have not developed CHD by the end of the study.

Let's include an intercept, two covariates, plus their interaction:

- A: age at study enrollment (`age`, recorded in years)
- P: personality type (`dibpat`):
  - $P = 1$ represents "Type A personality",
  - $P = 0$ represents "Type B personality".
- PA: the interaction of personality type and age (`dibpat:age`)
- $\tilde{X} = (1, A, P, PA)$

```
chd_glm_contrasts <-
  wcgs |>
  glm(
    "data" = _,
```

```
    "formula" = chd69 == "Yes" ~ dibpat * age,
    "family" = binomial(link = "logit")
  )

library(equatiomatic)
equatiomatic::extract_eq(chd_glm_contrasts)
```

$$\log\left[\frac { P(\operatorname{chd69} = \operatorname{Yes}) }{ 1 - P(\operatorname{chd69} = \operatorname{Yes}) } \right] = \alpha + \beta_{1}(\operatorname{dibpat}_{\operatorname{Type\ A}}) + \beta_{2}(\operatorname{age}) + \beta_{3}(\operatorname{dibpat}_{\operatorname{Type\ A}} \times \operatorname{age}) \tag{46}$$

Or in more formal notation:

$$\begin{aligned} Y_i|\tilde{X}_i &\sim_{\perp\!\!\!\perp} \text{Ber}(\pi(\tilde{X}_i)) \\ \pi(\tilde{x}) &= \text{expit}(\eta(\tilde{x})) \\ \eta(\tilde{x}) &= \beta_0 + \beta_P p + \beta_A a + \beta_{PA} pa \end{aligned} \tag{47}$$

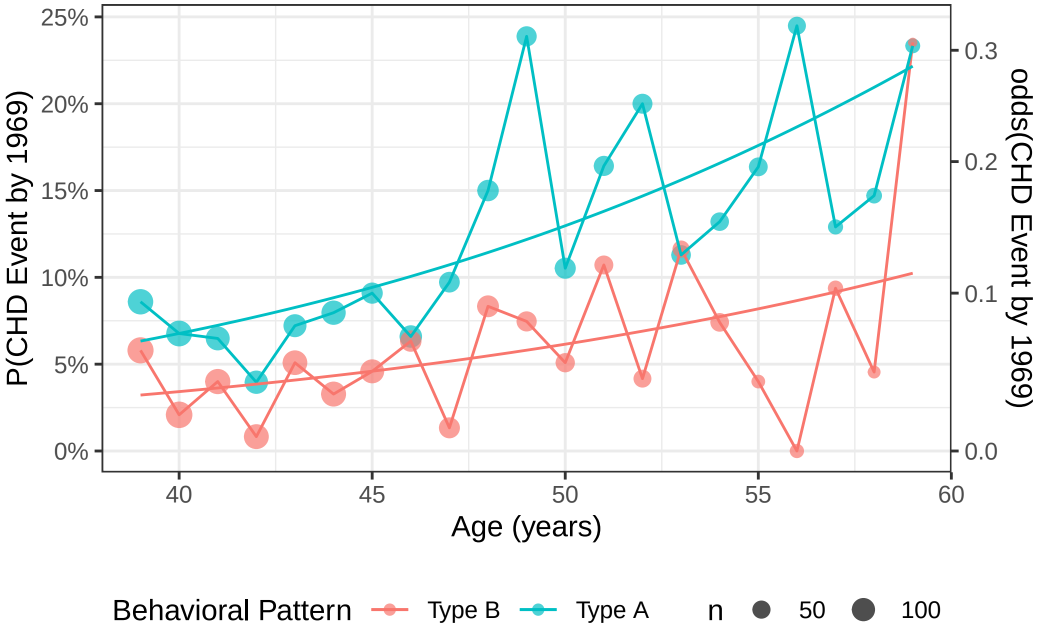
7.2.2 Models superimposed on data

We can graph our fitted models on each scale (probability, odds, log-odds).

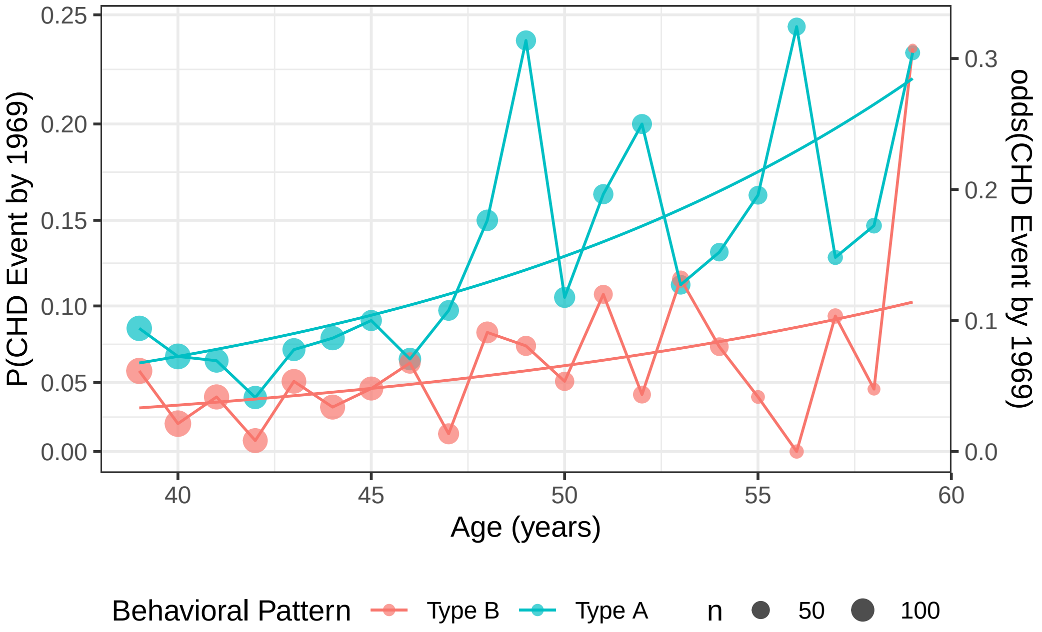
---

probability scale

```
curve_type_A <- function(x) { # nolint: object_name_linter
  chd_glm_contrasts |> predict(
    type = "response",
    newdata = tibble(age = x, dibpat = "Type A")
  )
}

curve_type_B <- function(x) { # nolint: object_name_linter
  chd_glm_contrasts |> predict(
    type = "response",
    newdata = tibble(age = x, dibpat = "Type B")
  )
}

chd_plot_probs_2 <-
  chd_plot_probs +
  geom_function(
    fun = curve_type_A,
    aes(col = "Type A")
  ) +
  geom_function(
    fun = curve_type_B,
    aes(col = "Type B")
  )
print(chd_plot_probs_2)
```



```r
chd_plot_odds_2 <-
  chd_plot_odds +
  geom_function(
    fun = curve_type_A,
    aes(col = "Type A")
  ) +
  geom_function(
    fun = curve_type_B,
    aes(col = "Type B")
  )
print(chd_plot_odds_2)
```



odds scale

---

log-odds (logit) scale

```r
chd_plot_logit_2 <-
  chd_plot_logit +
  geom_function(
    fun = curve_type_A,
    aes(col = "Type A")
  ) +
  geom_function(
    fun = curve_type_B,
    aes(col = "Type B")
  )

print(chd_plot_logit_2)
```

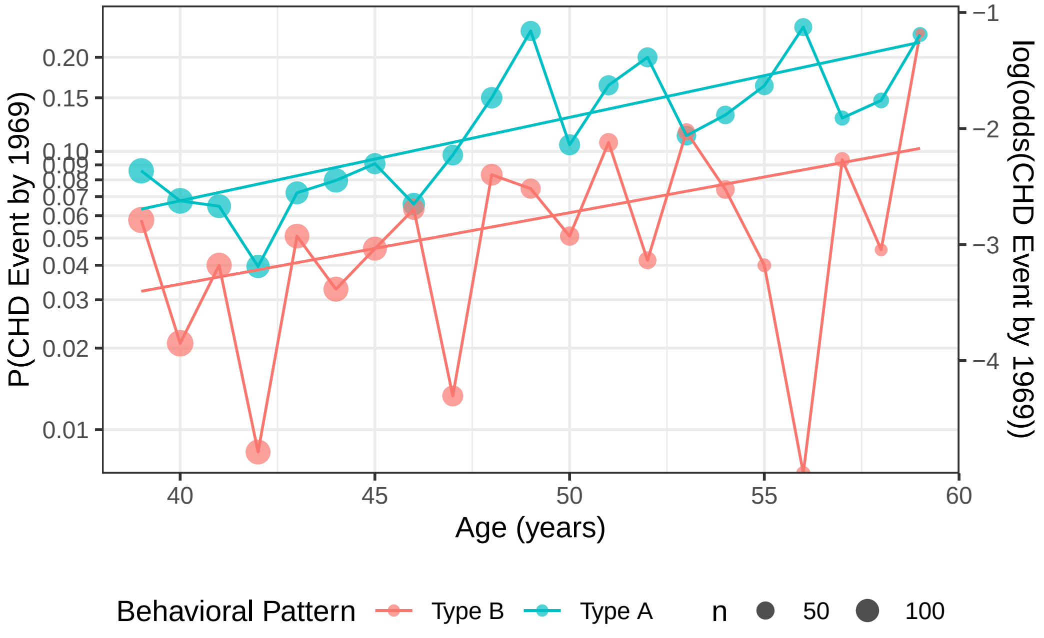


Figure 15

7.2.3 Interpreting the model parameters

> **Exercise 7.2.** For Equation 47, derive interpretations of β_0, β_P, β_A, and β_{PA} on the odds **and** log-odds scales, State the interpretations concisely in math **and** in words.

Solution

Solution 7.2.

```r
# include: false
age_offset = 0L
```

$$\begin{aligned}\eta(P=0,A=0) &= \beta_0 + \beta_P 0 + \beta_A 0 \\ &= \beta_0 + 0 + 0 \\ &= \beta_0\end{aligned}$$

Therefore:

$$\beta_0 = \eta(P=0,A=0) \tag{48}$$

β_0 is the natural logarithm of the odds ("log-odds") of experiencing CHD for a 0 year-old person with a type B personality; that is,

---

e^{β_0} is the odds of experiencing CHD for a 0 year-old with a type B personality,

$$\begin{aligned}\exp\{\beta_0\} &= \frac{\Pr(Y=1|P=0,A=0)}{1-\Pr(Y=1|P=0,A=0)} \\ &= \frac{\Pr(Y=1|P=0,A=0)}{\Pr(Y=0|P=0,A=0)}\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial a}\eta(P=0,A=a) &= \frac{\partial}{\partial a}(\beta_0 + \beta_P 0 + \beta_A a + \beta_{PA}(0 \cdot a)) \\ &= \frac{\partial}{\partial a}\beta_0 + \frac{\partial}{\partial a}\beta_P 0 + \frac{\partial}{\partial a}\beta_A a + \frac{\partial}{\partial a}\beta_{PA}(0 \cdot a)) \\ &= 0 + 0 + \beta_A + 0 \\ &= \beta_A\end{aligned}$$

Therefore:

$$\beta_A = \frac{\partial}{\partial a}\eta(P=0,A=a) \tag{49}$$

β_A is the slope of the log-odds of CHD with respect to age, for individuals with personality type B.
Alternatively:

$$\beta_A = \eta(P=0,A=a+1) - \eta(P=0,A=a)$$

That is, β_A is the difference in log-odds of experiencing CHD experiencing CHD per one-year difference in age between two individuals with type B personalities.

$$\begin{aligned}\exp\{\beta_A\} &= \exp\{\eta(P=0,A=a+1) - \eta(P=0,A=a)\} \\ &= \frac{\exp\{\eta(P=0,A=a+1)\}}{\exp\{\eta(P=0,A=a)\}} \\ &= \frac{\omega(P=0,A=a+1)}{\omega(P=0,A=a)} \\ &= \frac{\text{odds}(Y=1|P=0,A=a+1)}{\text{odds}(Y=1|P=0,A=a)} \\ &= \theta_\omega(\Delta a = 1|P=0)\end{aligned}$$

- The odds ratio of experiencing CHD (aka "the odds ratio") differs by a factor of e^{β_A} per one-year difference in age between individuals with type B personality.

β_P is the difference in log-odds of experiencing CHD for a 0 year-old person with type A personality compared to a 0 year-old person with type B personality; that is,

$$\beta_P = \eta(P=1,A=0) - \eta(P=0,A=0) \tag{50}$$

- e^{β_P} is the ratio of the odds (aka "the odds ratio") of experiencing CHD, for a 0-year old individual with type A personality vs a 0-year old individual with type B personality; that is,

$$\exp\{\beta_P\} = \frac{\text{odds}(Y=1|P=1,A=0)}{\text{odds}(Y=1|P=0,A=0)}$$

$$\begin{aligned}
\frac{\partial}{\partial a}\eta(P=1,A=a) &= \beta_A + \beta_{PA} \\
\frac{\partial}{\partial a}\eta(P=0,A=a) &= \beta_A
\end{aligned}$$

Therefore:

$$\begin{aligned}
\frac{\partial}{\partial a}\eta(P=1,A=a) - \frac{\partial}{\partial a}\eta(P=0,A=a) &= \beta_A + \beta_{PA} - \beta_A \\
&= \beta_{PA}
\end{aligned}$$

That is,

$$\begin{aligned}
\beta_{PA} &= \frac{\partial}{\partial a}\eta(P=1,A=a) - \frac{\partial}{\partial a}\eta(P=0,A=a) \\
&= \frac{\partial}{\partial a}\eta(P=1,A=a) - \frac{\partial}{\partial a}\eta(P=0,A=a)
\end{aligned}$$

β_{PA} is the difference in the slopes of log-odds over age between participants with Type A personalities and participants with Type B personalities.

Accordingly, the odds ratio of experiencing CHD per one-year difference in age differs by a factor of $e^{\beta_{PA}}$ for participants with type A personality compared to participants with type B personality; that is,

$$\theta_\omega(\Delta a = 1|P=1) = \exp\{\beta_{PA}\} \times \theta_\omega(\Delta a = 1|P=0)$$

or equivalently:

$$\exp\{\beta_{PA}\} = \frac{\theta_\omega(\Delta a = 1|P=1)}{\theta_\omega(\Delta a = 1|P=0)}$$

See Section 5.1.1[15] of Vittinghoff et al. (2012) for another perspective, also using the `wcgs` data as an example.

7.2.4 Interpreting the model parameter estimates

Table 20 shows the fitted model.

```
library(parameters)
chd_glm_contrasts |>
  parameters() |>
  print_md()
```

---

[15] https://link.springer.com/chapter/10.1007/978-1-4614-1353-0_5#Sec2_5

Table 20: CHD model (corner-point parametrization)

Parameter	Log-Odds	SE	95% CI	z	p
(Intercept)	-5.80	0.98	(-7.73, -3.90)	-5.95	$<$ .001
dibpat (Type A)	0.30	1.18	(-2.02, 2.63)	0.26	0.797
age	0.06	0.02	(0.02, 0.10)	3.01	0.003
dibpat (Type A) × age	0.01	0.02	(-0.04, 0.06)	0.42	0.674

We can get the corresponding odds ratio estimates ($e^{\hat{\beta}}$s) by passing `exponentiate = TRUE` to `parameters()`:

```r
chd_glm_contrasts |>
  parameters(exponentiate = TRUE) |>
  print_md()
```

Table 21: Odds ratio estimates for CHD model

Parameter	Odds Ratio	SE	95% CI	z	p
(Intercept)	3.02e-03	2.94e-03	(4.40e-04, 0.02)	-5.95	$<$ .001
dibpat (Type A)	1.36	1.61	(0.13, 13.88)	0.26	0.797
age	1.06	0.02	(1.02, 1.11)	3.01	0.003
dibpat (Type A) × age	1.01	0.02	(0.96, 1.06)	0.42	0.674

7.2.5 Stratified parametrization

We could instead use a stratified parametrization:

```r
chd_glm_strat <- glm(
  "formula" = chd69 == "Yes" ~ dibpat + dibpat:age - 1,
  "data" = wcgs,
  "family" = binomial(link = "logit")
)
equatiomatic::extract_eq(chd_glm_strat)
```

$$\log\left[\frac{P(\text{chd69} = \text{Yes})}{1 - P(\text{chd69} = \text{Yes})}\right] = \beta_1(\text{dibpat}_{\text{Type B}}) + \beta_2(\text{dibpat}_{\text{Type A}}) + \beta_3(\text{dibpat}_{\text{Type B}} \times \text{dibpat}_{\text{age}}) + \beta_4(\text{dibpat}_{\text{Type A}} \times \text{dibp} \tag{51}$$

```r
chd_glm_strat |>
  parameters() |>
  print_md()
```

Table 22: CHD model, stratified parametrization

Parameter	Log-Odds	SE	95% CI	z	p
dibpat (Type B)	-5.80	0.98	(-7.73, -3.90)	-5.95	$<$ .001
dibpat (Type A)	-5.50	0.67	(-6.83, -4.19)	-8.18	$<$ .001
dibpat (Type B) × age	0.06	0.02	(0.02, 0.10)	3.01	0.003
dibpat (Type A) × age	0.07	0.01	(0.05, 0.10)	5.24	$<$ .001

Again, we can get the corresponding odds ratios (e^{β}s) by passing `exponentiate = TRUE` to `parameters()`:

```
chd_glm_strat |>
  parameters(exponentiate = TRUE) |>
  print_md()
```

Table 23: Odds ratio estimates for CHD model

Parameter	Odds Ratio	SE	95% CI	z	p
dibpat (Type B)	3.02e-03	2.94e-03	(4.40e-04, 0.02)	-5.95	< .001
dibpat (Type A)	4.09e-03	2.75e-03	(1.08e-03, 0.02)	-8.18	< .001
dibpat (Type B) × age	1.06	0.02	(1.02, 1.11)	3.01	0.003
dibpat (Type A) × age	1.07	0.01	(1.05, 1.10)	5.24	< .001

Compare with Table 20.

Exercise 7.3. If I give you model 1, how would you get the coefficients of model 2?

8 Model comparisons for logistic models

8.0.1 Deviance test

We can compare the maximized log-likelihood of our model, $\ell(\hat{\beta}; \mathbf{x})$, versus the log-likelihood of the full model (aka saturated model aka maximal model), ℓ_{full}, which has one parameter per covariate pattern. With enough data, $2(\ell_{\text{full}} - \ell(\hat{\beta}; \mathbf{x})) \dot{\sim} \chi^2(N - p)$, where N is the number of distinct covariate patterns and p is the number of β parameters in our model. A significant p-value for this **deviance** statistic indicates that there's some detectable pattern in the data that our model isn't flexible enough to catch.

> Caution
>
> The deviance statistic needs to have a large amount of data **for each covariate pattern** for the χ^2 approximation to hold. A guideline from Dobson is that if there are q distinct covariate patterns $x_1 ..., x_q$, with $n_1, ..., n_q$ observations per pattern, then the expected frequencies $n_k \cdot \pi(x_k)$ should be at least 1 for every pattern $k \in 1 : q$.

If you have covariates measured on a continuous scale, you may not be able to use the deviance tests to assess goodness of fit.

8.0.2 Hosmer-Lemeshow test

If our covariate patterns produce groups that are too small, a reasonable solution is to make bigger groups by merging some of the covariate-pattern groups together.

Hosmer and Lemeshow (1980) proposed that we group the patterns by their predicted probabilities according to the model of interest. For example, you could group all of the observations with predicted probabilities of 10% or less together, then group the observations with 11%-20% probability together, and so on; $g = 10$ categories in all.

Then we can construct a statistic

$$X^2 = \sum_{c=1}^{g} \frac{(o_c - e_c)^2}{e_c}$$

where o_c is the number of events *observed* in group c, and e_c is the number of events expected in group c (based on the sum of the fitted values $\hat{\pi}_i$ for observations in group c).

If each group has enough observations in it, you can compare X^2 to a χ^2 distribution; by simulation, the degrees of freedom has been found to be approximately $g - 2$.

For our CHD model, this procedure would be:

```r
wcgs <-
  wcgs |>
  mutate(
    pred_probs_glm1 = chd_glm_contrasts |> fitted(),
    pred_prob_cats1 = pred_probs_glm1 |>
      cut(
        breaks = seq(0, 1, by = .1),
        include.lowest = TRUE
      )
  )

HL_table <- # nolint: object_name_linter
  wcgs |>
  summarize(
    .by = pred_prob_cats1,
    n = n(),
    o = sum(chd69 == "Yes"),
    e = sum(pred_probs_glm1)
  )

library(pander)
HL_table |> pander()
```

pred_prob_cats1	n	o	e
(0.1,0.2]	785	116	108
(0.2,0.3]	64	12	13.77
[0,0.1]	2,305	129	135.2

```r
X2 <- HL_table |> # nolint: object_name_linter
  summarize(
    `X^2` = sum((o - e)^2 / e)
  ) |>
  pull(`X^2`)
print(X2)
#> [1] 1.11029

pval1 <- pchisq(X2, lower = FALSE, df = nrow(HL_table) - 2)
```

Our statistic is $X^2 = 1.110287$; $p(\chi^2(1) > 1.110287) = 0.29202$, which is our p-value for detecting a lack of goodness of fit.

Unfortunately that grouping plan left us with just three categories with any observations, so instead of grouping by 10% increments of predicted probability, typically analysts use deciles of the predicted probabilities:

```r
wcgs <-
  wcgs |>
  mutate(
    pred_probs_glm1 = chd_glm_contrasts |> fitted(),
    pred_prob_cats1 = pred_probs_glm1 |>
      cut(
        breaks = quantile(pred_probs_glm1, seq(0, 1, by = .1)),
        include.lowest = TRUE
      )
  )
```

```
HL_table <- # nolint: object_name_linter
  wcgs |>
  summarize(
    .by = pred_prob_cats1,
    n = n(),
    o = sum(chd69 == "Yes"),
    e = sum(pred_probs_glm1)
  )

HL_table |> pander()
```

pred_prob_cats1	n	o	e
(0.114,0.147]	275	48	36.81
(0.147,0.222]	314	51	57.19
(0.0774,0.0942]	371	27	32.56
(0.0942,0.114]	282	30	29.89
(0.0633,0.069]	237	17	15.97
(0.069,0.0774]	306	20	22.95
(0.0487,0.0633]	413	27	24.1
(0.0409,0.0487]	310	14	14.15
[0.0322,0.0363]	407	16	13.91
(0.0363,0.0409]	239	7	9.48

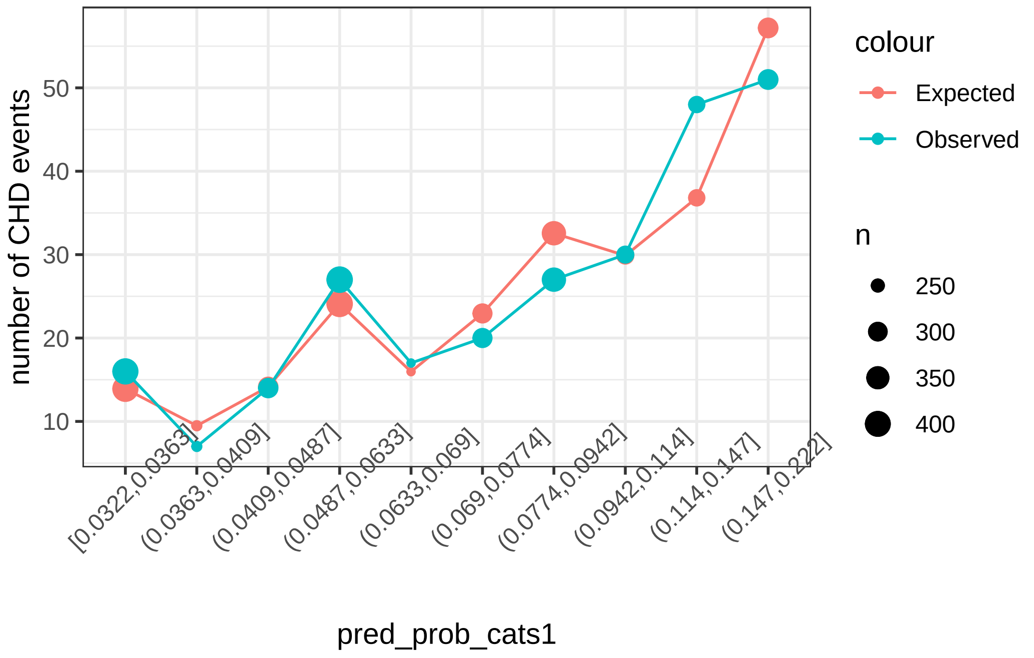
```
X2 <- HL_table |> # nolint: object_name_linter
  summarize(
    `X^2` = sum((o - e)^2 / e)
  ) |>
  pull(`X^2`)

print(X2)
#> [1] 6.78114

pval1 <- pchisq(X2, lower = FALSE, df = nrow(HL_table) - 2)
```

Now we have more evenly split categories. The p-value is 0.56042, still not significant.

Graphically, we have compared:

```
HL_plot <- # nolint: object_name_linter
  HL_table |>
  ggplot(aes(x = pred_prob_cats1)) +
  geom_line(
    aes(y = e, x = pred_prob_cats1, group = "Expected", col = "Expected")
  ) +
  geom_point(aes(y = e, size = n, col = "Expected")) +
  geom_point(aes(y = o, size = n, col = "Observed")) +
  geom_line(aes(y = o, col = "Observed", group = "Observed")) +
  scale_size(range = c(1, 4)) +
  theme_bw() +
  ylab("number of CHD events") +
  theme(axis.text.x = element_text(angle = 45))
```

```
print(HL_plot)
```



8.0.3 Comparing models

- AIC $= -2 * \ell(\hat{\theta}) + 2 * p$ [lower is better]
- BIC $= -2 * \ell(\hat{\theta}) + p * \log(n)$ [lower is better]
- likelihood ratio [higher is better]

9 Residual-based diagnostics

9.0.1 Logistic regression residuals only work for grouped data

```
library(haven)
url <- paste0(
  # I'm breaking up the url into two chunks for readability
  "https://regression.ucsf.edu/sites/g/files/",
  "tkssra6706/f/wysiwyg/home/data/wcgs.dta"
)
library(here) # provides the `here()` function
library(fs) # provides the `path()` function
here::here() |>
  fs::path("Data/wcgs.rda") |>
  load()
chd_glm_contrasts <-
  wcgs |>
  glm(
    "data" = _,
    "formula" = chd69 == "Yes" ~ dibpat * age,
    "family" = binomial(link = "logit")
  )
library(ggfortify)
chd_glm_contrasts |> autoplot()
```

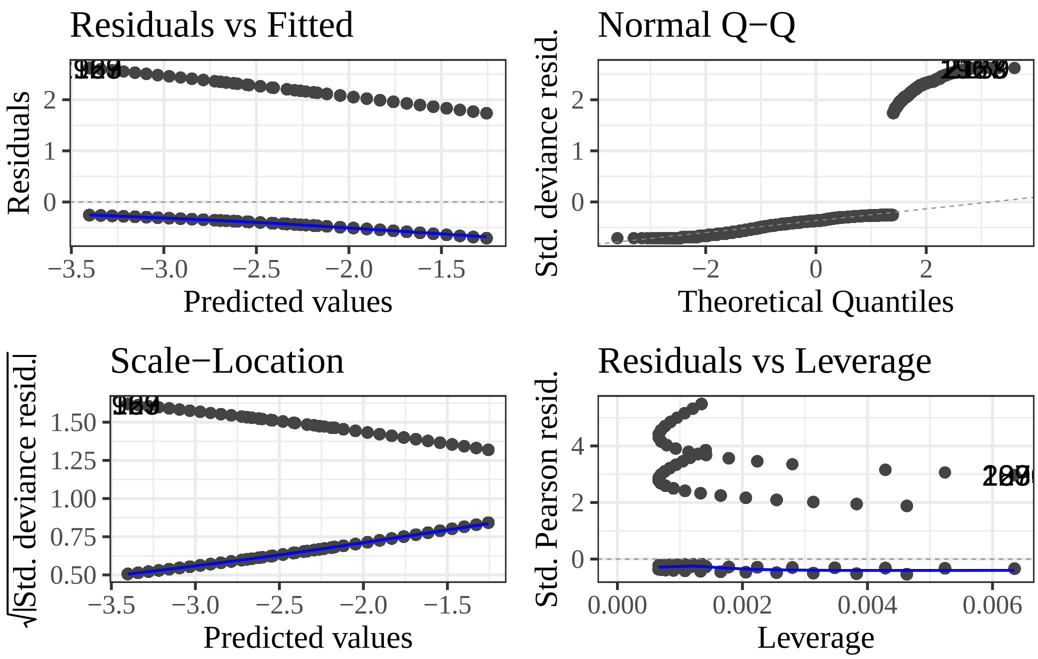


Figure 16: Residual diagnostics for WCGS model with individual-level observations

Residuals only work if there is more than one observation for most covariate patterns.

Here we will create the grouped-data version of our CHD model from the WCGS study:

```r
library(dplyr)
wcgs_grouped <-
  wcgs |>
  summarize(
    .by = c(dibpat, age),
    n = n(),
    chd = sum(chd69 == "Yes"),
    no_chd = sum(chd69 == "No")
  ) |>
  mutate(p_chd = chd/n)

chd_glm_contrasts_grouped <- glm(
  "formula" = cbind(chd, no_chd) ~ dibpat*age,
  "data" = wcgs_grouped,
  "family" = binomial(link = "logit")
)
chd_glm_contrasts_grouped |> equatiomatic::extract_eq()
```

$$\log\left[\frac{P(\operatorname{chd})}{1-P(\operatorname{chd})}\right] = \alpha + \beta_{1}(\operatorname{dibpat}_{\operatorname{Type\ A}}) + \beta_{2}(\operatorname{age}) + \beta_{3}(\operatorname{dibpat}_{\operatorname{Type\ A}} \times \operatorname{age}) \tag{52}$$

```r
library(parameters)
chd_glm_contrasts_grouped |>
  parameters() |>
  print_md()
```

Table 24: CHD model with grouped `wcgs` data

Parameter	Log-Odds	SE	95% CI	z	p
(Intercept)	-5.80	0.98	(-7.73, -3.90)	-5.95	< .001
dibpat (Type A)	0.30	1.18	(-2.02, 2.63)	0.26	0.797
age	0.06	0.02	(0.02, 0.10)	3.01	0.003
dibpat (Type A) × age	0.01	0.02	(-0.04, 0.06)	0.42	0.674

```
chd_glm_contrasts_grouped |>
  sjPlot::plot_model(type = "pred", terms = c("age", "dibpat")) +
  geom_point(data = wcgs_grouped |> mutate(group_col = dibpat),
             aes(x = age, y = p_chd))
```

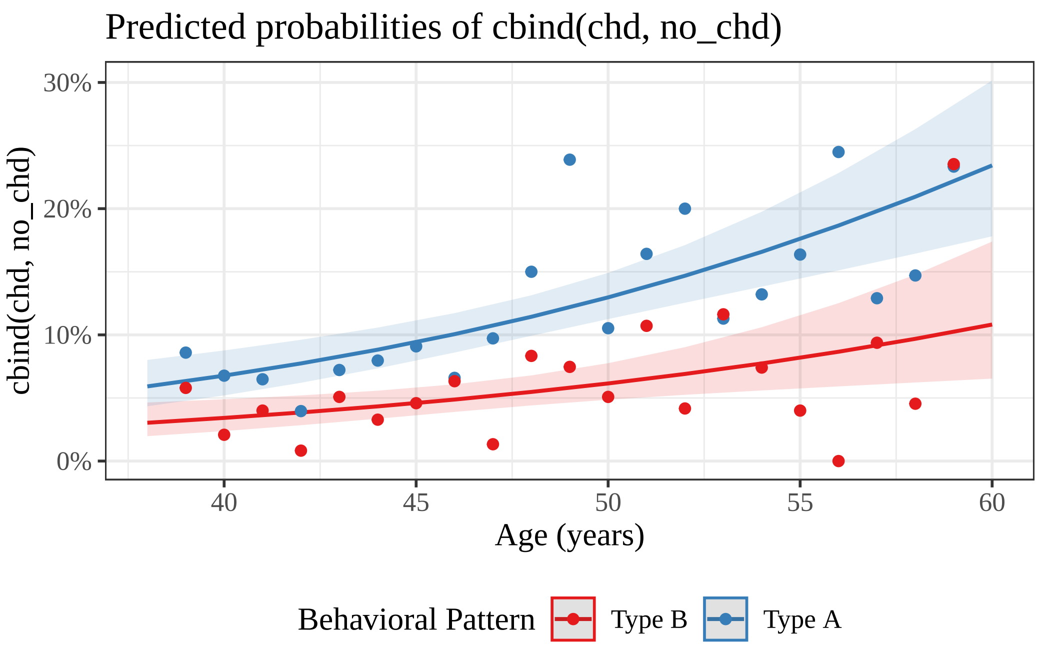
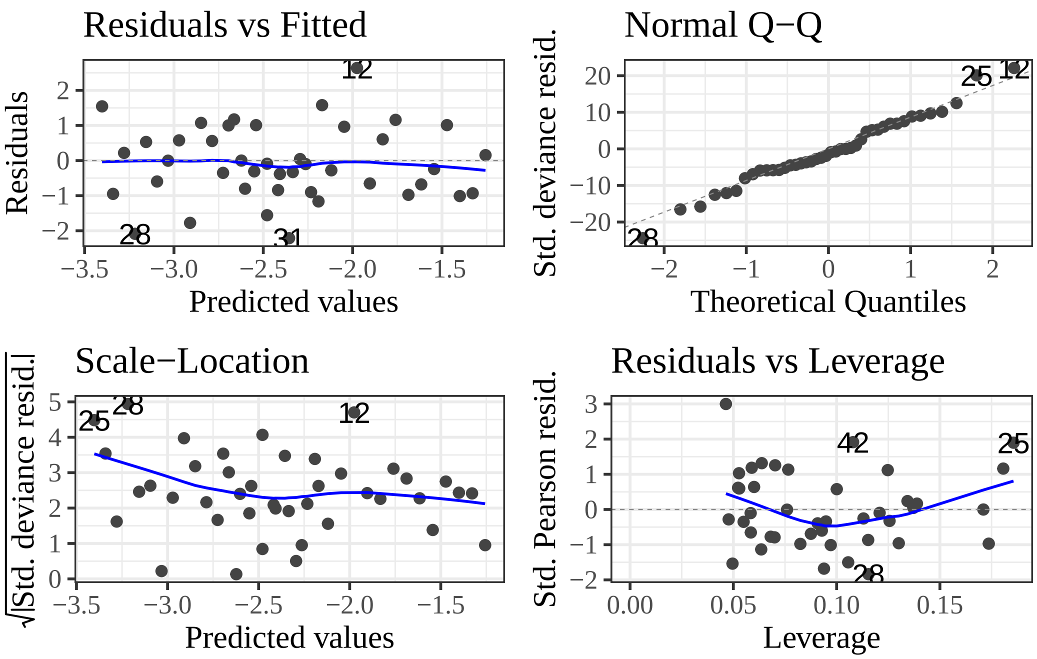


Figure 17: CHD model with grouped `wcgs` data

```
library(ggfortify)
chd_glm_contrasts_grouped |> autoplot()
```



9.0.2 (Response) residuals

$$e_k \overset{\text{def}}{=} \bar{y}_k - \hat{\pi}(x_k)$$

(k indexes the covariate patterns)

We can graph these residuals e_k against the fitted values $\hat{\pi}(x_k)$:

```
odds <- function(pi) pi/(1-pi)
logit <- function(pi) log(odds(pi))
wcgs_grouped <-
  wcgs_grouped |>
  mutate(
    fitted = chd_glm_contrasts_grouped |> fitted(),
    fitted_logit = fitted |> logit(),
    response_resids = chd_glm_contrasts_grouped |> resid(type = "response")
  )

wcgs_response_resid_plot <-
  wcgs_grouped |>
  ggplot(
    mapping = aes(
      x = fitted,
      y = response_resids
    )
  ) +
  geom_point(
    aes(col = dibpat)
  ) +
  geom_hline(yintercept = 0) +
  geom_smooth(                                                                ①
    se = TRUE,
    method.args = list(
      span = 2 / 3,
      degree = 1,
      family = "symmetric",
      iterations = 3
```

```
    ),
    method = stats::loess
  )
```

① Don't worry about these options for now; I chose them to match `autoplot()` as closely as I can. `plot.glm` and `autoplot` use `stats::lowess` instead of `stats::loess`; `stats::lowess` is older, hard to use with `geom_smooth`, and hard to match exactly with `stats::loess`; see https://support.bioconductor.org/p/2323/.]

```
wcgs_response_resid_plot |> print()
```

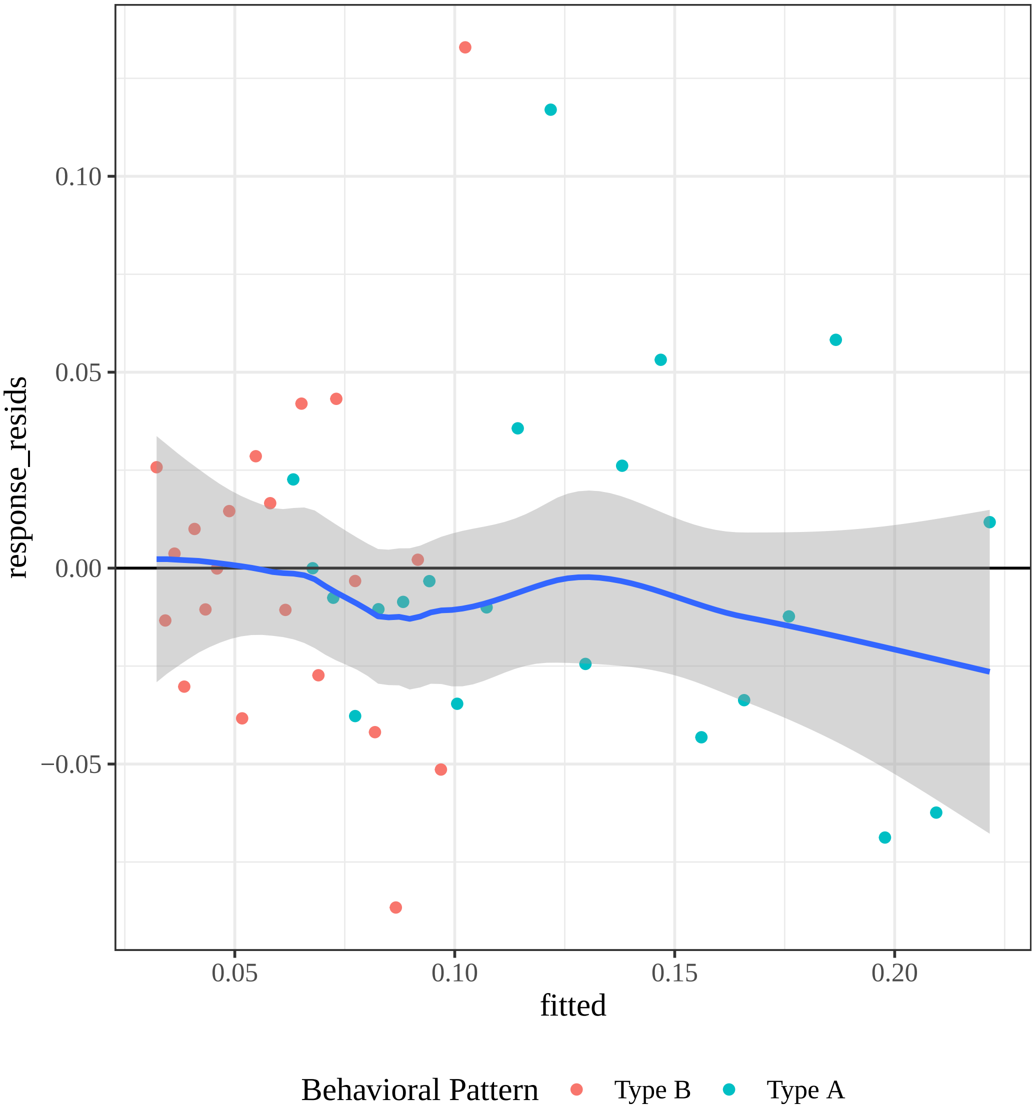


Figure 18: residuals plot for `wcgs` model

We can see a slight fan-shape here: observations on the right have larger variance (as expected since $var(\bar{y}) = \pi(1 - \pi)/n$ is maximized when $\pi = 0.5$).

9.0.3 Pearson residuals

The fan-shape in the response residuals plot isn't necessarily a concern here, since we haven't made an assumption of constant residual variance, as we did for linear regression.

However, we might want to divide by the standard error in order to make the graph easier to interpret. Here's one way to do that:

The Pearson (chi-squared) residual for covariate pattern k is:

$$X_k = \frac{\bar{y}_k - \hat{\pi}_k}{\sqrt{\hat{\pi}_k(1-\hat{\pi}_k)/n_k}}$$

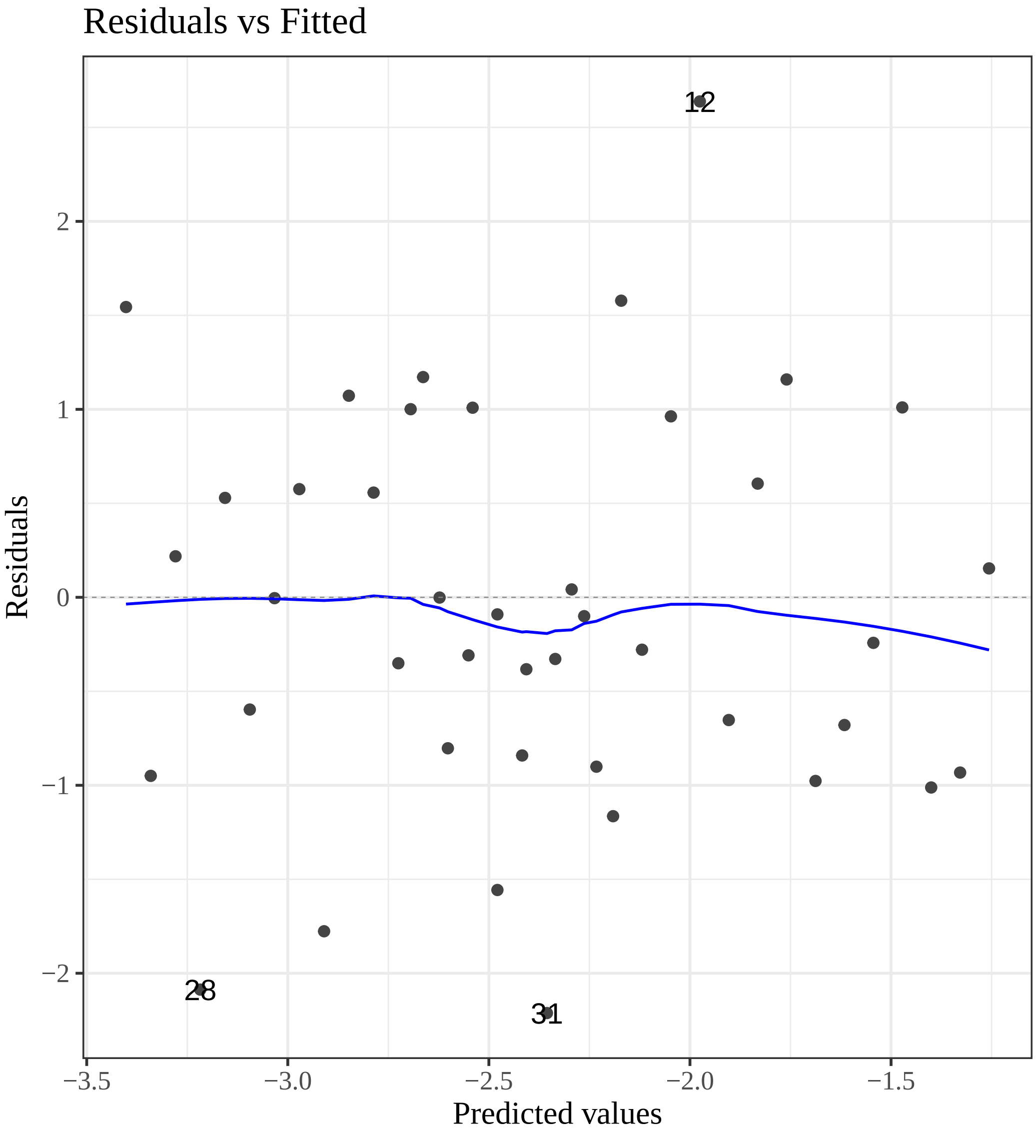
where

$$\begin{aligned}
\hat{\pi}_k &\overset{\text{def}}{=} \hat{\pi}(x_k) \\
&\overset{\text{def}}{=} \hat{P}(Y=1|X=x_k) \\
&\overset{\text{def}}{=} \text{expit}(x_i'\hat{\beta}) \\
&\overset{\text{def}}{=} \text{expit}(\hat{\beta}_0 + \sum_{j=1}^{p} \hat{\beta}_j x_{ij})
\end{aligned}$$

Let's take a look at the Pearson residuals for our CHD model from the WCGS data (graphed against the fitted values on the logit scale):

```r
library(ggfortify)
```

```r
autoplot(chd_glm_contrasts_grouped, which = 1, ncol = 1) |> print()
```

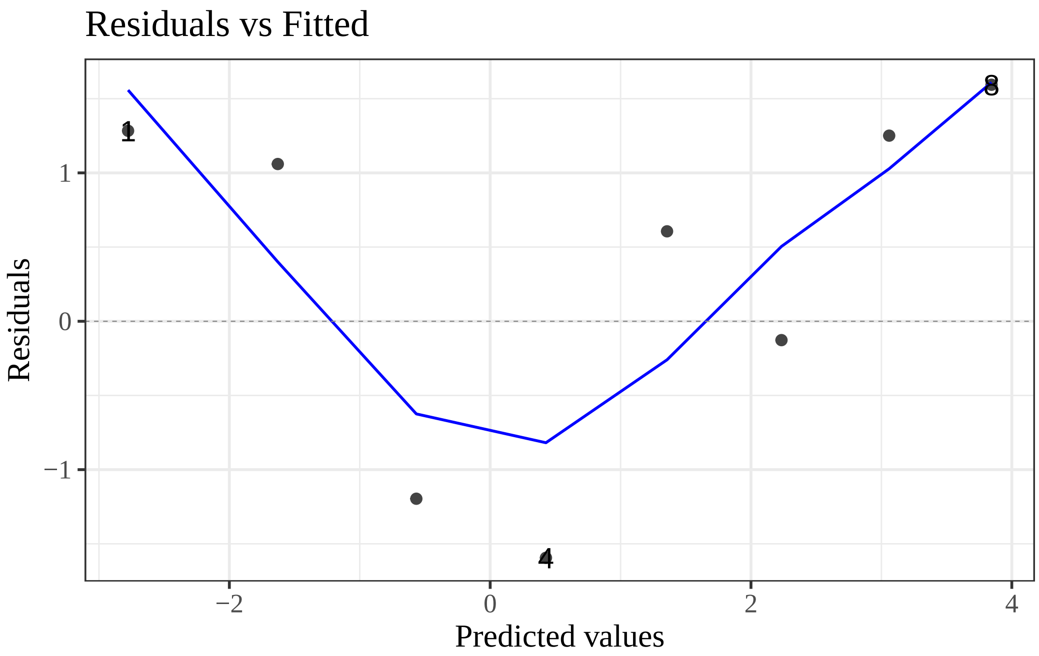


The fan-shape is gone, and these residuals don't show any obvious signs of model fit issues.

Pearson residuals plot for Beetles Data

If we create the same plot for the `beetles` model, we see some strong evidence of a lack of fit:

```r
library(glmx)
library(dplyr)
data(BeetleMortality)
beetles <- BeetleMortality |>
  mutate(
    pct = died / n,
    survived = n - died,
    dose_c = dose - mean(dose)
  )
beetles_glm_grouped <- beetles |>
  glm(
    formula = cbind(died, survived) ~ dose,
    family = "binomial"
  )
autoplot(beetles_glm_grouped, which = 1, ncol = 1) |> print()
```

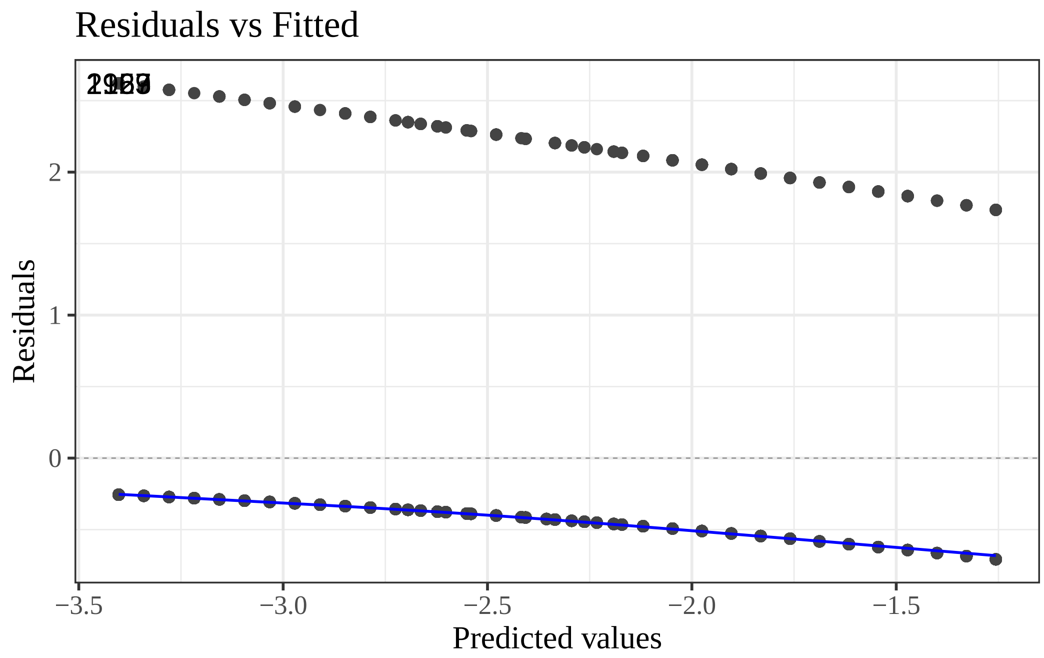


Pearson residuals with individual (ungrouped) data

What happens if we try to compute residuals without grouping the data by covariate pattern?

```r
library(ggfortify)
```

```r
chd_glm_strat <- glm(
  "formula" = chd69 == "Yes" ~ dibpat + dibpat:age - 1,
  "data" = wcgs,
  "family" = binomial(link = "logit")
)

autoplot(chd_glm_strat, which = 1, ncol = 1) |> print()
```



Meaningless.

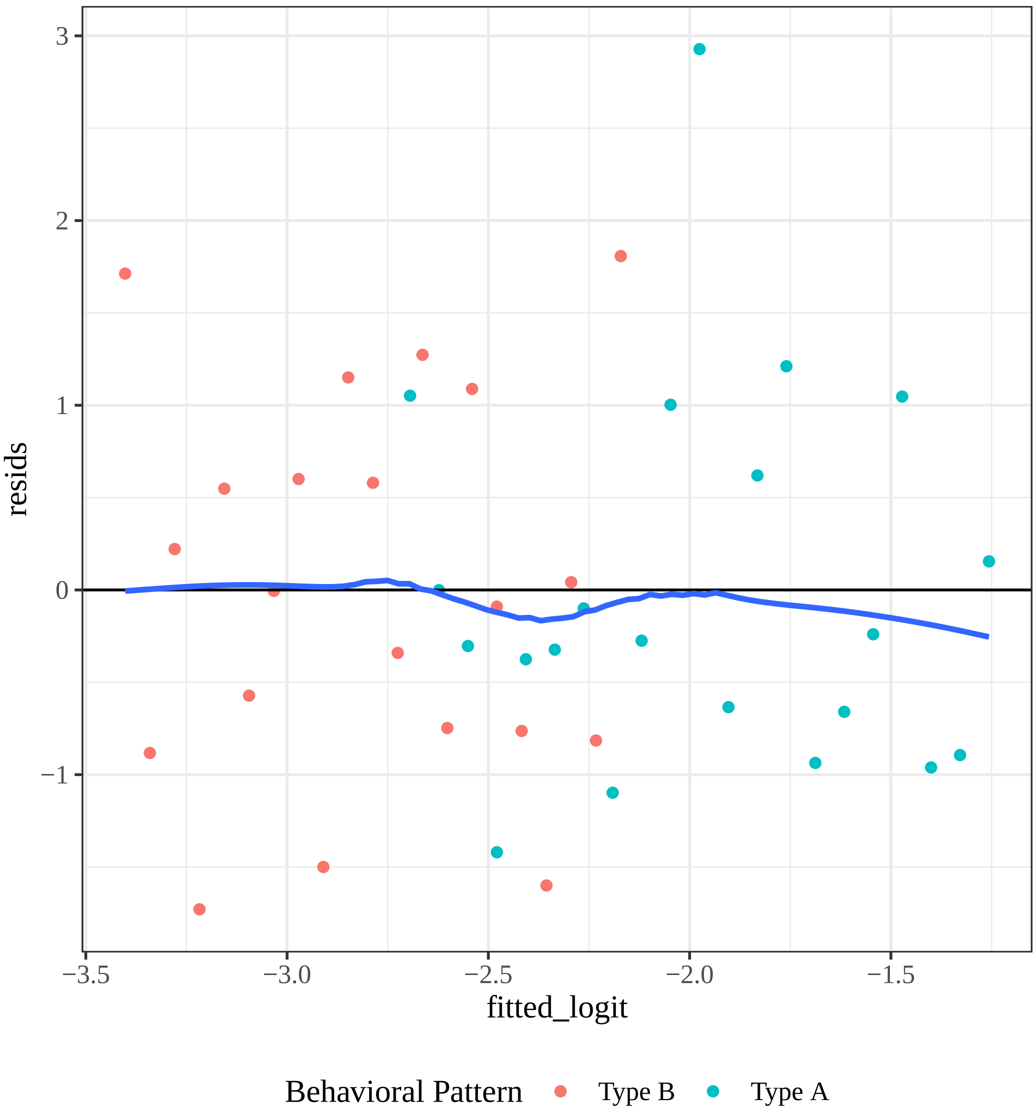
Residuals plot by hand

If you want to check your understanding of what these residual plots are, try building them yourself:

```
wcgs_grouped <-
  wcgs_grouped |>
  mutate(
    fitted = chd_glm_contrasts_grouped |> fitted(),
    fitted_logit = fitted |> logit(),
    resids = chd_glm_contrasts_grouped |> resid(type = "pearson")
  )

wcgs_resid_plot1 <-
  wcgs_grouped |>
  ggplot(
    mapping = aes(
      x = fitted_logit,
      y = resids
    )
  ) +
  geom_point(
    aes(col = dibpat)
  ) +
  geom_hline(yintercept = 0) +
  geom_smooth(
    se = FALSE,
    method.args = list(
      span = 2 / 3,
      degree = 1,
      family = "symmetric",
      iterations = 3,
      surface = "direct"
    ),
    method = stats::loess
  )
```

```
# plot.glm and autoplot use stats::lowess, which is hard to use with
# geom_smooth and hard to match exactly;
# see https://support.bioconductor.org/p/2323/
```

```
wcgs_resid_plot1 |> print()
```



Pearson chi-squared goodness of fit test

The Pearson chi-squared goodness of fit statistic is:

$$X^2 = \sum_{k=1}^{m} X_k^2$$

Under the null hypothesis that the model in question is correct (i.e., sufficiently complex), $X^2 \dot{\sim} \chi^2(N-p)$.

```
x_pearson <- chd_glm_contrasts_grouped |>
  resid(type = "pearson")

chisq_stat <- sum(x_pearson^2)
```

```r
pval <- pchisq(
  chisq_stat,
  lower = FALSE,
  df = length(x_pearson) - length(coef(chd_glm_contrasts_grouped))
)
```

For our CHD model, the p-value for this test is 0.265236; no significant evidence of a lack of fit at the 0.05 level.

Standardized Pearson residuals

Especially for small data sets, we might want to adjust our residuals for leverage (since outliers in X add extra variance to the residuals):

$$r_{P_k} = \frac{X_k}{\sqrt{1 - h_k}}$$

where h_k is the leverage of X_k. The functions `autoplot()` and `plot.lm()` use these for some of their graphs.

9.0.4 Deviance residuals

For large sample sizes, the Pearson and deviance residuals will be approximately the same. For small sample sizes, the deviance residuals from covariate patterns with small sample sizes can be unreliable (high variance).

$$d_k = \text{sign}(y_k - n_k\hat{\pi}_k)\left\{\sqrt{2[\ell_{\text{full}}(x_k) - \ell(\hat{\beta}; x_k)]}\right\}$$

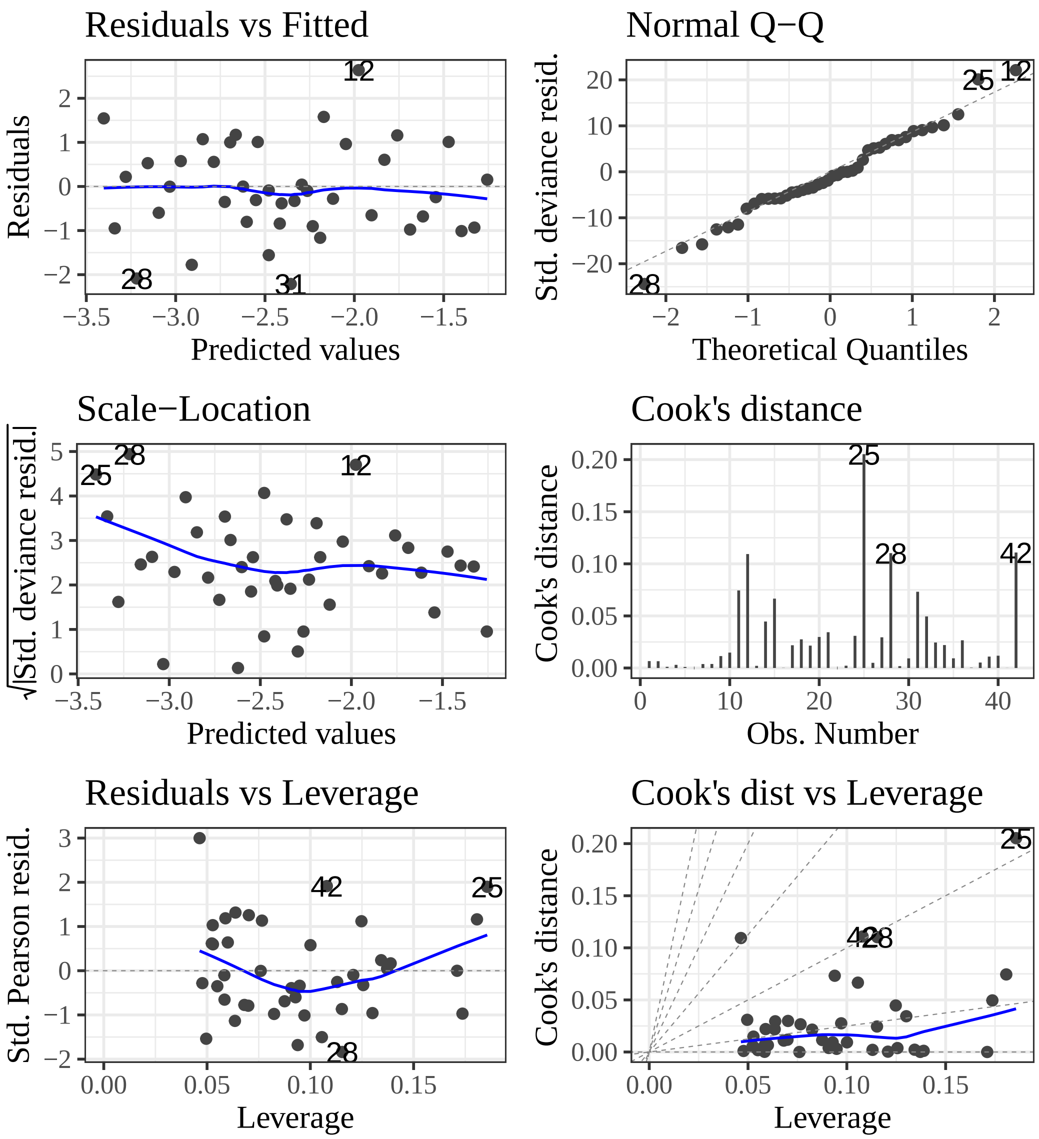
Standardized deviance residuals

$$r_{D_k} = \frac{d_k}{\sqrt{1 - h_k}}$$

9.0.5 Diagnostic plots

Let's take a look at the full set of `autoplot()` diagnostics now for our `CHD` model:

```r
chd_glm_contrasts_grouped |>
  autoplot(which = 1:6) |>
  print()
```


Residuals vs Fitted

Normal Q−Q

Scale−Location

Cook's distance

Residuals vs Leverage

Cook's dist vs Leverage

Figure 19: Diagnostics for CHD model

Things look pretty good here. The QQ plot is still usable; with large samples; the residuals should be approximately Gaussian.

Beetles

Let's look at the beetles model diagnostic plots for comparison:

```r
beetles_glm_grouped |>
  autoplot(which = 1:6) |>
  print()
```

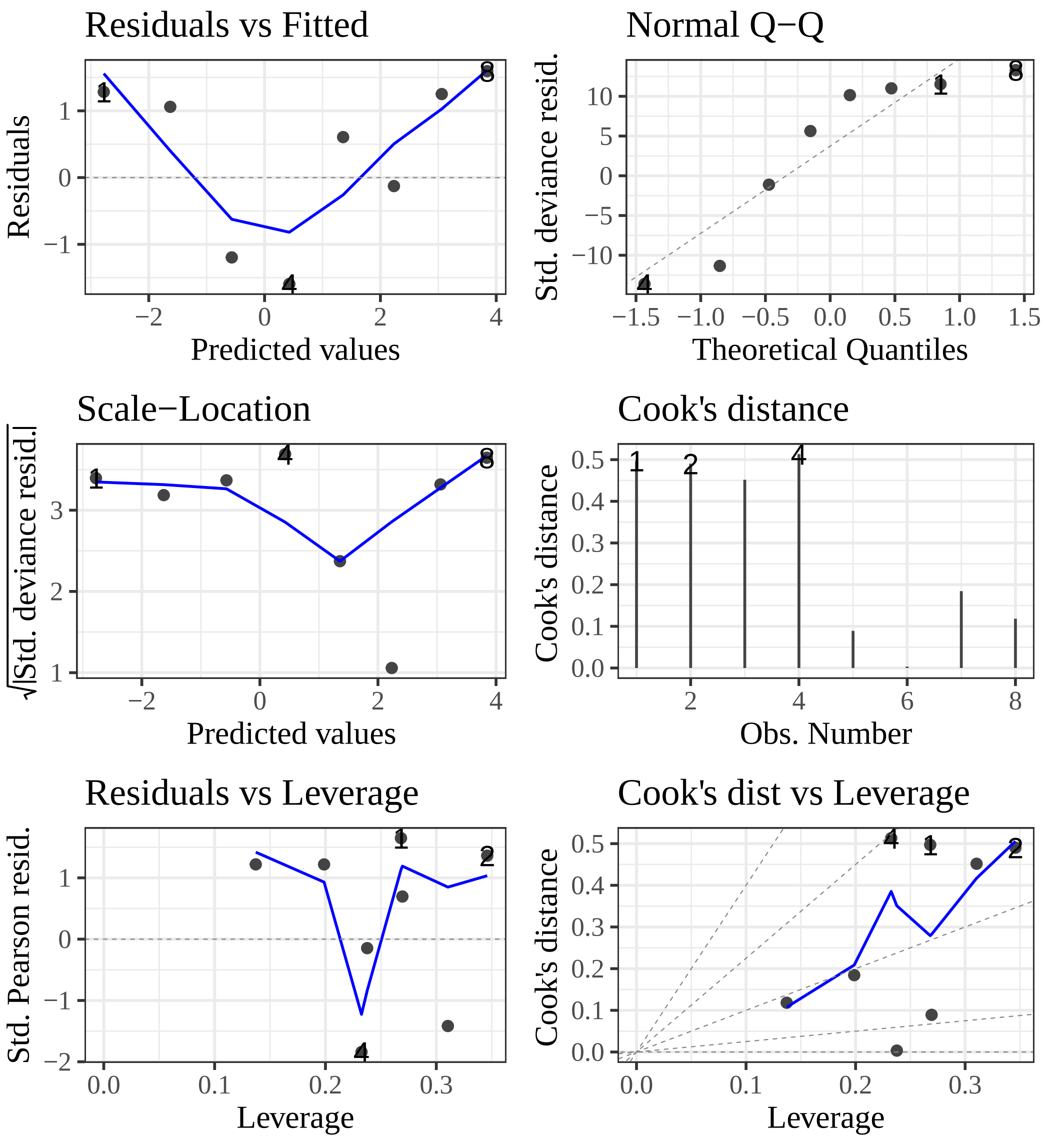


Figure 20: Diagnostics for logistic model of `BeetleMortality` data

Hard to tell much from so little data, but there might be some issues here.

10 Alternatives to reporting odds ratios

10.0.1 Objections to odds ratios

Some scholars have raised objections to the use of odds ratios as an effect measurement (Sackett et al. 1996; Norton et al. 2024).

As we saw in Figure 3, the odds ratio is not very closely correlated with the risk difference, and the risk difference is typically the metric that ultimately matters for policy decisions.

Another objection is that odds ratios (and risk ratios, and risk differences) depend on the set of covariates in a logistic regression model, even when those covariates are independent of the exposure of interest and do not interact with that exposure. For example, consider the following model:

$$\text{P}(Y = y|X = x, C = c) = \pi(x, c)^y(1 - \pi(x, c))^{1-y}$$

$$\pi(x,c) = \text{expit}\{\eta_0 + \beta_X x + \beta_C c\}$$

Then:

$$\begin{aligned}
\text{E}[Y|X=x] &= \text{E}[\text{E}[Y|X,C]|X=x] \\
&= \text{E}[\pi(X,C)|X=x] \\
&= \text{E}[\text{expit}\{\eta_0 + \beta_X X + \beta_C C\}|X=x] \\
&= \int_c \text{expit}\{\eta_0 + \beta_X x + \beta_C c\} \;\; \text{p}(C=c|X=x)\ \partial c \\
&= \int_c \pi(x,c) \;\; \text{p}(C=c|X=x)\ \partial c
\end{aligned}$$

Since the expit{} function is nonlinear, we can't change the order of the expectation and expit{} operators:

$$\text{E}[\text{expit}\{\eta_0 + \beta_X X + \beta_C C\}|X] \neq \text{expit}\{\text{E}[\eta_0 + \beta_X X + \beta_C C]|X\}$$

In contrast, consider a model with an identity link function:

$$\text{P}(Y=y|X=x,C=c) = \pi(x,c)^y(1-\pi(x,c))^{1-y}$$

$$\pi(x,c) = \eta_0 + \beta_X x + \beta_C c$$

Then:

$$\begin{aligned}
\text{E}[Y|X=x] &= \text{E}[\text{E}[Y|X,C]|X=x] \\
&= \text{E}[\eta_0 + \beta_X X + \beta_C C|X=x] \\
&= \text{E}[\eta_0|X=x] + \text{E}[\beta_X X|X=x] + \text{E}[\beta_C C|X=x] \\
&= \eta_0 + \beta_X x + \beta_C\,\text{E}[C|X=x] \\
&= (\eta_0 + \beta_C\,\text{E}[C|X=x]) + \beta_X x
\end{aligned}$$

If $C \perp\!\!\!\perp X$, then $\text{E}[C|X=x] = \text{E}[C]$, and we can simplify further:

$$\begin{aligned}
\text{E}[Y|X=x] &= (\eta_0 + \beta_C\,\text{E}[C|X=x]) + \beta_X x \\
&= (\eta_0 + \beta_C\,\text{E}[C]) + \beta_X x \\
&= \eta_0^* + \beta_X x
\end{aligned}$$

Then:

$$\frac{\partial}{\partial x}\text{E}[Y|X=x] = \beta_X = \frac{\partial}{\partial x}\text{E}[Y|X=x,C=c]$$

In other words, for a model with an identity link function, if covariates X and C are independent, then the slope with respect to X doesn't depend on whether C is included in the model (and an analogous result holds if X is discrete or categorical).

Exercise 10.1. What are the expressions for $\text{E}[Y|X=x]$ and $\frac{\partial}{\partial x}\text{E}[Y|X=x]$ for the model above, if $\text{E}[C|X=x] = \gamma_0 + \gamma_x x$?

Solution

Solution 10.1. Left to the reader.

Exercise 10.2. What are the expressions for $\text{E}[Y|X=x]$ and $\frac{\partial}{\partial x}\text{E}[Y|X=x]$, if instead of the model above,

$$\pi(x,c) = \eta_0 + \beta_X x + \beta_C c + \beta_{XC} xc$$

and $\text{E}[C|X=x] = \gamma_0 + \gamma_x x$?

Solution

Solution 10.2. Left to the reader.
Hint: does adding the interaction term change the functional form of $\text{E}[Y|X=x]$?

10.0.2 Deriving risk ratios and risk differences from logistic regression models

If you want to report risk differences or risk ratios instead of odds ratios, you can obtain estimates from logistic regression models, as long as you didn't stratify sampling by the outcome; in other words, not in case-control studies (see Section 1.3.3).

To compute risk ratios from logistic regression models:

- Apply the expit function to the linear predictor for each covariate pattern to compute the (estimated) risks,
- Then take the differences or ratios of the risks, as needed.

To quantify uncertainty for risk difference or risk ratio estimates derived from logistic regression models (e.g., to calculate SEs, CIs, and p-values), you will need to use the bootstrap, the multivariate delta method, or some other special technique.

Adapted from (Vittinghoff et al. 2012, sec. 3.6, p. 62), (Hastie et al. 2009, sec. 7.11, p. 249), and (James et al. 2021, chap. 5, Section 5.2, p. 209).

Bootstrap workflow for derived risk measures

When using nonparametric bootstrap inference for a derived quantity like a marginal risk difference or risk ratio:

1. Fit the logistic model on the observed data.
2. Compute the target estimand (for example, a g-computation risk difference or risk ratio).
3. Repeat for $b = 1, \dots, B$: draw a bootstrap sample of size n with replacement, refit the model, and recompute the target estimand.
4. Use the empirical standard deviation of the B bootstrap estimates as the bootstrap standard error.
5. Build a confidence interval from the bootstrap distribution (percentile or BCa intervals are common when the bootstrap distribution is skewed).

In practice, larger B is usually needed for interval estimation than for standard errors; for percentile or BCa intervals, it is common to use at least 1,000 resamples, and often 2,000 or more for stability.

Exm

Example 10.1 (Bootstrap CI for marginal risk difference and risk ratio (WCGS))**.** We estimate the marginal risk difference and risk ratio comparing Type A vs. Type B personality patterns in the WCGS study, using g-computation to derive the estimands and the nonparametric bootstrap to quantify uncertainty.

Steps 1–2: Point estimates via g-computation

```r
# Fit logistic model: CHD ~ behavioral pattern + age
fit_wcgs <- glm(
  chd69 ~ dibpat + age,
  family = binomial,
  data = wcgs
)

# G-computation: set everyone to Type A, then to Type B,
# and average the predicted risks
dibpat_levels <- levels(wcgs$dibpat)

newdata_A <- wcgs |> mutate(dibpat = factor("Type A", levels = dibpat_levels))
newdata_B <- wcgs |> mutate(dibpat = factor("Type B", levels = dibpat_levels))

risk_A <- mean(predict(fit_wcgs, newdata = newdata_A, type = "response"))
risk_B <- mean(predict(fit_wcgs, newdata = newdata_B, type = "response"))

tibble::tibble(
  measure   = c(
    "Risk (Type A)", "Risk (Type B)",
    "Risk difference", "Risk ratio"
  ),
  estimate  = c(risk_A, risk_B, risk_A - risk_B, risk_A / risk_B)
)
#> # A tibble: 4 x 2
#>   measure         estimate
#>   <chr>              <dbl>
#> 1 Risk (Type A)     0.109
#> 2 Risk (Type B)     0.0523
#> 3 Risk difference   0.0562
#> 4 Risk ratio        2.07
```

Steps 3–5: Bootstrap SE and BCa CIs

```
library(boot)
library(dplyr)

boot_gcomp <- function(data, indices) {
  d <- data[indices, ]
  fit <- glm(chd69 ~ dibpat + age, family = binomial, data = d)
  lev <- levels(d$dibpat)
  risk_A <- mean(
    predict(fit, newdata = mutate(d, dibpat = factor("Type A", levels = lev)),
            type = "response")
  )
  risk_B <- mean(
    predict(fit, newdata = mutate(d, dibpat = factor("Type B", levels = lev)),
            type = "response")
  )
  c(RD = risk_A - risk_B, RR = risk_A / risk_B)
}

set.seed(42)
boot_wcgs <- boot(data = wcgs, statistic = boot_gcomp, R = 1000)

boot_wcgs
#>
#> ORDINARY NONPARAMETRIC BOOTSTRAP
#>
#>
#> Call:
#> boot(data = wcgs, statistic = boot_gcomp, R = 1000)
#>
#>
#> Bootstrap Statistics :
#>      original       bias    std. error
#> t1* 0.0561584 -1.75742e-05  0.00953337
#> t2* 2.0729167  2.92369e-02  0.27591700
```

```
# BCa CI for risk difference (index = 1)
boot.ci(boot_wcgs, type = "bca", index = 1)
#> BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
#> Based on 1000 bootstrap replicates
#>
#> CALL :
#> boot.ci(boot.out = boot_wcgs, type = "bca", index = 1)
#>
#> Intervals :
#> Level       BCa
#> 95%   ( 0.0377,  0.0754 )
#> Calculations and Intervals on Original Scale
```

```
# BCa CI for risk ratio (index = 2)
boot.ci(boot_wcgs, type = "bca", index = 2)
#> BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
#> Based on 1000 bootstrap replicates
#>
#> CALL :
#> boot.ci(boot.out = boot_wcgs, type = "bca", index = 2)
#>
#> Intervals :
#> Level       BCa
#> 95%   ( 1.599,  2.695 )
#> Calculations and Intervals on Original Scale
```

The bootstrap standard errors and BCa intervals provide valid inference for both the risk difference and risk ratio without requiring any closed-form delta-method derivation.

10.0.3 Other link functions for Bernoulli outcomes

Alternatively, if you want to estimate risk ratios more directly from the model, you can sometimes change the link function from logit{} to log{}; then you can obtain risk ratios by exponentiating coefficients [16], just like we did for odds ratios with the logit link:

```
data(anthers, package = "dobson")
anthers_sum <- aggregate(
  anthers[c("n", "y")],
  by = anthers[c("storage")], FUN = sum
)

anthers_glm_log <- glm(
  formula = cbind(y, n - y) ~ storage,
  data = anthers_sum,
  family = binomial(link = "log")
)

anthers_glm_log |>
  parameters() |>
  print_md()
```

Parameter	Log-Risk	SE	95% CI	z	p
(Intercept)	-0.80	0.12	(-1.04, -0.58)	-6.81	$< .001$
storage	0.17	0.07	(0.02, 0.31)	2.31	0.021

Now $\exp\{\beta\}$ gives us risk ratios instead of odds ratios:

```
anthers_glm_log |>
  parameters(exponentiate = TRUE) |>
  print_md()
```

---

[16] or linear combinations of coefficients, depending on what covariate patterns you are contrasting

Parameter	Risk Ratio	SE	95% CI	z	p
(Intercept)	0.45	0.05	(0.35, 0.56)	-6.81	< .001
storage	1.18	0.09	(1.03, 1.36)	2.31	0.021

Let's compare this model with a logistic model:

```r
anthers_glm_logit <- glm(
  formula = cbind(y, n - y) ~ storage,
  data = anthers_sum,
  family = binomial(link = "logit")
)

anthers_glm_logit |>
  parameters(exponentiate = TRUE) |>
  print_md()
```

Parameter	Odds Ratio	SE	95% CI	z	p
(Intercept)	0.76	0.20	(0.45, 1.27)	-1.05	0.296
storage	1.49	0.26	(1.06, 2.10)	2.29	0.022

[to add: fitted plots on each outcome scale]

When I try to use `link ="log"` in practice, I often get errors about not finding good starting values for the estimation procedure. This is likely because the model is producing fitted probabilities greater than 1.

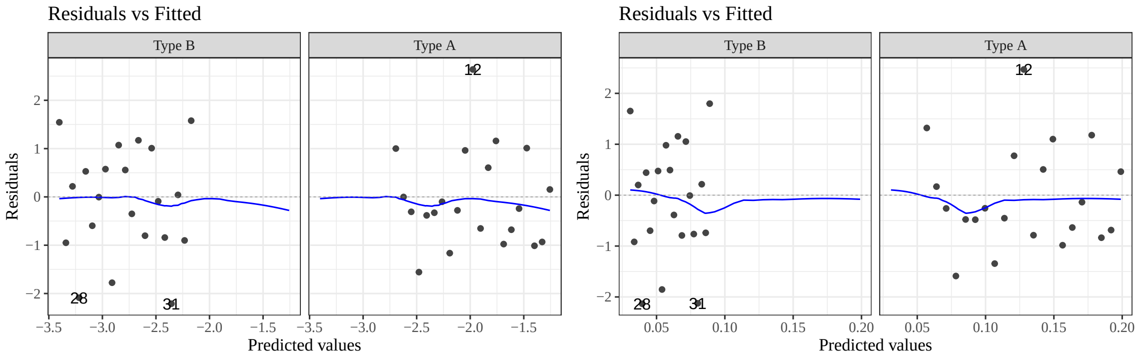
When this happens, you can try to fit Poisson regression models instead (we will see those soon!). But then the outcome distribution isn't quite right, and you won't get warnings about fitted probabilities greater than 1. In my opinion, the Poisson model for binary outcomes is confusing and not very appealing.

10.0.4 WCGS: link functions

```r
wcgs_glm_logit_link <- chd_grouped_data |>
  mutate(type = relevel(dibpat, ref = "Type B")) |>
  glm(
    "formula" = cbind(x, `n - x`) ~ dibpat * age,
    "data" = _,
    "family" = binomial(link = "logit")
  )

wcgs_glm_identity_link <-
  chd_grouped_data |>
  mutate(type = relevel(dibpat, ref = "Type B")) |>
  glm(
    "formula" = cbind(x, `n - x`) ~ dibpat * age,
    "data" = _,
    "family" = binomial(link = "identity")
  )
wcgs_glm_identity_link |>
  coef() |>
  pander()
```

(Intercept)	dibpatType A	age	dibpatType A:age
-0.08257	-0.1374	0.002906	0.004194

```
library(ggfortify)
wcgs_glm_logit_link |> autoplot(which = c(1), ncol = 1) + facet_wrap(~dibpat)
wcgs_glm_identity_link |> autoplot(which = c(1), ncol = 1) + facet_wrap(~dibpat)
```

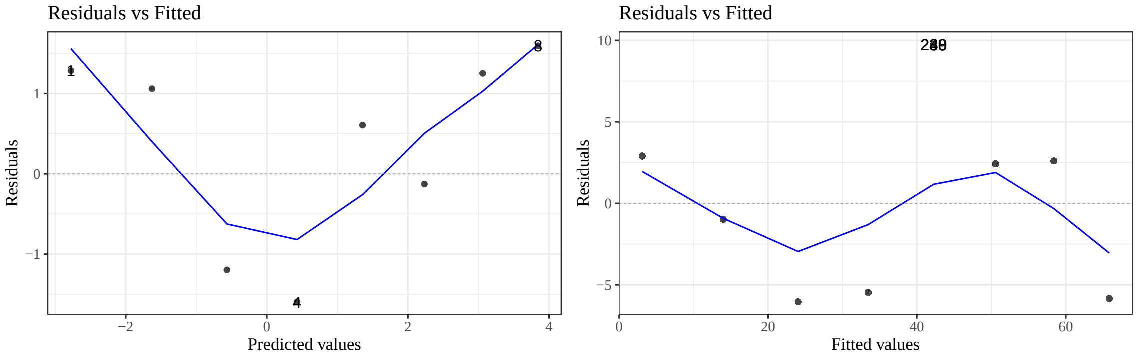


(a) Logistic link

(b) Identity link

Figure 21: Residuals vs Fitted plot for `wcgs` models

```
beetles_lm <-
  beetles_long |>
  lm(formula = died ~ dose)

beetles_glm_grouped <- beetles |>
  glm(formula = cbind(died, survived) ~ dose, family = "binomial")


beetles <-
  beetles |> mutate(
    resid_logit = beetles_glm_grouped |> resid(type = "response")
  )
beetles_glm_grouped |> autoplot(which = c(1), ncol = 1)
beetles_lm |> autoplot(which = c(1), ncol = 1)
```



(a) Logistic link

(b) Identity link

Figure 22: Residuals vs Fitted plot for `BeetleMortality` models

10.0.5 Quasibinomial

See Hua Zhou[17]'s lecture notes[18]

11 Further reading

- Hosmer et al. (2013) is a classic textbook on logistic regression

Exercises

Exercise 11.1 (Choosing a link function for binary outcomes)**.** (adapted from Dunn and Smyth (2018), Chapter 3)
Two researchers are modeling the probability $\pi(x)$ that a patient experiences a side effect, as a function of dose $x > 0$:

- Researcher A uses the **logit** link: $\text{logit}(\pi) = \beta_0 + \beta_1 x$
- Researcher B uses the **log** link: $\log\{\pi\} = \beta_0 + \beta_1 x$

(a) For each model, write $\pi(x)$ as an explicit function of x.
(b) For the log-link model (Researcher B), what constraint on the parameters ensures $\pi(x) \leq 1$ for all $x > 0$?
(c) Which link is more commonly used for binary outcomes? Give one practical advantage of that link.

Solution

Solution. **(a)**
Logit link (Researcher A):

$$\pi(x) = \frac{e^{\beta_0+\beta_1 x}}{1+e^{\beta_0+\beta_1 x}} = \text{expit}\{\beta_0 + \beta_1 x\}$$

This is always in $(0,1)$, regardless of the values of β_0, β_1, or x.
Log link (Researcher B):

$$\pi(x) = e^{\beta_0+\beta_1 x}$$

This is always positive, but may exceed 1.
(b)
For the log-link model, $\pi(x) \leq 1$ requires $e^{\beta_0+\beta_1 x} \leq 1$.
Since the exponential function is increasing, this is equivalent to

$$\beta_0 + \beta_1 x \leq 0 \qquad \text{for all } x > 0.$$

Because this must hold for all positive x, a positive slope $\beta_1 > 0$ is not possible on this unbounded domain: for sufficiently large x, we would have $\beta_0 + \beta_1 x > 0$. Thus we need $\beta_1 \leq 0$. Also, to keep $\beta_0 + \beta_1 x \leq 0$ for x arbitrarily close to 0, we need $\beta_0 \leq 0$. So the parameter constraint is $\beta_0 \leq 0$ and $\beta_1 \leq 0$.
(c)
The **logit link** is more commonly used for binary outcomes.
One practical advantage: the logit link **automatically constrains** $\pi(x) \in (0,1)$ for any real values of β_0, β_1, and x, eliminating the risk of predicted probabilities outside $[0,1]$. Additionally, the logit link yields odds ratios as the natural measure of association, which are widely used in epidemiology (see Vittinghoff et al. (2012, chap. 5)).

---

[17] https://hua-zhou.github.io/

[18] https://ucla-biostat-200c-2020spring.github.io/slides/04-binomial/binomial.html#:~:text=0.05%20%27.%27%200.1%20%27%20%27%201-,Quasi%2Dbinomial,-Another%20way%20to

Summary of definitions and results

Odds and log-odds

Odds

$$\omega \overset{\text{def}}{=} \frac{\Pr(A)}{\Pr(\neg A)}$$

Conditional odds

$$\omega(A|B) \overset{\text{def}}{=} \frac{\Pr(A|B)}{\Pr(\neg A|B)}$$

Odds function

$$\text{odds}\{\pi\} \overset{\text{def}}{=} \frac{\pi}{1-\pi}$$

Probability to odds

$$\omega = \frac{\pi}{1-\pi}$$

Odds function equals odds

$$\omega = \text{odds}\{\pi\}$$

Simplified odds expressions

$$\text{odds}\{\pi\} = \frac{1}{\pi^{-1}-1} = \left(\pi^{-1}-1\right)^{-1}$$

Odds of a non-event

$$\omega(\neg A) = \frac{1-\pi}{\pi} = \pi^{-1} - 1$$

Odds ratio

$$\theta(\omega_1, \omega_2) \overset{\text{def}}{=} \frac{\omega_1}{\omega_2}$$

OR as ratio of probability ratios

$$\begin{aligned}\theta(\omega_1, \omega_2) &= \frac{\omega_1}{\omega_2} \\ &= \frac{\left(\frac{\pi_1}{1-\pi_1}\right)}{\left(\frac{\pi_2}{1-\pi_2}\right)}\end{aligned}$$

Odds ratios are reversible

$$\theta_\omega(A|B) = \theta_\omega(B|A)$$

Conditional ORs are reversible

$$\theta_\omega(A|B,C) = \theta_\omega(B|A,C)$$

Inverse-odds and probability recovery

Odds to probability

$$\pi = \frac{\omega}{1+\omega}$$

Inverse-odds function

$$\text{invodds}\{\omega\} \overset{\text{def}}{=} \frac{\omega}{1+\omega}$$

Probability as inverse-odds

$$\pi = \text{invodds}\{\omega\}$$

Simplified inverse-odds

$$\text{invodds}\{\omega\} = \frac{1}{1+\omega^{-1}} = (1+\omega^{-1})^{-1}$$

One minus inverse-odds

$$1 - \pi = \frac{1}{1+\omega}$$

Complement of inverse-odds

$$1 + \omega = \frac{1}{1-\pi}$$

Log-odds (logit) and expit

Log-odds

$$\eta \overset{\text{def}}{=} \log\{\omega\}$$

Log-odds from probability

$$\eta = \log\left\{\frac{\pi}{1-\pi}\right\}$$

Logit function

$$\text{logit}(\pi) \overset{\text{def}}{=} \log\{\text{odds}\{\pi\}\}$$

Logit expanded

$$\text{logit}(\pi) = \log\left\{\frac{\pi}{1-\pi}\right\}$$

Log-odds equals logit

$$\eta = \text{logit}\{\pi\}$$

Odds from log-odds

$$\omega = \exp\{\eta\}$$

Probability from log-odds

$$\pi = \frac{\exp\{\eta\}}{1+\exp\{\eta\}}$$

Expit / inverse-logit function

$$\text{expit}(\eta) \overset{\text{def}}{=} \text{invodds}\{\exp\{\eta\}\}$$

Expit expressions

$$\text{expit}(\eta) = \frac{\exp\{\eta\}}{1+\exp\{\eta\}} = (1+\exp\{-\eta\})^{-1}$$

Probability as expit

$$\pi = \text{expit}\{\eta\} \tag{53}$$

Logit and expit are inverses

$$\text{logit}\{\text{expit}\{\eta\}\} = \eta \qquad \text{expit}\{\text{logit}\{\pi\}\} = \pi$$

$$\left[\pi \overset{\text{def}}{=} \Pr(Y=1|\tilde{X}=\tilde{x})\right] \underbrace{\overbrace{\underset{\xleftarrow[\frac{\omega}{1+\omega}]{}}{\xrightarrow{\frac{\pi}{1-\pi}}} \left[\omega \overset{\text{def}}{=} \text{odds}(Y=1|\tilde{X}=\tilde{x})\right] \underset{\xleftarrow[\exp\{\eta\}]{}}{\xrightarrow{\log\{\omega\}}}}^{\text{logit}(\pi)}}_{\text{expit}(\eta)} \left[\eta(\tilde{x}) \overset{\text{def}}{=} \text{log-odds}(Y=1|\tilde{X}=\tilde{x})\right]$$

Figure 23: Diagram of logistic regression link and inverse link functions

Rare events

Odds minus probability

$$\omega - \pi = \frac{\pi^2}{1-\pi}, \quad \text{where } \omega = \frac{\pi}{1-\pi}$$

Derivatives

	π	ω	η	$\tilde{x}$	$\tilde{\beta}$
π	1	$(1+\omega)^2$	$\frac{(1+\omega)^2}{\omega}$	undef	undef
ω	$(1-\pi)^2$	1	$\frac{1}{\omega}$	undef	undef
η	$\pi(1-\pi)$	ω	1	undef	undef
$\tilde{x}$	$\tilde{\beta}\pi(1-\pi)$	$\tilde{\beta}\omega$	$\tilde{\beta}$	$\mathbb{I}$	$\mathbf{0}$
$\tilde{\beta}$	$\tilde{x}\pi(1-\pi)$	$\tilde{x}\omega$	$\tilde{x}$	$\mathbf{0}$	$\mathbb{I}$

Column labels indicate the numerators of the derivatives; row labels indicate the denominators.

Log-likelihood and score function

Log-likelihood component

$$\ell_i(\pi_i) = y_i \eta_i - \log\{1 + \omega_i\}$$

Score function as sum

$$\tilde{\ell}'(\tilde{\beta}) = \sum_{i=1}^{n} \tilde{\ell}_i'(\tilde{\beta})$$

Score component

$$\ell_i'(\tilde{\beta}) = \tilde{x}_i e_i$$

Score function

$$\tilde{\ell}'(\tilde{\beta}) = \sum_{i=1}^{n} \tilde{x}_i e_i = \mathbf{X}^\top \tilde{e}$$

MLE

One-sample MLE for odds

$$\hat{\omega} = \frac{x}{n-x}$$

Odds ratios in logistic regression

General OR formula

$$\theta_\omega(\tilde{x}, \tilde{x}^*) = \exp\{\eta(\tilde{x}) - \eta(\tilde{x}^*)\}$$

Difference in log-odds

$$\Delta\eta \overset{\text{def}}{=} \eta(\tilde{x}) - \eta(\tilde{x}^*)$$

OR in terms of $\Delta\eta$

$$\theta_\omega(\tilde{x}, \tilde{x}^*) = \exp\{\Delta\eta\}$$

$\Delta\eta$ from covariates

$$\Delta\eta = (\tilde{x} - \tilde{x}^*) \cdot \tilde{\beta}$$

Difference in covariate patterns

$$\Delta\tilde{x} \overset{\text{def}}{=} \tilde{x} - \tilde{x}^*$$

$\Delta\eta$ from $\Delta\tilde{x}$

$$\Delta\eta = \Delta\tilde{x} \cdot \tilde{\beta}$$

OR in terms of $\Delta\tilde{x}$

$$\theta_\omega(\tilde{x}, \tilde{x}^*) = \exp\Big\{(\Delta\tilde{x}) \cdot \tilde{\beta}\Big\}$$

Log OR equals $\Delta\eta$

$$\log\{\theta_\omega(\tilde{x}, \tilde{x}^*)\} = \Delta\eta$$

Inference for log-odds and odds ratios

Estimated SE of log-odds

$$\begin{aligned}\widehat{\text{Var}}(\hat{\eta}(\tilde{x})) &= \tilde{x}^\top \hat{\Sigma} \tilde{x} \\ \widehat{\text{SE}}(\hat{\eta}(\tilde{x})) &= \sqrt{\tilde{x}^\top \hat{\Sigma} \tilde{x}}\end{aligned}$$

Estimated SE of $\Delta\hat{\eta}$

$$\begin{aligned}\widehat{\text{Var}}(\Delta\hat{\eta}) &= \Delta\tilde{x}^\top \hat{\Sigma}(\Delta\tilde{x}) \\ \widehat{\text{SE}}(\Delta\hat{\eta}) &= \sqrt{\Delta\tilde{x}^\top \hat{\Sigma}(\Delta\tilde{x})}\end{aligned}$$

Comparing probabilities

Risk difference

$$\delta(\pi_1, \pi_2) \stackrel{\text{def}}{=} \pi_1 - \pi_2$$

Risk ratio

$$\rho(\pi_1, \pi_2) \stackrel{\text{def}}{=} \frac{\pi_1}{\pi_2}$$

Relative risk difference

$$\xi(\pi_1, \pi_2) \stackrel{\text{def}}{=} \frac{\delta(\pi_1, \pi_2)}{\pi_2}$$

RRD equals RR minus 1

$$\xi(\pi_1, \pi_2) = \rho(\pi_1, \pi_2) - 1$$

Logistic regression model

Logistic regression

$$Y_i|\tilde{X}_i \ \sim_{\perp\!\!\!\perp}\ \text{Ber}(\pi(\tilde{X}_i)), \qquad \text{logit}\{\pi(\tilde{x})\} = \tilde{x}^\top \tilde{\beta}$$

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