Linear (Gaussian) Models

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
```

```r
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
```

Here are some R settings I use in this document:

```r
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
include_reference_lines <- FALSE
```

Note

This content is adapted from:

- Dobson and Barnett (2018), Chapters 2-6
- Dunn and Smyth (2018), Chapters 2-3
- Vittinghoff et al. (2012), Chapter 4

There are numerous textbooks specifically for linear regression, including:

- Kutner et al. (2005): used for UCLA Biostatistics MS level linear models class
- Chatterjee and Hadi (2015): used for Stanford MS-level linear models class
- Seber and Lee (2012): used for UCLA Biostatistics PhD level linear models class and UC Davis STA 108.
- Kleinbaum et al. (2014): same first author as Kleinbaum and Klein (2010) and Kleinbaum and Klein (2012)
- *Linear Models with R* (Faraway 2025)
- *Applied Linear Regression* by Sanford Weisberg (Weisberg 2005)

For more recommendations, see the discussion on Reddit[a].

- see also https://web.stanford.edu/class/stats191 [1]

[a] https://www.reddit.com/r/statistics/comments/qwgctl/q_books_on_applied_linear_modelsregression_for/

1 Overview

1.1 Why this course includes linear regression

- This course is about *generalized linear models* (for non-Gaussian outcomes)
- UC Davis STA 108 ("Applied Statistical Methods: Regression Analysis") is a prerequisite for this course, so everyone here should have some understanding of linear regression already.
- We will review linear regression to:
- make sure everyone is caught up
- provide an epidemiological perspective on model interpretation.

1.2 Chapter overview

- Section 2: how to interpret linear regression models
- Section 3: how to estimate linear regression models
- Section 4: how to quantify uncertainty about our estimates
- Section 6.3: how to tell if your model is insufficiently complex

2 Understanding Gaussian Linear Regression Models

2.1 Motivating example: birthweights and gestational age

Suppose we want to learn about the distributions of birthweights (*outcome* Y) for (human) babies born at different gestational ages (*covariate* A) and with different chromosomal sexes (*covariate* S) (Dobson and Barnett (2018) Example 2.2.2).

2.2 Dobson `birthweight` data

2.2.1 Data as table

2.2.2 Reshape data for graphing

2.2.3 Data as graph

```
plot1 <- bw |>
  ggplot(aes(
    x = age,
    y = weight,
    shape = sex,
    col = sex
  )) +
  theme_bw() +
  xlab("Gestational age (weeks)") +
  ylab("Birthweight (grams)") +
  theme(legend.position = "bottom") +
  # expand_limits(y = 0, x = 0) +
  geom_point(alpha = .7)
print(plot1 + facet_wrap(~sex))
```

[1] the current version of the first regression course I ever took

Table 1: `birthweight` data (Dobson and Barnett (2018) Example 2.2.2)

```
library(dobson)
data("birthweight", package = "dobson")
birthweight
#> # A tibble: 12 x 4
#>    `boys gestational age` `boys weight` `girls gestational age` `girls weight`
#>                    <dbl>         <dbl>                   <dbl>          <dbl>
#>  1                     40          2968                      40           3317
#>  2                     38          2795                      36           2729
#>  3                     40          3163                      40           2935
#>  4                     35          2925                      38           2754
#>  5                     36          2625                      42           3210
#>  6                     37          2847                      39           2817
#>  7                     41          3292                      40           3126
#>  8                     40          3473                      37           2539
#>  9                     37          2628                      36           2412
#> 10                     38          3176                      38           2991
#> 11                     40          3421                      39           2875
#> 12                     38          2975                      40           3231
```

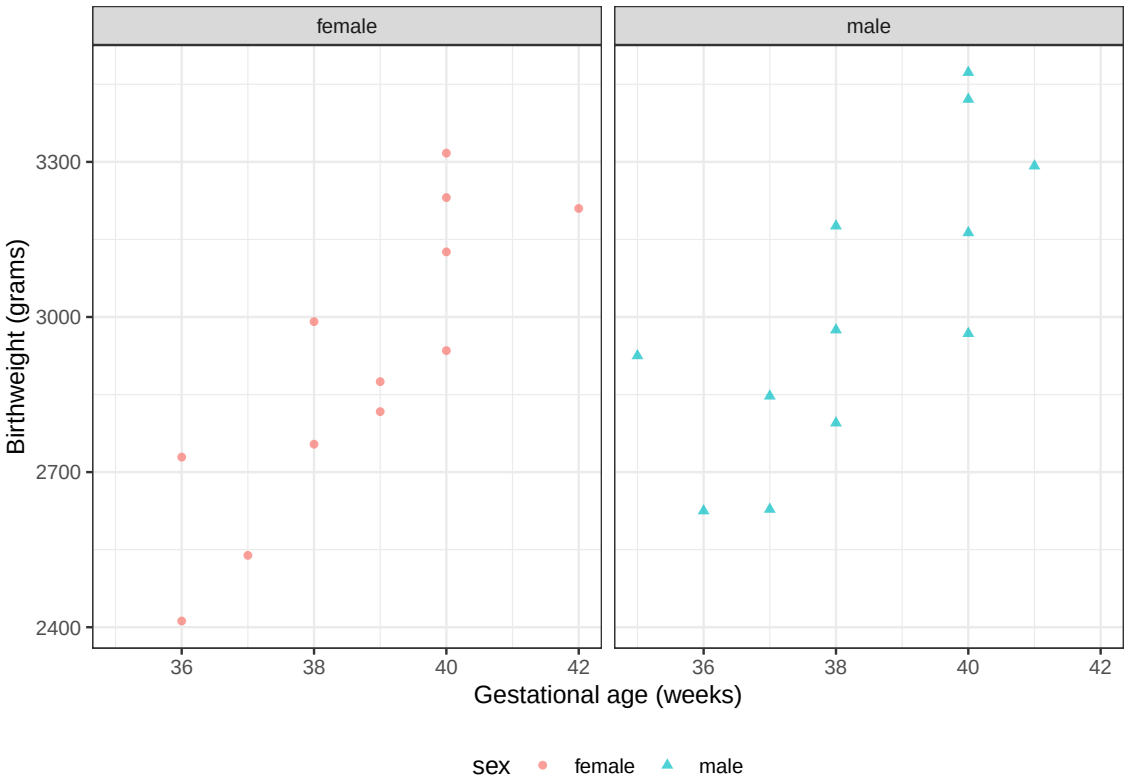


Figure 1: `birthweight` data (Dobson and Barnett (2018) Example 2.2.2)

2.2.4 Data notation

Let's define some notation to represent this data:

- Y: birthweight (measured in grams)
- S: chromosomal sex: "male" (XY) or "female" (XX)

Table 2: `birthweight` data reshaped

```
library(tidyverse)
bw <-
  birthweight |>
  pivot_longer(
    cols = everything(),
    names_to = c("sex", ".value"),
    names_sep = "s "
  ) |>
  rename(age = `gestational age`) |>
  mutate(
    id = row_number(),
    sex = sex |>
      case_match(
        "boy" ~ "male",
        "girl" ~ "female"
      ) |>
      factor(levels = c("female", "male")),
    male = sex == "male",
    female = sex == "female"
  )

bw
#> # A tibble: 24 x 6
#>    sex      age weight    id male  female
#>    <fct>  <dbl>  <dbl> <int> <lgl> <lgl>
#>  1 male      40   2968     1 TRUE  FALSE
#>  2 female    40   3317     2 FALSE TRUE
#>  3 male      38   2795     3 TRUE  FALSE
#>  4 female    36   2729     4 FALSE TRUE
#>  5 male      40   3163     5 TRUE  FALSE
#>  6 female    40   2935     6 FALSE TRUE
#>  7 male      35   2925     7 TRUE  FALSE
#>  8 female    38   2754     8 FALSE TRUE
#>  9 male      36   2625     9 TRUE  FALSE
#> 10 female    42   3210    10 FALSE TRUE
#> # i 14 more rows
```

- M: indicator variable for $S =$ "male"[2]
- $M = 0$ if $S =$ "female"
- $M = 1$ if $S =$ "male"
- F: indicator variable for $S =$ "female"[3]
- $F = 1$ if $S =$ "female"
- $F = 0$ if $S =$ "male"
- A: estimated gestational age at birth (measured in weeks).

Female is the **reference level** for the categorical variable S (chromosomal sex) and corresponding indicator variable M . The choice of a reference level is arbitrary and does not limit what we can do with the resulting model; it only makes it more computationally convenient to make inferences about comparisons involving that reference group.

M and F are called **dummy variables**; together, they are a numeric representation of the categorical variable S. Dummy variables with values 0 and 1 are also called **indicator variables**. There are other ways to construct dummy variables, such as using the values -1 and 1 (see Dobson and Barnett (2018) §2.4 for details).

2.3 Parallel lines regression

(c.f. Dunn and Smyth (2018) §2.10.3[4])

We don't have enough data to model the distribution of birth weight separately for each combination of gestational age and sex, so let's instead consider a (relatively) simple model for how that distribution varies with gestational age and sex:

$$\begin{aligned} Y|M, A &\sim_{\text{ciid}} N(\mu(M, A), \sigma^2) \\ \mu(m, a) &= \beta_0 + \beta_M m + \beta_A a \end{aligned} \tag{1}$$

Table 3 shows the parameter estimates from R. Figure 2 shows the estimated model, superimposed on the data.

```
bw_lm1 <- lm(
  formula = weight ~ sex + age,
  data = bw
)

library(parameters)
bw_lm1 |>
  parameters::parameters() |>
  parameters::print_md(
    include_reference = include_reference_lines,
    select = "{estimate}"
  )
```

Table 3: Regression parameter estimates for Model 1 of `birthweight` data

Parameter	Coefficient
(Intercept)	-1773.32
sex (male)	163.04
age	120.89

[2] M is implicitly a deterministic function of S
[3] F is implicitly a deterministic function of S
[4] https://link.springer.com/chapter/10.1007/978-1-4419-0118-7_2#Sec31

```r
bw <-
  bw |>
  mutate(`E[Y|X=x]` = fitted(bw_lm1)) |>
  arrange(sex, age)

plot2 <-
  plot1 %+% bw +
  geom_line(aes(y = `E[Y|X=x]`))

print(plot2)
```

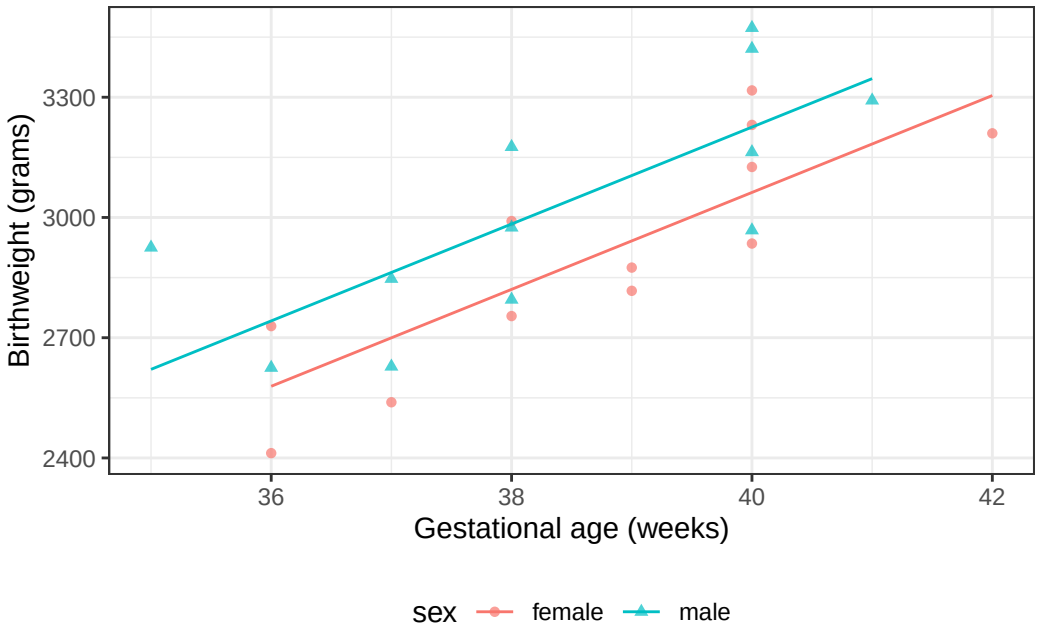


Figure 2: Graph of Model 1 for `birthweight` data

2.3.1 Model assumptions and predictions

To learn what this model is assuming, let's plug in a few values.

Exercise 2.1. What's the mean birthweight for a female born at 36 weeks?

Table 4: Estimated coefficients for model 1

Parameter	Coefficient
(Intercept)	-1773.32
sex (male)	163.04
age	120.89

Solution.

Table 5: Estimated coefficients for model 1

Parameter	Coefficient
(Intercept)	-1773.32
sex (male)	163.04
age	120.89

```
pred_female <- coef(bw_lm1)["(Intercept)"] + coef(bw_lm1)["age"] * 36
## or using built-in prediction:
pred_female_alt <- predict(bw_lm1, newdata = tibble(sex = "female", age = 36))
```

$$\begin{aligned} E[Y|M=0, A=36] &= \beta_0 + (\beta_M \cdot 0) + (\beta_A \cdot 36) \\ &= -1773.321839 + (163.039303 \cdot 0) + (120.894327 \cdot 36) \\ &= 2578.873934 \end{aligned}$$

Exercise 2.2. What's the mean birthweight for a male born at 36 weeks?

Table 6: Estimated coefficients for model 1

Parameter	Coefficient
(Intercept)	-1773.32
sex (male)	163.04
age	120.89

Solution.

Table 7: Estimated coefficients for model 1

Parameter	Coefficient
(Intercept)	-1773.32
sex (male)	163.04
age	120.89

```
pred_male <-
  coef(bw_lm1)["(Intercept)"] +
  coef(bw_lm1)["sexmale"] +
  coef(bw_lm1)["age"] * 36
```

$$\begin{aligned} E[Y|M=1, A=36] &= \beta_0 + \beta_M \cdot 1 + \beta_A \cdot 36 \\ &= 2741.913237 \end{aligned}$$

Exercise 2.3. What's the difference in mean birthweights between males born at 36 weeks and females born at 36 weeks?

```
coef(bw_lm1)
#> (Intercept)     sexmale         age
#>   -1773.322     163.039     120.894
```

Solution.

$$\begin{aligned}
&E[Y|M=1, A=36] - E[Y|M=0, A=36] \\
&= 2741.913237 - 2578.873934 \\
&= 163.039303
\end{aligned}$$

Shortcut:

$$\begin{aligned}
&E[Y|M=1, A=36] - E[Y|M=0, A=36] \\
&= (\beta_0 + \beta_M \cdot 1 + \beta_A \cdot 36) - (\beta_0 + \beta_M \cdot 0 + \beta_A \cdot 36) \\
&= \beta_M \\
&= 163.039303
\end{aligned}$$

Age cancels out in this difference. In other words, according to this model, the difference between females and males with the same gestational age is the same for every age.

This characteristic is an assumption of the model specified by Equation 1. It's hardwired into the parametric model structure, even before we estimated values for those parameters.

2.3.2 Coefficient Interpretation

Recall Model 1:

$$E[Y|M=m, A=a] = \mu(m,a) = \beta_0 + \beta_M m + \beta_A a$$

Slope (of the mean with respect to age) for males:

$$\begin{aligned}
\frac{d}{da}\mu(1,a) &= \frac{d}{da}(\beta_0 + \beta_M 1 + \beta_A a) \\
&= \left(\frac{d}{da}\beta_0 + \frac{d}{da}\beta_M 1 + \frac{d}{da}\beta_A a\right) \\
&= (0 + 0 + \beta_A) \\
&= \beta_A
\end{aligned}$$

Slope for females:

$$\begin{aligned}
\frac{d}{da}\mu(0,a) &= \frac{d}{da}(\beta_0 + \beta_M 0 + \beta_A a) \\
&= \left(\frac{d}{da}\beta_0 + \frac{d}{da}\beta_M 0 + \frac{d}{da}\beta_A a\right) \\
&= (0 + 0 + \beta_A) \\
&= \beta_A
\end{aligned}$$

Exercise 2.4. What is the interpretation of β_A in Model 1?

Solution.

$$\begin{aligned}
\frac{d}{da}\mu(m,a) &= \frac{d}{da}(\beta_0 + \beta_M m + \beta_A a) \\
&= \left(\frac{d}{da}\beta_0 + \frac{d}{da}\beta_M m + \frac{d}{da}\beta_A a\right) \\
&= (0 + 0 + \beta_A) \\
&= \beta_A
\end{aligned}$$

Conclusion:

$$\beta_A = \frac{d}{da}\mu(m,a)$$

β_A is the slope of mean birthweight with respect to gestational age, adjusting for sex.

Or we can plug in the definition of slope:

$$\beta_A = E[Y|M=m, A=a+1] - E[Y|M=m, A=a]$$

Exchangeability and consistency have not been assessed; so we are not discussing potential outcomes (causality), only observed outcomes.

Exercise 2.5. What is the interpretation of β_M in Model 1?

Solution.

More precisely written:

$$\mathrm{E}[Y|M=m, A=a] = \mu(m,a) = \begin{cases} \beta_0 + \beta_M m + \beta_A a, & \text{for } m \in \{0,1\} \\ \text{undefined}, & \text{for } m \notin \{0,1\} \end{cases}$$

The model is undefined for $m \notin \{0,1\}$, so the derivative with respect to m doesn't exist.

$$\begin{aligned} E[Y|M=1, A=a] &= \beta_0 + \beta_M 1 + \beta_A a \\ &= \beta_0 + \beta_M + \beta_A a \\ E[Y|M=0, A=a] &= \beta_0 + \beta_M 0 + \beta_A a \\ &= \beta_0 + \beta_A a \end{aligned}$$

So:

$$\begin{aligned} E[Y|M=1, A=a] - E[Y|M=0, A=a] &= (\beta_0 + \beta_M + \beta_A a) - (\beta_0 + \beta_A a) \\ &= \beta_M \end{aligned}$$

Therefore:

$$\begin{aligned} \beta_M &= E[Y|M=1, A=a] - E[Y|M=0, A=a] \\ &= \mu(1,a) - \mu(0,a) \end{aligned}$$

In words: β_M is the difference in mean birthweight between males and females adjusting for age.

Exercise 2.6. $\beta_0 = ?$

Solution.

$$\begin{aligned} \mathrm{E}[Y|M=0, A=0] &= \mu(0,0) \\ &= \beta_0 + \beta_M 0 + \beta_A 0 \\ &= \beta_0 \\ \beta_0 &= \mathrm{E}[Y|M=0, A=0] = \mu(0,0) \end{aligned}$$

β_0 is the mean birthweight for a female with gestational age 0 weeks.

Table 8: `hers` data

```
hers |> head()
#> # A tibble: 6 x 37
#>   HT              age raceth  nonwhite smoking drinkany exercise physact globrat
#>   <fct>         <dbl> <dbl+l> <dbl+lb> <dbl+l> <dbl+lb> <dbl+lb> <dbl+l> <dbl+l>
#> 1 placebo          70 2 [Afr~ 1 [yes]  0 [no]  0 [no]   0 [no]   5 [muc~ 3 [goo~
#> 2 placebo          62 2 [Afr~ 1 [yes]  0 [no]  0 [no]   0 [no]   1 [muc~ 3 [goo~
#> 3 hormone ther~    69 1 [Whi~ 0 [no]   0 [no]  0 [no]   0 [no]   3 [abo~ 3 [goo~
#> 4 placebo          64 1 [Whi~ 0 [no]   1 [yes] 1 [yes]  0 [no]   1 [muc~ 3 [goo~
#> 5 placebo          65 1 [Whi~ 0 [no]   0 [no]  0 [no]   0 [no]   2 [som~ 3 [goo~
#> 6 hormone ther~    68 2 [Afr~ 1 [yes]  0 [no]  1 [yes]  0 [no]   3 [abo~ 3 [goo~
#> # i 28 more variables: poorfair <dbl+lbl>, medcond <dbl>, htnmeds <dbl+lbl>,
#> #   statins <fct>, diabetes <dbl+lbl>, dmpills <dbl+lbl>, insulin <dbl+lbl>,
#> #   weight <dbl>, BMI <dbl>, waist <dbl>, WHR <dbl>, glucose <dbl>,
#> #   weight1 <dbl>, BMI1 <dbl>, waist1 <dbl>, WHR1 <dbl>, glucose1 <dbl>,
#> #   tchol <dbl>, LDL <dbl>, HDL <dbl>, TG <dbl>, tchol1 <dbl>, LDL1 <dbl>,
#> #   HDL1 <dbl>, TG1 <dbl>, SBP <dbl>, DBP <dbl>, age10 <dbl>
```

2.3.3 Motivating example: `hers` data

> **Note**
>
> This section is based on Vittinghoff et al. (2012), Chapter 4.

The "heart and estrogen/progestin study" (HERS) was a clinical trial of hormone therapy for prevention of recurrent heart attacks and death among 2,763 post-menopausal women with existing coronary heart disease (CHD) (Hulley et al. 1998).

```
library(haven)
hers <- haven::read_dta(
  paste0(
    "https://regression.ucsf.edu/sites/g/files",
    "/tkssra6706/f/wysiwyg/home/data/hersdata.dta"
  )
)
```

Data as table

Data as graph

```
library(ggplot2)
hers_scatter <-
  hers |>
  ggplot(aes(
    x = BMI,
    y = LDL,
    shape = HT,
    col = HT
  )) +
  theme_bw() +
  xlab("BMI (kg/m²)") +
  ylab("LDL cholesterol (mg/dL)") +
  theme(legend.position = "bottom") +
  geom_point(alpha = .3)
print(hers_scatter + facet_wrap(~HT))
```

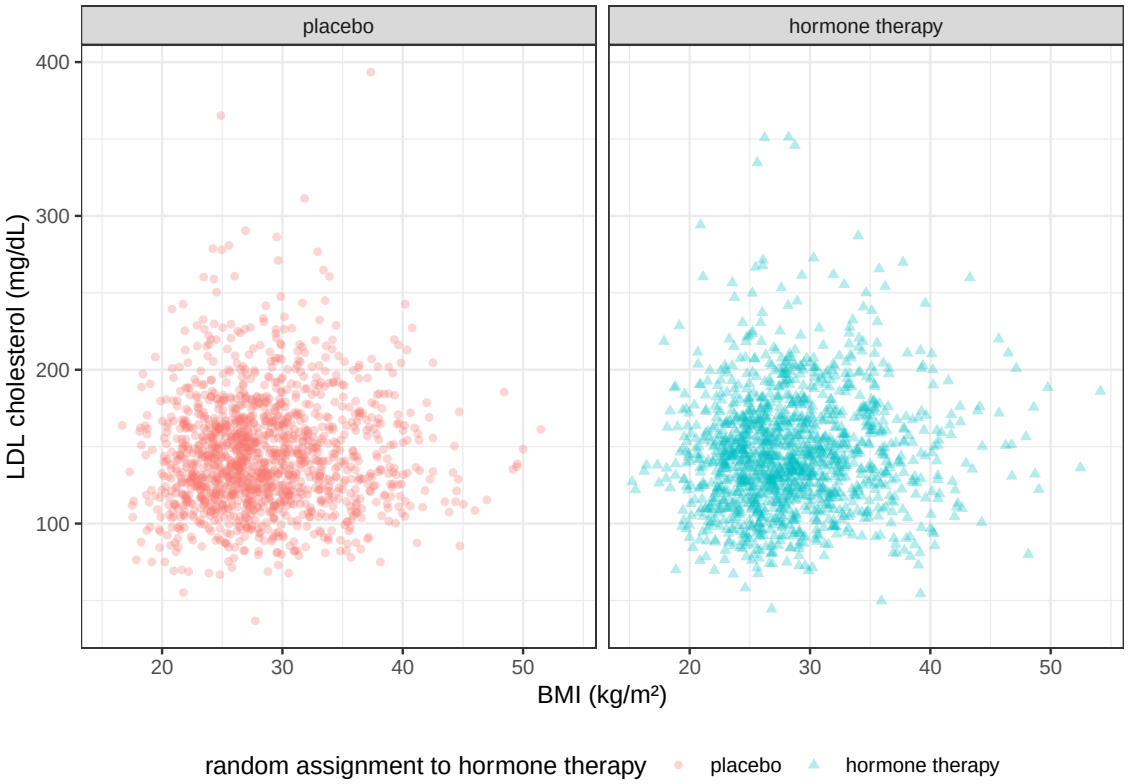


Figure 3: `hers` data (Vittinghoff et al. (2012))

Data notation

Let's define some notation to represent this data:

- Y: LDL cholesterol (mg/dL)
- T: hormone therapy treatment assignment ("placebo" or "hormone therapy")
- H: indicator variable for $T =$ "hormone therapy"
  - $H = 0$ if $T =$ "placebo"
  - $H = 1$ if $T =$ "hormone therapy"
- B: BMI (kg/m^2)
- U: statin use ("no" or "yes")
- V: indicator variable for $U =$ "yes"
  - $V = 0$ if $U =$ "no"
  - $V = 1$ if $U =$ "yes"

"Placebo" is the **reference level** for the categorical variable T, and "no" is the **reference level** for statin use U. The choice of reference level is arbitrary; it only affects the interpretation of the intercept and corresponding indicator coefficients.

2.3.4 Parallel lines regression for `hers` data

We model the distribution of LDL cholesterol as a linear function of BMI, with a separate intercept for each treatment group:

$$\begin{aligned} Y|H,B &\sim_{\text{ciid}} N(\mu(H,B),\sigma^2) \\ \mu(h,b) &= \beta_0 + \beta_H h + \beta_B b \end{aligned} \tag{2}$$

```r
library(dplyr)
hers_lm1 <- lm(
  formula = LDL ~ HT + BMI,
  data = hers,
  na.action = na.exclude
)

library(parameters)
hers_lm1 |>
  parameters::parameters() |>
  parameters::print_md(
    include_reference = include_reference_lines,
    select = "{estimate}"
  )
```

Table 9: Regression parameter estimates for Model 2

Parameter	Coefficient
(Intercept)	133.09
HT (hormone therapy)	0.21
BMI	0.41

```r
hers <-
  hers |>
  dplyr::mutate(`E[LDL|X=x]` = fitted(hers_lm1)) |>
  dplyr::arrange(HT, BMI)

hers_scatter2 <-
  hers_scatter +
  geom_line(data = hers, aes(y = `E[LDL|X=x]`))

print(hers_scatter2)
```

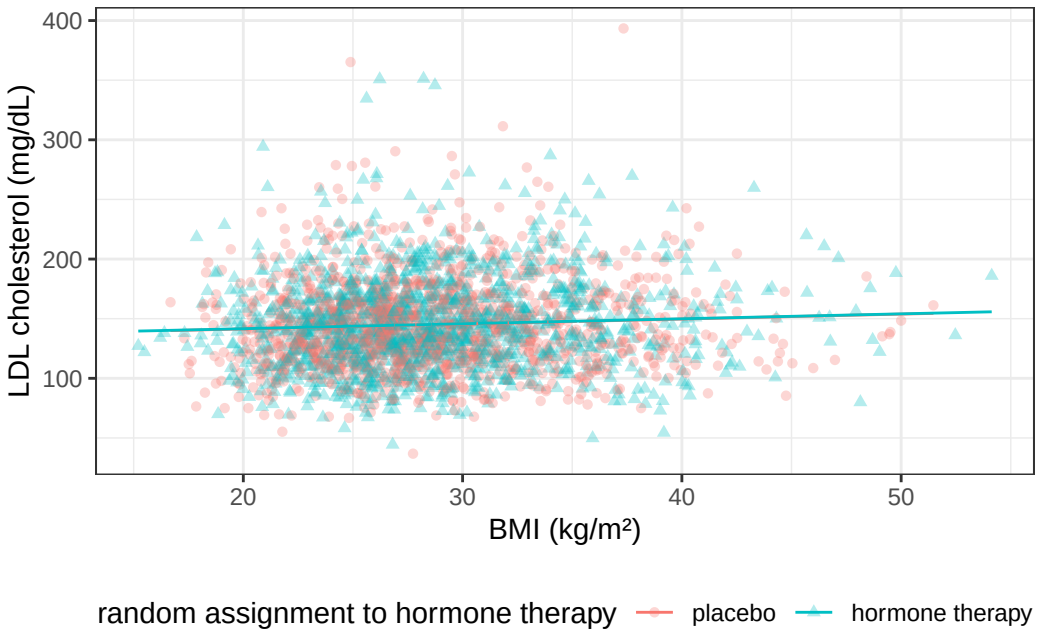


Figure 4: Graph of Model 2 for `hers` data

2.4 Interactions

What if we don't like that parallel lines assumption?

Then we need to allow an "interaction" between age A and sex S:

$$E[Y|S = s, A = a] = \beta_0 + \beta_A a + \beta_M m + \beta_{AM}(a \cdot m) \tag{3}$$

Now, the slope of mean birthweight $E[Y|A, S]$ with respect to gestational age A depends on the value of sex S.

```
bw_lm2 <- lm(weight ~ sex + age + sex:age, data = bw)
bw_lm2 |>
  parameters() |>
  parameters::print_md(
    include_reference = include_reference_lines,
    select = "{estimate}"
  )
```

Table 10: Birthweight model with interaction term

Parameter	Coefficient
(Intercept)	-2141.67
sex (male)	872.99
age	130.40
sex (male) × age	-18.42

```
bw <-
  bw |>
  mutate(
    predlm2 = predict(bw_lm2)
  ) |>
  arrange(sex, age)

plot1_interact <-
  plot1 %+% bw +
  geom_line(aes(y = predlm2))

print(plot1_interact)
```

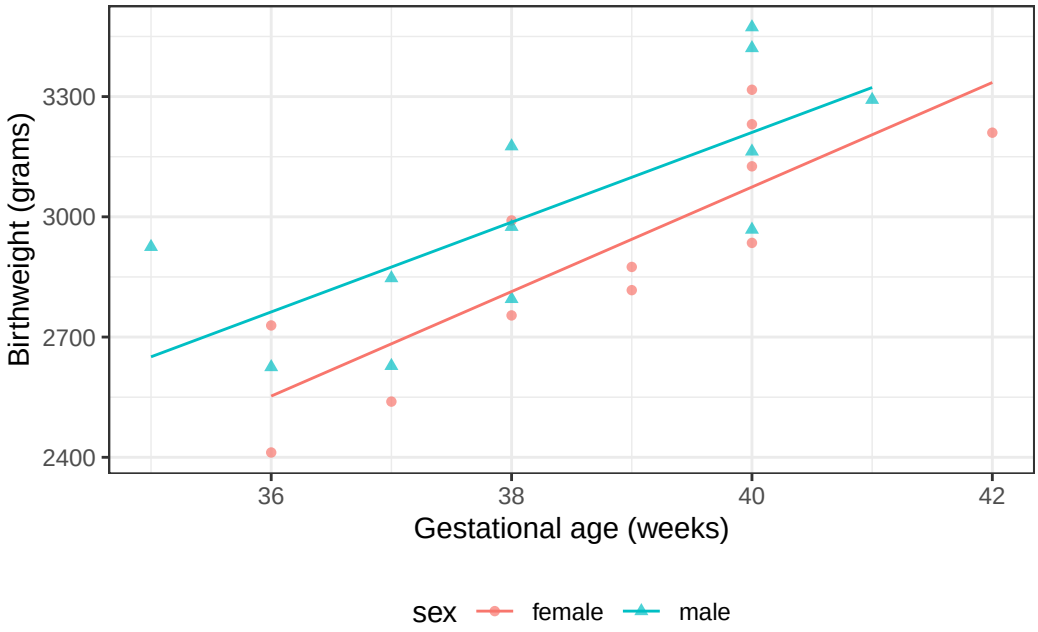


Figure 5: Birthweight model with interaction term

Now we can see that the lines aren't parallel.

Here's another way we could rewrite this model (by collecting terms involving S):

$$E[Y|M, A] = \beta_0 + \beta_M M + (\beta_A + \beta_{AM} M)A$$

If you want to understand a coefficient in a model with interactions, collect terms for the corresponding variable, and you will see which other covariates interact with the variable whose coefficient you are interested in. In this case, the association between A (age) varies between males and females (that is, by sex S). [5] So the slope of Y with respect to A depends on the value of M. According to this model, there is no such thing as "*the* slope of birthweight with respect to age". There are two slopes, one for each sex. We can only talk about "the slope of birthweight with respect to age among males" and "the slope of birthweight with respect to age among females". Then: each non-interaction slope coefficient is the difference in means per unit difference in its corresponding variable, when all interacting variables are set to 0.

To learn what this model is assuming, let's plug in a few values.

Exercise 2.7. According to this model, what's the mean birthweight for a female born at 36 weeks?

Parameter	Coefficient
(Intercept)	-2141.67
sex (male)	872.99
age	130.40
sex (male) × age	-18.42

---

[5] some call this kind of variation "interaction" or "effect modification", but "act", "effect", "modify", and "by" all suggest causality, which we are not prepared to assess here; let's try to avoid using causal terms, unless we are constructing a causal model.

Solution.

Parameter	Coefficient
(Intercept)	-2141.67
sex (male)	872.99
age	130.40
sex (male) × age	-18.42

```
pred_female <- coef(bw_lm2)["(Intercept)"] + coef(bw_lm2)["age"] * 36
```

$$E[Y|M = 0, A = 36] = \beta_0 + \beta_M \cdot 0 + \beta_A \cdot 36 + \beta_{AM} \cdot (0 * 36) = 2552.733333$$

Exercise 2.8. What's the mean birthweight for a male born at 36 weeks?

Parameter	Coefficient
(Intercept)	-2141.67
sex (male)	872.99
age	130.40
sex (male) × age	-18.42

Solution.

Parameter	Coefficient
(Intercept)	-2141.67
sex (male)	872.99
age	130.40
sex (male) × age	-18.42

```
pred_male <-
  coef(bw_lm2)["(Intercept)"] +
  coef(bw_lm2)["sexmale"] +
  coef(bw_lm2)["age"] * 36 +
  coef(bw_lm2)["sexmale:age"] * 36
```

$$\begin{aligned} E[Y|M = 1, A = 36] &= \beta_0 + \beta_M \cdot 1 + \beta_A \cdot 36 + \beta_{AM} \cdot 1 \cdot 36 \\ &= 2762.706897 \end{aligned}$$

Exercise 2.9. What's the difference in mean birthweights between males born at 36 weeks and females born at 36 weeks?

Solution.

$$\begin{aligned} &E[Y|M = 1, A = 36] - E[Y|M = 0, A = 36] \\ &= (\beta_0 + \beta_M \cdot 1 + \beta_A \cdot 36 + \beta_{AM} \cdot 1 \cdot 36) \\ &\quad - (\beta_0 + \beta_M \cdot 0 + \beta_A \cdot 36 + \beta_{AM} \cdot 0 \cdot 36) \\ &= \beta_M + \beta_{AM} \cdot 36 \\ &= 209.973563 \end{aligned}$$

Note that age now does show up in the difference: in other words, according to this model, the difference in mean birthweights between females and males with the same gestational age can vary by gestational age.

That's how the lines in the graph ended up non-parallel.

2.4.1 Coefficient Interpretation

Exercise 2.10. What is the interpretation of β_M in Model 3?

Solution.

Mean birthweight among males with gestational age 0 weeks:

$$\begin{aligned}\mu(1,0) &= \mathrm{E}[Y|M=1,A=0] \\ &= \beta_0 + \beta_M \cdot 1 + \beta_A \cdot 0 + \beta_{AM} \cdot 1 \cdot 0 \\ &= \beta_0 + \beta_M\end{aligned}$$

Mean birthweight among females with gestational age 0 weeks:

$$\begin{aligned}\mu(0,0) &= \mathrm{E}[Y|M=0,A=0] \\ &= \beta_0 + \beta_M \cdot 0 + \beta_A \cdot 0 + \beta_{AM} \cdot 0 \cdot 0 \\ &= \beta_0\end{aligned}$$

$$\begin{aligned}\beta_M &= \mu(1,0) - \mu(0,0) \\ &= \mathrm{E}[Y|M=1,A=0] - \mathrm{E}[Y|M=0,A=0]\end{aligned}$$

β_M is the difference in mean birthweight between males with gestational age 0 weeks and females with gestational age 0 weeks.

Exercise 2.11. What is the interpretation of β_{AM} in Model 3?

Solution.

Slope among males:

$$\begin{aligned}\frac{\partial}{\partial a}\mu(1,a) &= \frac{\partial}{\partial a}\left(\beta_0 + \beta_M \cdot 1 + \beta_A \cdot a + \beta_{AM} \cdot 1 \cdot a\right) \\ &= \frac{\partial}{\partial a}\left(\beta_0 + \beta_M + \beta_A \cdot a + \beta_{AM} \cdot a\right) \\ &= \beta_A + \beta_{AM}\end{aligned}$$

or

$$\begin{aligned}E[Y|1,a+1] - E[Y|1,a] =& \beta_0 + \beta_M 1 + \beta_A(a+1) + \beta_{AM}1(a+1) \\ &- (\beta_0 + \beta_M 1 + \beta_A(a) + \beta_{AM}1(a)) \\ =& \beta_A + \beta_{AM}\end{aligned}$$

Slope among females:

$$\begin{aligned}\frac{\partial}{\partial a}\mu(0,a) &= \frac{\partial}{\partial a}\left(\beta_0 + \beta_M \cdot 0 + \beta_A \cdot a + \beta_{AM} \cdot 0 \cdot a\right) \\ &= \frac{\partial}{\partial a}\left(\beta_0 + \beta_A \cdot a\right) \\ &= \beta_A\end{aligned}$$

or

$$\begin{aligned} E[Y|0,a+1] - E[Y|0,a] =& \beta_0 + \beta_M 0 + \beta_A(a+1) + \beta_{AM} 0(a+1) \\ & - (\beta_0 + \beta_M 0 + \beta_A(a) + \beta_{AM} 0(a)) \\ =& \beta_0 + \beta_A(a+1) - (\beta_0 + \beta_A(a)) \\ =& \beta_A \end{aligned}$$

Difference in slopes:

$$\begin{aligned} \frac{\partial}{\partial a}\mu(1,a) - \frac{\partial}{\partial a}\mu(0,a) &= \beta_A + \beta_{AM} - \beta_A \\ &= \beta_{AM} \end{aligned}$$

or

$$\begin{aligned} (E[Y|1,a+1] - E[Y|1,a]) - (E[Y|0,a+1] - E[Y|0,a]) &= \beta_A + \beta_{AM} - \beta_A \\ &= \beta_{AM} \end{aligned}$$

Therefore

$$\begin{aligned} \beta_{AM} =& \frac{\partial}{\partial a}\mu(1,a) - \frac{\partial}{\partial a}\mu(0,a) \\ =& (E[Y|M=1,A=a+1] - E[Y|M=1,A=a]) \\ & - (E[Y|M=0,A=a+1] - E[Y|M=0,A=a]) \end{aligned}$$

β_{AM} is the difference in slope of mean birthweight with respect to gestational age between males and females.

2.4.2 Compare coefficient interpretations

Table 11: Coefficient interpretations, by model structure

$\mu(m,a)$	$\beta_0 + \beta_M m + \beta_A a$	$\beta_0 + \beta_M m + \beta_A a + \beta_{AM} ma$
β_0	$\mu(0,0)$	$\mu(0,0)$
β_A	$\frac{\partial}{\partial a}\mu(m,a)$	$\frac{\partial}{\partial a}\mu(0,a)$
β_M	$\mu(1,a) - \mu(0,a)$	$\mu(1,0) - \mu(0,0)$
β_{AM}		$\frac{\partial}{\partial a}\mu(1,a) - \frac{\partial}{\partial a}\mu(0,a)$

In the model with an interaction term multiplying $A \times M$, the interpretation of β_A involves the reference level of M, and interpretation of β_M involves the reference level of A (Table 11).

2.4.3 Interactions in `hers` data

What if the slope of LDL with respect to BMI differs between statin users and non-users? Then we need an "interaction" between BMI B and statin use V:

$$\begin{aligned} Y|H,V,B &\sim_{\text{ciid}} N(\mu(H,V,B),\sigma^2) \\ \mu(h,v,b) &= \beta_0 + \beta_H h + \beta_V v + \beta_B b + \beta_{VB}(v \cdot b) \end{aligned} \tag{4}$$

Now the slope of mean LDL with respect to BMI B depends on statin use V:

$$\begin{aligned} \frac{\partial}{\partial b}\mu(H=h,V=0,B=b) &= \beta_B \\ \frac{\partial}{\partial b}\mu(H=h,V=1,B=b) &= \beta_B + \beta_{VB} \end{aligned}$$

```r
hers_lm2 <- lm(
  LDL ~ HT + BMI + statins + BMI:statins,
  data = hers,
  na.action = na.exclude
)

hers_lm2 |>
  parameters() |>
  parameters::print_md(
    include_reference = include_reference_lines,
    select = "{estimate}"
  )
```

Table 12: HERS interaction model

Parameter	Coefficient
(Intercept)	132.86
HT (hormone therapy)	-0.10
BMI	0.64
statins (yes)	3.86
BMI × statins (yes)	-0.72

```r
hers_scatter_statin <-
  hers |>
  ggplot(aes(
    x = BMI,
    y = LDL,
    shape = statins,
    col = statins
  )) +
  theme_bw() +
  xlab("BMI (kg/m²)") +
  ylab("LDL cholesterol (mg/dL)") +
  theme(legend.position = "bottom") +
  geom_point(alpha = .3)

hers <-
  hers |>
  dplyr::mutate(
    predlm2_hers = predict(hers_lm2)
  ) |>
  dplyr::arrange(statins, BMI)

hers_scatter_statin3 <-
  hers_scatter_statin +
  geom_line(data = hers, aes(y = predlm2_hers))

print(hers_scatter_statin3)
```

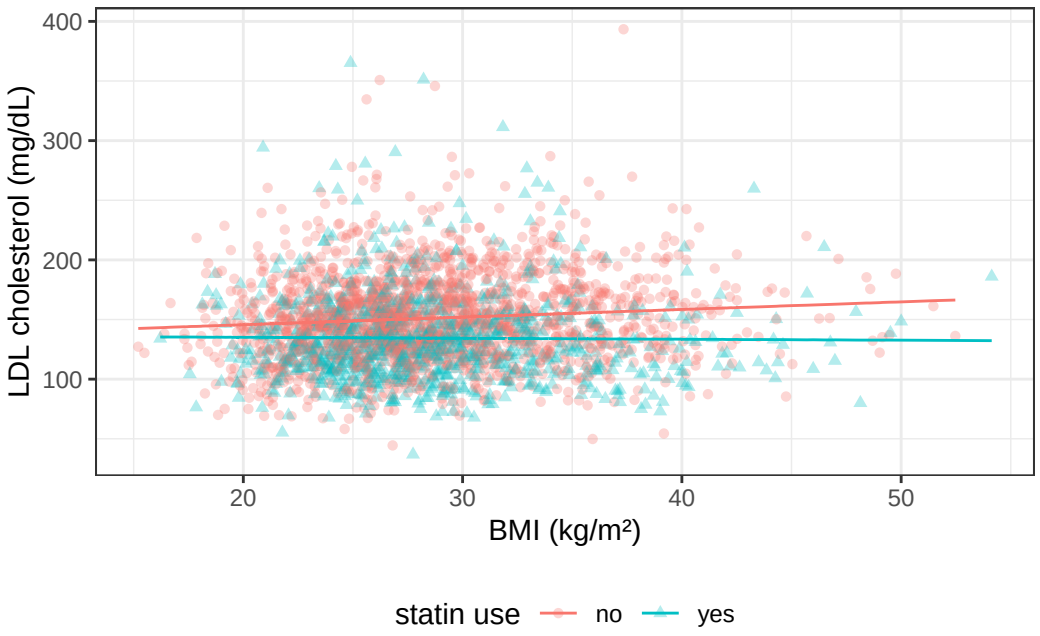


Figure 6: HERS interaction model fit (by statin use)

Graph of Model 4 for `hers` data

2.5 Stratified regression

We could re-write the interaction model as a stratified model, with a slope and intercept for each sex:

$$\mathrm{E}[Y|A=a,S=s] = \beta_M m + \beta_{AM}(a \cdot m) + \beta_F f + \beta_{AF}(a \cdot f) \tag{5}$$

Compare this stratified model (Equation 5) with our interaction model, Equation 3:

$$\mathrm{E}[Y|A=a,S=s] = \beta_0 + \beta_A a + \beta_M m + \beta_{AM}(a \cdot m)$$

In the stratified model, the intercept term β_0 has been relabeled as β_F.

```
bw_lm2 <- lm(weight ~ sex + age + sex:age, data = bw)
bw_lm2 |>
  parameters() |>
  print_md(
    include_reference = include_reference_lines,
    select = "{estimate}"
  )
```

Table 13: Birthweight model with interaction term

Parameter	Coefficient
(Intercept)	-2141.67
sex (male)	872.99
age	130.40
sex (male) × age	-18.42

```r
bw_lm_strat <-
  bw |>
  lm(
    formula = weight ~ sex + sex:age - 1,
    data = _
  )

bw_lm_strat |>
  parameters() |>
  print_md(
    select = "{estimate}"
  )
```

Table 14: Birthweight model - stratified betas

Parameter	Coefficient
sex (female)	-2141.67
sex (male)	-1268.67
sex (female) × age	130.40
sex (male) × age	111.98

2.6 Curved-line regression

If we transform some of our covariates (Xs) and plot the resulting model on the original covariate scale, we end up with curved regression lines:

```r
bw_lm3 <- lm(weight ~ sex:log(age) - 1, data = bw)

ggbw <-
  bw |>
  ggplot(
    aes(x = age, y = weight)
  ) +
  geom_point() +
  xlab("Gestational Age (weeks)") +
  ylab("Birth Weight (g)")

ggbw2 <- ggbw +
  stat_smooth(
    method = "lm",
    formula = y ~ log(x),
    geom = "smooth"
  ) +
  xlab("Gestational Age (weeks)") +
  ylab("Birth Weight (g)")


ggbw2 |> print()
```

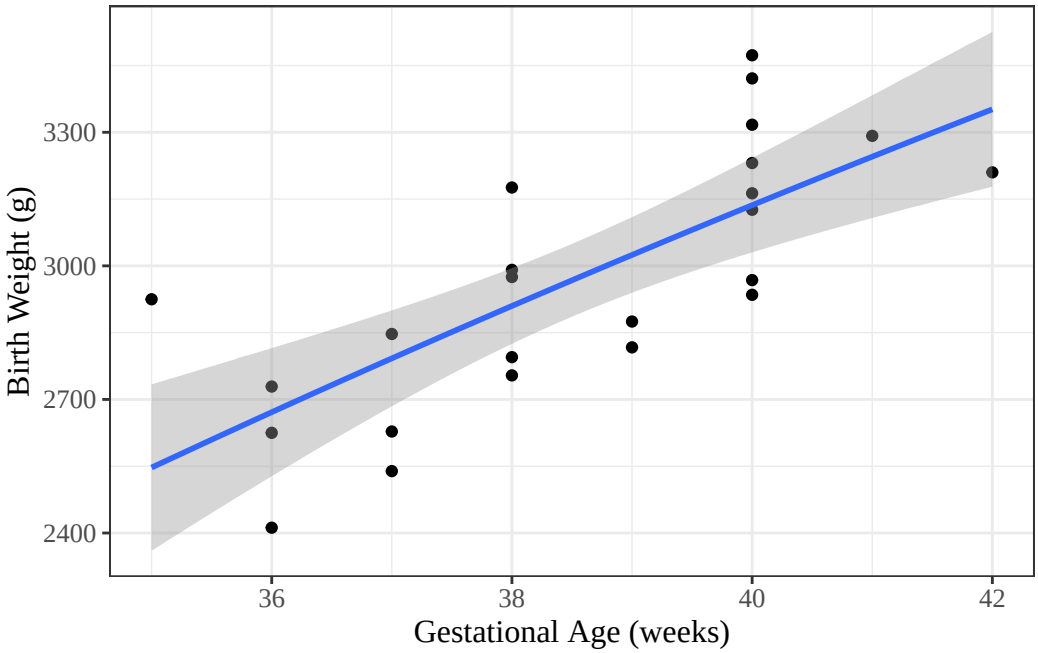


Figure 7: `birthweight` model with `age` entering on log scale

Below is an example with a slightly more obvious curve.

```
library(palmerpenguins)

ggpenguins <-
  palmerpenguins::penguins |>
  dplyr::filter(species == "Adelie") |>
  ggplot(
    aes(x = bill_length_mm, y = body_mass_g)
  ) +
  geom_point() +
  xlab("Bill length (mm)") +
  ylab("Body mass (g)")

ggpenguins2 <- ggpenguins +
  stat_smooth(
    method = "lm",
    formula = y ~ log(x),
    geom = "smooth"
  ) +
  xlab("Bill length (mm)") +
  ylab("Body mass (g)")


ggpenguins2 |> print()
```

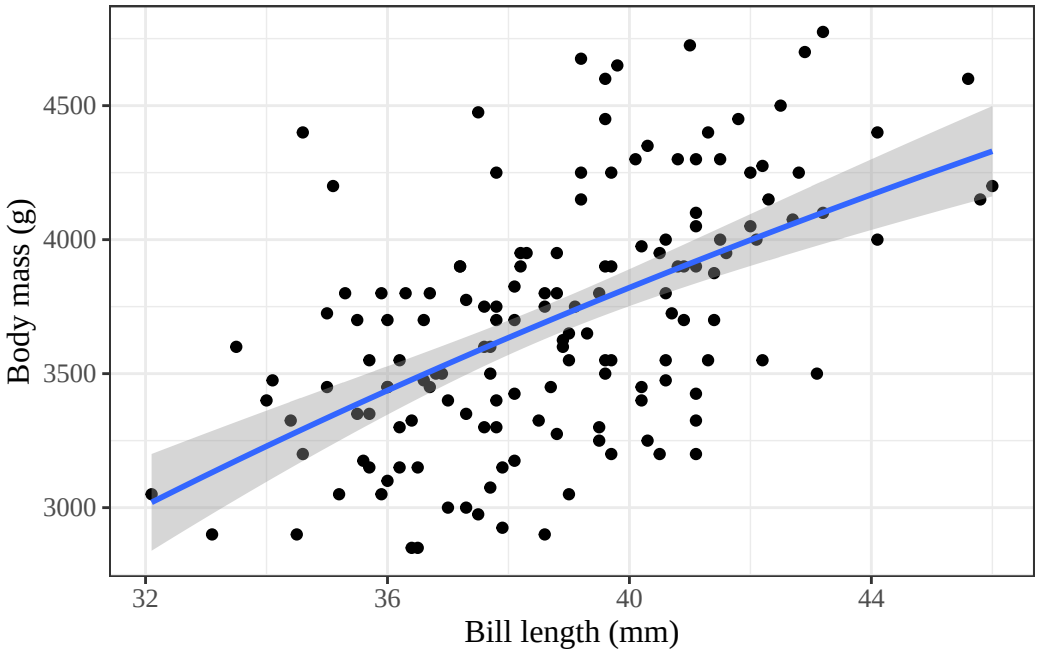


Figure 8: `palmerpenguins` model with `bill_length` entering on log scale

2.7 Rescaling

Centering covariates (subtracting a constant from them) can make coefficient interpretations more meaningful, particularly for the intercept and main effect terms in models with interactions.

2.7.1 Rescale age

For example, the intercept β_0 in our interaction model represents the mean birthweight for females at age = 0 weeks, which is not a biologically plausible scenario. If we center age at 36 weeks instead, β_0 will represent the mean birthweight for females at 36 weeks, which is more interpretable.

Exercise 2.12. Let $A^* = A - 32$ weeks.

Consider a new version of Model 3, with A^* in place of A:

$$\mathrm{E}[Y|M = m, A^* = a^*] = \gamma_0 + \gamma_M m + \gamma_{A^*} a^* + \gamma_{A^*M}(m \cdot a^*) \tag{6}$$

Let the coefficients of this model be γs instead of βs.

What are the interpretations of the γs? How do they relate to the βs in Model 3? Which have the same interpretation? Which are different, and how do they differ? What is the pattern?

Solution. **Interpretation of γ_0:**

From Model 6, γ_0 is the mean birthweight among females ($M = 0$) with $A^* = 0$ (i.e., $A = 32$ weeks):

$$\gamma_0 = \mathrm{E}[Y|M = 0, A^* = 0] = \mathrm{E}[Y|M = 0, A = 32]$$

Substituting into Model 3:

$$\begin{aligned}\gamma_0 &= \beta_0 + \beta_M \cdot 0 + \beta_A \cdot 32 + \beta_{AM} \cdot 0 \cdot 32 \\ &= \beta_0 + 32\beta_A\end{aligned}$$

This differs from $\beta_0 = \mathrm{E}[Y|M=0, A=0]$, which is the mean birthweight among females at $A=0$ weeks.

Interpretation of γ_M:

From Model 6, γ_M is the sex difference in mean birthweight at $A^*=0$ (i.e., $A=32$ weeks):

$$\begin{aligned}\gamma_M &= \mathrm{E}[Y|M=1, A^*=0] - \mathrm{E}[Y|M=0, A^*=0] \\ &= \mathrm{E}[Y|M=1, A=32] - \mathrm{E}[Y|M=0, A=32]\end{aligned}$$

Substituting into Model 3:

$$\begin{aligned}\gamma_M &= (\beta_0 + \beta_M + \beta_A \cdot 32 + \beta_{AM} \cdot 32) - (\beta_0 + \beta_A \cdot 32) \\ &= \beta_M + 32\beta_{AM}\end{aligned}$$

This differs from β_M, which is the sex difference at $A=0$ weeks.

Interpretation of γ_{A^*}:

From Model 6, γ_{A^*} is the slope of mean birthweight with respect to A^* among females ($M=0$):

$$\begin{aligned}\gamma_{A^*} &= \frac{d}{da^*}\mathrm{E}[Y|M=0, A^*=a^*] \\ &= \frac{d}{da^*}\mathrm{E}[Y|M=0, A=a^*+32] \\ &= \frac{d}{da}\mathrm{E}[Y|M=0, A=a]\end{aligned}$$

Substituting into Model 3:

$$\begin{aligned}\gamma_{A^*} &= \frac{d}{da}(\beta_0 + \beta_A \cdot a) \\ &= \beta_A\end{aligned}$$

Since shifting A by a constant does not change the slope, $\gamma_{A^*} = \beta_A$: these two coefficients have the same value and interpretation.

Interpretation of γ_{A^*M}:

From Model 6, γ_{A^*M} is the difference in slope with respect to A^* between males and females:

$$\begin{aligned}\gamma_{A^*M} &= \frac{d}{da^*}\mathrm{E}[Y|M=1, A^*=a^*] - \frac{d}{da^*}\mathrm{E}[Y|M=0, A^*=a^*] \\ &= \frac{d}{da}\mathrm{E}[Y|M=1, A=a] - \frac{d}{da}\mathrm{E}[Y|M=0, A=a]\end{aligned}$$

Substituting into Model 3:

$$\begin{aligned}\gamma_{A^*M} &= (\beta_A + \beta_{AM}) - \beta_A \\ &= \beta_{AM}\end{aligned}$$

Since shifting A by a constant does not change slopes, $\gamma_{A^*M} = \beta_{AM}$: these two coefficients have the same value and interpretation.

The pattern:

Slope coefficients (γ_{A^*} and γ_{A^*M}) are unchanged by rescaling: they have the same values and interpretations as the corresponding βs.

Coefficients change only for variables that have interactions with the rescaled variable A. This includes the intercept (which can be viewed as the main effect of a variable that interacts with A via

β_A), and the main effect of M (which interacts with A via β_{AM}). Shifting A by 32 weeks changes the reference point from $A = 0$ to $A = 32$, so these coefficients now represent quantities evaluated at $A = 32$ weeks rather than at $A = 0$ weeks.

Exercise 2.13. Using R, fit the rescaled interaction model with $A^* = A - 36$ weeks in place of A in Model 3. Compare the coefficient estimates with those from the original model. Which coefficients change, and which remain the same?

Solution.

```
bw <-
  bw |>
  mutate(
    `age - mean` = age - mean(age),
    `age - 36wks` = age - 36
  )

lm1_c <- lm(weight ~ sex + `age - 36wks`, data = bw)

lm2_c <- lm(weight ~ sex + `age - 36wks` + sex:`age - 36wks`, data = bw)

parameters(lm2_c, ci_method = "wald") |> print_md()
```

Parameter	Coefficient	SE	95% CI	t(20)	p
(Intercept)	2552.73	97.59	(2349.16, 2756.30)	26.16	< .001
sex (male)	209.97	129.75	(-60.68, 480.63)	1.62	0.121
age - 36wks	130.40	30.00	(67.82, 192.98)	4.35	< .001
sex (male) × age - 36wks	-18.42	41.76	(-105.52, 68.68)	-0.44	0.664

Compare with what we got without rescaling:

```
parameters(bw_lm2, ci_method = "wald") |> print_md()
```

Parameter	Coefficient	SE	95% CI	t(20)	p
(Intercept)	-2141.67	1163.60	(-4568.90, 285.56)	-1.84	0.081
sex (male)	872.99	1611.33	(-2488.18, 4234.17)	0.54	0.594
age	130.40	30.00	(67.82, 192.98)	4.35	< .001
sex (male) × age	-18.42	41.76	(-105.52, 68.68)	-0.44	0.664

Notice that the slope coefficients (`age - 36wks` and `sexmale:age - 36wks`) remain the same, but the intercept and `sexmale` coefficient have changed to reflect means at age = 36 weeks rather than age = 0 weeks.

2.8 Categorical covariates with more than two levels

2.8.1 Example: `birthweight`

In the birthweight example, the variable `sex` had only two observed values:

```
unique(bw$sex)
#> [1] female male
#> Levels: female male
```

If there are more than two observed values, we can't just use a single variable with 0s and 1s.

Table 15: The `iris` data

```
head(iris)
#> # A tibble: 6 x 5
#>   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
#>          <dbl>       <dbl>        <dbl>       <dbl> <fct>
#> 1          5.1         3.5          1.4         0.2 setosa
#> 2          4.9         3            1.4         0.2 setosa
#> 3          4.7         3.2          1.3         0.2 setosa
#> 4          4.6         3.1          1.5         0.2 setosa
#> 5          5           3.6          1.4         0.2 setosa
#> 6          5.4         3.9          1.7         0.4 setosa
```

Table 16: Summary statistics for the `iris` data

	setosa (N=50)	**versicolor (N=50)**	**virginica (N=50)**
Sepal.Length			
Mean (SD)	5.01 (0.352)	5.94 (0.516)	6.59 (0.636)
Median [Min, Max]	5.00 [4.30, 5.80]	5.90 [4.90, 7.00]	6.50 [4.90, 7.90]
Sepal.Width			
Mean (SD)	3.43 (0.379)	2.77 (0.314)	2.97 (0.322)
Median [Min, Max]	3.40 [2.30, 4.40]	2.80 [2.00, 3.40]	3.00 [2.20, 3.80]
Petal.Length			
Mean (SD)	1.46 (0.174)	4.26 (0.470)	5.55 (0.552)
Median [Min, Max]	1.50 [1.00, 1.90]	4.35 [3.00, 5.10]	5.55 [4.50, 6.90]
Petal.Width			
Mean (SD)	0.246 (0.105)	1.33 (0.198)	2.03 (0.275)
Median [Min, Max]	0.200 [0.100, 0.600]	1.30 [1.00, 1.80]	2.00 [1.40, 2.50]

2.8.2 Example: `iris`

For example, Table 15 shows the (in)famous[6] `iris` data (Anderson (1935)), and Table 16 provides summary statistics. The data include three species: "setosa", "versicolor", and "virginica".

```
library(table1)
table1(
  x = ~ . | Species,
  data = iris,
  overall = FALSE
)
```

If we want to model `Sepal.Length` by species, we could create a variable X that represents "setosa" as $X = 1$, "virginica" as $X = 2$, and "versicolor" as $X = 3$.

Then we could fit a model like:

```
iris_lm1 <- lm(Sepal.Length ~ X, data = iris)
iris_lm1 |>
  parameters() |>
  print_md()
```

[6] https://www.meganstodel.com/posts/no-to-iris/

Table 17: `iris` data with numeric coding of species

```
data(iris) # this step is not always necessary, but ensures you're starting
# from the original version of a dataset stored in a loaded package

iris <-
  iris |>
  tibble() |>
  mutate(
    X = case_when(
      Species == "setosa" ~ 1,
      Species == "virginica" ~ 2,
      Species == "versicolor" ~ 3
    )
  )

iris |>
  distinct(Species, X)
#> # A tibble: 3 x 2
#>   Species        X
#>   <fct>      <dbl>
#> 1 setosa         1
#> 2 versicolor     3
#> 3 virginica      2
```

Table 18: Model of `iris` data with numeric coding of `Species`

Parameter	Coefficient	SE	95% CI	t(148)	p
(Intercept)	4.91	0.16	(4.60, 5.23)	30.83	< .001
X	0.46	0.07	(0.32, 0.61)	6.30	< .001

2.8.3 Let's see how that model looks:

```
iris_plot1 <- iris |>
  ggplot(
    aes(
      x = X,
      y = Sepal.Length
    )
  ) +
  geom_point(alpha = .1) +
  geom_abline(
    intercept = coef(iris_lm1)[1],
    slope = coef(iris_lm1)[2]
  ) +
  theme_bw(base_size = 18)
print(iris_plot1)
```

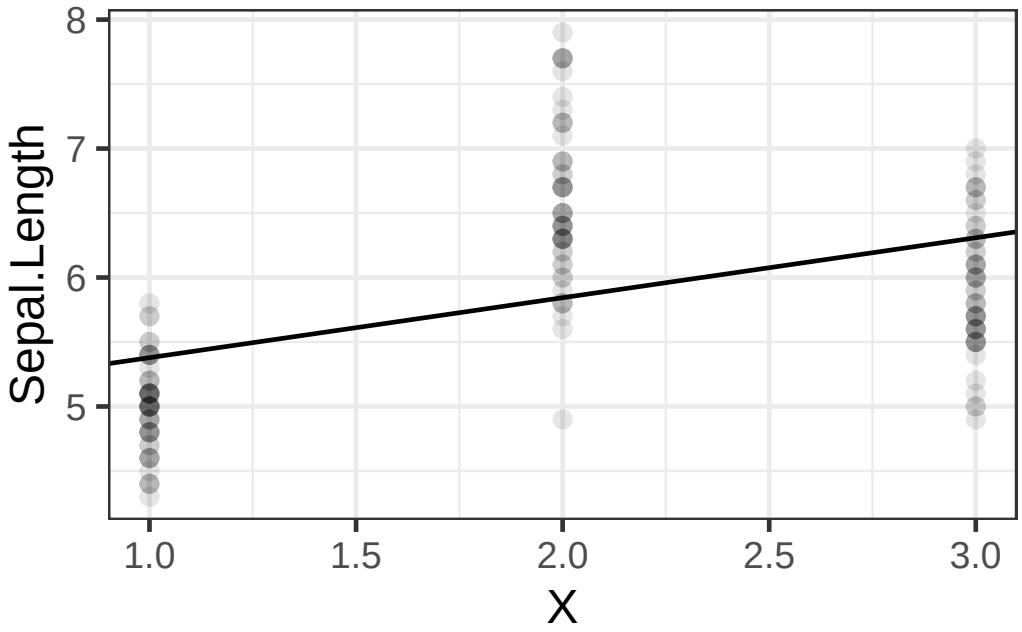


Figure 9: Model of `iris` data with numeric coding of `Species`

We have forced the model to use a straight line for the three estimated means. Maybe not a good idea?

2.8.4 Let's see what R does with categorical variables by default:

```
iris_lm2 <- lm(Sepal.Length ~ Species, data = iris)
iris_lm2 |>
  parameters() |>
  print_md()
```

Table 19: Model of `iris` data with `Species` as a categorical variable

Parameter	Coefficient	SE	95% CI	t(147)	p
(Intercept)	5.01	0.07	(4.86, 5.15)	68.76	< .001
Species (versicolor)	0.93	0.10	(0.73, 1.13)	9.03	< .001
Species (virginica)	1.58	0.10	(1.38, 1.79)	15.37	< .001

2.8.5 Re-parametrize with no intercept

If you don't want the default and offset option, you can use "-1" like we've seen previously:

```
iris_lm2_no_int <- lm(Sepal.Length ~ Species - 1, data = iris)
iris_lm2_no_int |>
  parameters() |>
  print_md()
```

Table 20

Parameter	Coefficient	SE	95% CI	t(147)	p
Species (setosa)	5.01	0.07	(4.86, 5.15)	68.76	< .001
Species (versicolor)	5.94	0.07	(5.79, 6.08)	81.54	< .001
Species (virginica)	6.59	0.07	(6.44, 6.73)	90.49	< .001

2.8.6 Let's see what these new models look like:

```
iris_plot2 <-
  iris |>
  mutate(
    predlm2 = predict(iris_lm2)
  ) |>
  arrange(X) |>
  ggplot(aes(x = X, y = Sepal.Length)) +
  geom_point(alpha = .1) +
  geom_line(aes(y = predlm2), col = "red") +
  geom_abline(
    intercept = coef(iris_lm1)[1],
    slope = coef(iris_lm1)[2]
  ) +
  theme_bw(base_size = 18)

print(iris_plot2)
```

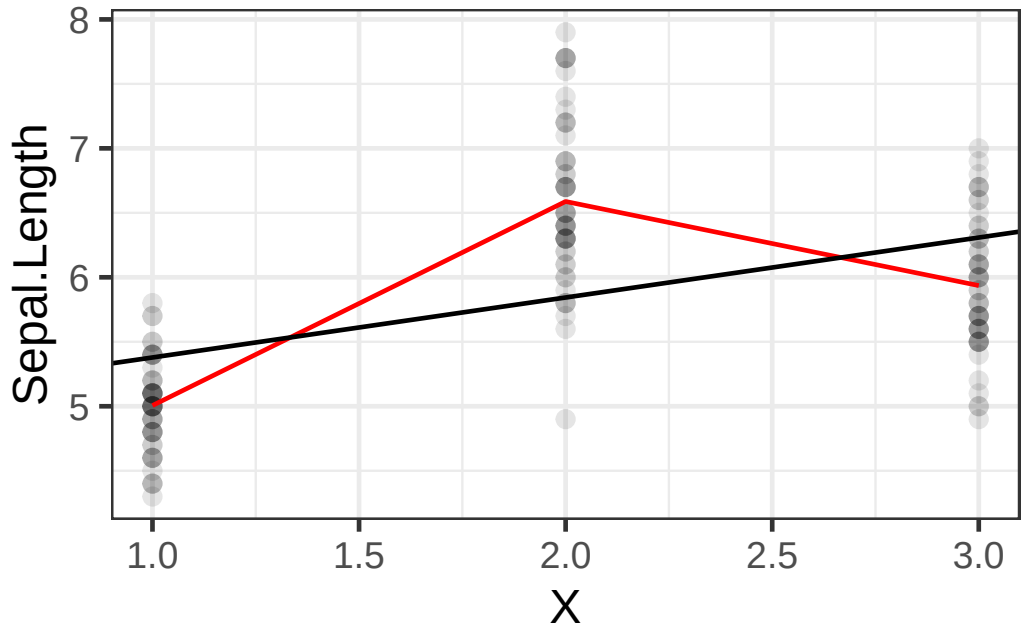


Figure 10

2.8.7 Let's see how R did that:

This format is called a "corner point parametrization" (e.g., in Dobson and Barnett (2018)) or "treatment coding" (e.g., in Dunn and Smyth (2018)).

The default contrasts are controlled by `options("contrasts")`:

```
options("contrasts")
#> $contrasts
#>         unordered           ordered
#> "contr.treatment"      "contr.poly"
```

See `?options` for more details.

This format is called a "group point parametrization" (e.g., in Dobson and Barnett (2018)).

Table 21

```
formula(iris_lm2)
#> Sepal.Length ~ Species
model.matrix(iris_lm2) |>
  as_tibble() |>
  unique()
#> # A tibble: 3 x 3
#>   `(Intercept)` Speciesversicolor Speciesvirginica
#>           <dbl>             <dbl>            <dbl>
#> 1             1                 0                0
#> 2             1                 1                0
#> 3             1                 0                1
```

Table 22

```
formula(iris_lm2_no_int)
#> Sepal.Length ~ Species - 1
model.matrix(iris_lm2_no_int) |>
  as_tibble() |>
  unique()
#> # A tibble: 3 x 3
#>   Speciessetosa Speciesversicolor Speciesvirginica
#>           <dbl>             <dbl>            <dbl>
#> 1             1                 0                0
#> 2             0                 1                0
#> 3             0                 0                1
```

There are more options; see Dobson and Barnett (2018) §6.4.1 and the `codingMatrices` package[7] vignette[8] (Venables (2023)).

2.9 Ordinal covariates

(c.f. Dobson and Barnett (2018) §2.4.4)

We can create ordinal variables in R using the `ordered()` function[9].

Example 2.1.

```
url <- paste0(
  "https://regression.ucsf.edu/sites/g/files/tkssra6706/",
  "f/wysiwyg/home/data/hersdata.dta"
)
library(haven)
hers <- read_dta(url)
```

For ordinal variables, we might want to use contrasts that respect the ordering of the categories. The default treatment contrasts don't account for ordering.

[7] https://CRAN.R-project.org/package=codingMatrices
[8] https://cran.r-project.org/web/packages/codingMatrices/vignettes/codingMatrices.pdf
[9] or equivalently, `factor(ordered = TRUE)`

Table 23: HERS dataset

```
hers |> head()
#> # A tibble: 6 x 37
#>   HT              age raceth  nonwhite smoking drinkany exercise physact globrat
#>   <dbl+lbl>     <dbl> <dbl+l> <dbl+lb> <dbl+l> <dbl+lb> <dbl+lb> <dbl+l> <dbl+l>
#> 1 0 [placebo]      70 2 [Afr~ 1 [yes]  0 [no]  0 [no]   0 [no]   5 [muc~ 3 [goo~
#> 2 0 [placebo]      62 2 [Afr~ 1 [yes]  0 [no]  0 [no]   0 [no]   1 [muc~ 3 [goo~
#> 3 1 [hormone t~    69 1 [Whi~ 0 [no]   0 [no]  0 [no]   0 [no]   3 [abo~ 3 [goo~
#> 4 0 [placebo]      64 1 [Whi~ 0 [no]   1 [yes] 1 [yes]  0 [no]   1 [muc~ 3 [goo~
#> 5 0 [placebo]      65 1 [Whi~ 0 [no]   0 [no]  0 [no]   0 [no]   2 [som~ 3 [goo~
#> 6 1 [hormone t~    68 2 [Afr~ 1 [yes]  0 [no]  1 [yes]  0 [no]   3 [abo~ 3 [goo~
#> # i 28 more variables: poorfair <dbl+lbl>, medcond <dbl>, htnmeds <dbl+lbl>,
#> #   statins <dbl+lbl>, diabetes <dbl+lbl>, dmpills <dbl+lbl>,
#> #   insulin <dbl+lbl>, weight <dbl>, BMI <dbl>, waist <dbl>, WHR <dbl>,
#> #   glucose <dbl>, weight1 <dbl>, BMI1 <dbl>, waist1 <dbl>, WHR1 <dbl>,
#> #   glucose1 <dbl>, tchol <dbl>, LDL <dbl>, HDL <dbl>, TG <dbl>, tchol1 <dbl>,
#> #   LDL1 <dbl>, HDL1 <dbl>, TG1 <dbl>, SBP <dbl>, DBP <dbl>, age10 <dbl>
```

Working with ordinal variables

When working with ordinal covariates in linear models:

1. Use `ordered()` or `factor(ordered = TRUE)` to create the variable
2. Consider using polynomial contrasts (`contr.poly`) which respect ordering
3. Alternatively, treat the ordinal variable as numeric if equal spacing is reasonable
4. Check `?codingMatrices::contr.diff` for additional contrast options

See Dobson and Barnett (2018) §2.4.4 for more details on contrasts for ordinal variables.

3 Estimating Linear Models via Maximum Likelihood

In EPI 203 and our review of MLEs[10], we learned how to fit outcome-only models of the form $p(X = x|\theta)$ to iid data $\tilde{x} = (x_1, ..., x_n)$ using maximum likelihood estimation.

Now, we apply the same procedure to linear regression models:

3.1 Likelihood

$$
\begin{aligned}
\mathcal{L}_i &\stackrel{\text{def}}{=} p(Y_i = y_i|\tilde{X}_i = \tilde{x}_i) \\
&= (2\pi\sigma^2)^{-1/2}\exp\left\{-\frac{1}{2\sigma^2}\varepsilon_i^2\right\} \\
\varepsilon_i &\stackrel{\text{def}}{=} y_i - \mu_i \\
\mu_i &\stackrel{\text{def}}{=} \mu(x_i) \\
&= x_i \cdot \beta
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{L} &\stackrel{\text{def}}{=} \mathcal{L}(\tilde{y}|\mathbf{x}, \tilde{\beta}, \sigma^2) \\
&\stackrel{\text{def}}{=} \mathrm{p}(\tilde{Y} = \tilde{y}|\mathbf{X} = \mathbf{x}) \\
&= \prod_{i=1}^{n} \mathcal{L}_i
\end{aligned}
\tag{7}
$$

---

[10] intro-MLEs.qmd#sec-intro-MLEs

3.2 Log-likelihood

$$
\begin{aligned}
\ell_i &\stackrel{\text{def}}{=} \log\{\mathcal{L}_i\} \\
&= \log\left\{(2\pi\sigma^2)^{-1/2}\exp\left\{-\frac{1}{2\sigma^2}\varepsilon_i^2\right\}\right\} \\
&= -\frac{1}{2}\log\{2\pi\sigma^2\} - \frac{1}{2\sigma^2}\varepsilon_i^2
\end{aligned}
$$

$$
\begin{aligned}
\ell &\stackrel{\text{def}}{=} \ell(\tilde{y}|\mathbf{x},\beta,\sigma^2) \\
&\stackrel{\text{def}}{=} \log\{\mathcal{L}(\tilde{y}|\mathbf{x},\beta,\sigma^2)\} \\
&= \log\left\{\prod_{i=1}^{n}\mathcal{L}_i\right\} \\
&= \sum_{i=1}^{n}\log\{\mathcal{L}_i\} \\
&= \sum_{i=1}^{n}\ell_i \\
&= \sum_{i=1}^{n}\left(-\frac{1}{2}\log\{2\pi\sigma^2\} - \frac{1}{2\sigma^2}\varepsilon_i^2\right) \\
&= -\frac{n}{2}\log\{2\pi\sigma^2\} - \frac{1}{2\sigma^2}\sum_{i=1}^{n}\varepsilon_i^2 \\
&= -\frac{n}{2}\log\{2\pi\sigma^2\} - \frac{1}{2\sigma^2}(\tilde{\varepsilon}\cdot\tilde{\varepsilon}) \\
&= -\frac{n}{2}\log\{2\pi\sigma^2\} - \frac{1}{2\sigma^2}((\tilde{y}-\tilde{\mu})\cdot(\tilde{y}-\tilde{\mu})) \\
&= -\frac{n}{2}\log\{2\pi\sigma^2\} - \frac{1}{2\sigma^2}\big((\tilde{y}-\mathbf{X}\tilde{\beta})\cdot(\tilde{y}-\mathbf{X}\tilde{\beta})\big) \\
&= -\frac{n}{2}\log\{2\pi\sigma^2\} - \frac{1}{2\sigma^2}\sum_{i=1}^{n}\big(y_i - \big(\tilde{x}_i\cdot\tilde{\beta}\big)\big)^2
\end{aligned}
\tag{8}
$$

3.3 Score function

$$
\begin{aligned}
\mu_i' &\stackrel{\text{def}}{=} \frac{\partial}{\partial\tilde{\beta}}\mu_i \\
&= \frac{\partial}{\partial\tilde{\beta}}\big(\tilde{x}_i\cdot\tilde{\beta}\big) \\
&= \left(\frac{\partial}{\partial\tilde{\beta}}\tilde{\beta}\right)\tilde{x}_i \\
&= \mathbb{I}\tilde{x}_i \\
&= \tilde{x}_i
\end{aligned}
$$

$$
\begin{aligned}
\varepsilon_i' &\stackrel{\text{def}}{=} \frac{\partial}{\partial\tilde{\beta}}\varepsilon_i \\
&= \frac{\partial}{\partial\tilde{\beta}}(y_i-\mu_i) \\
&= \frac{\partial}{\partial\tilde{\beta}}y_i - \frac{\partial}{\partial\tilde{\beta}}\mu_i \\
&= 0 - \tilde{x}_i \\
&= -\tilde{x}_i
\end{aligned}
$$

$$
\begin{aligned}
\ell_i' &\stackrel{\text{def}}{=} \frac{\partial}{\partial \tilde{\beta}} \ell_i \\
&= \frac{\partial}{\partial \tilde{\beta}} \Big(-\frac{1}{2} \log\{2\pi\sigma^2\} - \frac{1}{2\sigma^2} \varepsilon_i^2 \Big) \\
&= \frac{\partial}{\partial \tilde{\beta}} \Big(-\frac{1}{2} \log\{2\pi\sigma^2\} \Big) - \frac{\partial}{\partial \tilde{\beta}} \frac{1}{2\sigma^2} \varepsilon_i^2 \\
&= 0 - \frac{1}{2\sigma^2} \frac{\partial}{\partial \tilde{\beta}} \varepsilon_i^2 \\
&= -\frac{1}{2\sigma^2} 2(\varepsilon_i') \varepsilon_i \\
&= -\frac{1}{\sigma^2} (-\tilde{x}_i \varepsilon_i) \\
&= \frac{1}{\sigma^2} \tilde{x}_i \varepsilon_i
\end{aligned}
$$

$$
\begin{aligned}
\ell_{\tilde{\beta}}' &\stackrel{\text{def}}{=} \frac{\partial}{\partial \tilde{\beta}} \ell_{\tilde{\beta}} \\
&= \frac{\partial}{\partial \tilde{\beta}} \sum_{i=1}^{n} \ell_i \\
&= \sum_{i=1}^{n} \frac{\partial}{\partial \tilde{\beta}} \ell_i \\
&= \sum_{i=1}^{n} \ell_i' \\
&= \sum_{i=1}^{n} \frac{1}{\sigma^2} \tilde{x}_i \varepsilon_i \\
&= \frac{1}{\sigma^2} \sum_{i=1}^{n} \tilde{x}_i \varepsilon_i \\
&= \frac{1}{\sigma^2} \mathbf{X}^\top \tilde{\varepsilon}
\end{aligned}
$$

3.4 Hessian

$$
\begin{aligned}
\ell_i'' &\stackrel{\text{def}}{=} \frac{\partial}{\partial \tilde{\beta}^\top} \frac{\partial}{\partial \tilde{\beta}} \ell_i \\
&= \frac{\partial}{\partial \tilde{\beta}^\top} \ell_i' \\
&= \frac{\partial}{\partial \tilde{\beta}^\top} \Big(\frac{1}{\sigma^2} \tilde{x}_i \varepsilon_i \Big) \\
&= \frac{1}{\sigma^2} \tilde{x}_i \varepsilon_i'^\top \\
&= \frac{1}{\sigma^2} \tilde{x}_i (-\tilde{x}_i^\top) \\
&= -\frac{1}{\sigma^2} \tilde{x}_i \tilde{x}_i^\top
\end{aligned}
$$

$$
\begin{aligned}
\ell'' &\stackrel{\text{def}}{=} \frac{\partial}{\partial \tilde{\beta}^\top} \frac{\partial}{\partial \tilde{\beta}} \ell \\
&= \frac{\partial}{\partial \tilde{\beta}^\top} \ell' \\
&= \frac{\partial}{\partial \tilde{\beta}^\top} \sum_{i=1}^{n} \ell_i' \\
&= \sum_{i=1}^{n} \frac{\partial}{\partial \tilde{\beta}^\top} \ell_i' \\
&= \sum_{i=1}^{n} \ell_i'' \\
&= \sum_{i=1}^{n} -\frac{1}{\sigma^2} \tilde{x}_i \tilde{x}_i^\top \\
&= -\frac{1}{\sigma^2} \sum_{i=1}^{n} \tilde{x}_i \tilde{x}_i^\top \\
&= -\frac{1}{\sigma^2} \mathbf{X}^\top \mathbf{X}
\end{aligned}
$$

That is,

$$
\ell'' = -\frac{1}{\sigma^2} \sum_{i=1}^{n} \tilde{x}_i \tilde{x}_i^\top \tag{9}
$$

3.5 Alternative approach using matrix derivatives

$$
\begin{aligned}
\ell'_{\tilde{\beta}}(\tilde{y}|\mathbf{x}, \tilde{\beta}, \sigma^2) &\stackrel{\text{def}}{=} \frac{\partial}{\partial \tilde{\beta}} \ell_{\tilde{\beta}}(\tilde{y}|\mathbf{x}, \tilde{\beta}, \sigma^2) \\
&= -\frac{1}{2\sigma^2} \frac{\partial}{\partial \tilde{\beta}} \left(\sum_{i=1}^{n} \left(y_i - \left(\tilde{x}_i \cdot \tilde{\beta} \right) \right)^2 \right)
\end{aligned} \tag{10}
$$

Let's switch to matrix-vector notation:

$$
\sum_{i=1}^{n} (y_i - \tilde{x}_i^\top \tilde{\beta})^2 = (\tilde{y} - \mathbf{X}\tilde{\beta}) \cdot (\tilde{y} - \mathbf{X}\tilde{\beta})
$$

So

$$
\begin{aligned}
(\tilde{y} - \mathbf{X}\tilde{\beta})'(\tilde{y} - \mathbf{X}\tilde{\beta}) &= (\tilde{y}' - \tilde{\beta}' X')(\tilde{y} - \mathbf{X}\tilde{\beta}) \\
&= \tilde{y}'\tilde{y} - \tilde{\beta}' X' \tilde{y} - \tilde{y}' \mathbf{X} \tilde{\beta} + \tilde{\beta}' \mathbf{X}' \mathbf{X} \beta \\
&= \tilde{y}'\tilde{y} - 2\tilde{y}' \mathbf{X} \beta + \beta' \mathbf{X}' \mathbf{X} \beta
\end{aligned}
$$

We will use some results from vector calculus[11]:

[11] math-prereqs.qmd#sec-vector-calculus

$$
\begin{aligned}
\frac{\partial}{\partial \tilde{\beta}}\left(\sum_{i=1}^{n}(y_i - x_i'\beta)^2\right) &= \frac{\partial}{\partial \tilde{\beta}}(\tilde{y} - X\beta)'(\tilde{y} - X\beta) \\
&= \frac{\partial}{\partial \tilde{\beta}}(y'y - 2y'X\beta + \beta'\mathbf{X}'\mathbf{X}\beta) \\
&= (-2X'y + 2\mathbf{X}'\mathbf{X}\beta) \\
&= -2X'(y - X\beta) \\
&= -2X'(y - \mathrm{E}[y]) \\
&= -2X'\varepsilon(y)
\end{aligned}
\tag{11}
$$

So if $\ell'(\beta, \sigma^2) = 0$, then

$$
\begin{aligned}
0 &= (-2X'y + 2\mathbf{X}'\mathbf{X}\beta) \\
2X'y &= 2\mathbf{X}'\mathbf{X}\beta \\
X'y &= \mathbf{X}'\mathbf{X}\beta \\
(\mathbf{X}'\mathbf{X})^{-1}X'y &= \beta
\end{aligned}
$$

3.5.1 Hessian

The Hessian (second derivative matrix) is:

$$
\ell''_{\beta,\beta'}(\beta, \sigma^2; \tilde{y}, \mathbf{X}) = -\frac{1}{2\sigma^2}\mathbf{X}'\mathbf{X}
$$

$\ell''_{\beta,\beta'}(\beta, \sigma^2; \mathbf{X}, \tilde{y})$ is negative definite at $\beta = (\mathbf{X}'\mathbf{X})^{-1}X'y$, so $\hat{\beta}_{ML} = (\mathbf{X}'\mathbf{X})^{-1}X'y$ is the MLE for β.

Similarly (not shown):

$$
\hat{\sigma}^2_{ML} = \frac{1}{n}(Y - X\hat{\beta})'(Y - X\hat{\beta})
$$

3.6 Residual Standard Deviation

$\hat{\sigma}$ represents an *estimate* of the *Residual Standard Deviation* parameter, σ. We can extract $\hat{\sigma}$ from the fitted model, using the `sigma()` function:

```
sigma(bw_lm2)
#> [1] 180.613
```

3.6.1 σ is NOT "Residual standard error"

In the `summary.lm()` output, this estimate is labeled as `"Residual standard error"`:

```
summary(bw_lm2)
#>
#> Call:
#> lm(formula = weight ~ sex + age + sex:age, data = bw)
#>
#> Residuals:
#>    Min     1Q Median     3Q    Max
#> -246.7 -138.1  -39.1  176.6  274.3
```

```
#>
#> Coefficients:
#>             Estimate Std. Error t value Pr(>|t|)
#> (Intercept)  -2141.7     1163.6   -1.84  0.08057 .
#> sexmale        873.0     1611.3    0.54  0.59395
#> age            130.4       30.0    4.35  0.00031 ***
#> sexmale:age    -18.4       41.8   -0.44  0.66389
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#> Residual standard error: 181 on 20 degrees of freedom
#> Multiple R-squared:  0.643,  Adjusted R-squared:  0.59
#> F-statistic:   12 on 3 and 20 DF,  p-value: 0.000101
```

However, this is a misnomer: see note in `?stats::sigma`

4 Inference about Gaussian Linear Regression Models

4.1 Motivating example: `birthweight` data

Research question: is there really an interaction between sex and age?

$H_0 : \beta_{AM} = 0$

$H_A : \beta_{AM} \neq 0$

$P(|\hat{\beta}_{AM}| > |-18.417241| \mid H_0) = ?$

4.2 Inference for individual predictor coefficients

4.2.1 Sampling distribution of $\hat{\beta}$

The Fisher information[12] for β is:

$$\begin{aligned} \mathcal{I}_\beta &= \mathrm{E}\big[-\ell''_{\beta,\beta'}(Y|X,\beta,\sigma^2)\big] \\ &= \frac{1}{\sigma^2}\mathbf{X}'\mathbf{X} \end{aligned}$$

Therefore:

$$\mathrm{Var}\big(\hat{\beta}\big) \approx (\mathcal{I}_\beta)^{-1} = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$$

and

$$\hat{\beta} \dot{\sim} N(\beta, \mathcal{I}_\beta^{-1})$$

These are all results you have hopefully seen before.

In the Gaussian linear regression case, we also have exact results:

$$\frac{\hat{\beta}_j}{\widehat{\mathrm{se}}\big(\hat{\beta}_j\big)} \sim t_{n-p}$$

---

[12] intro-MLEs.qmd

Table 24: Covariance matrix of $\hat{\tilde{\beta}}$ for `birthweight` model 3 (with interaction term)

```
bw_lm2 |> vcov()
#>             (Intercept)  sexmale        age sexmale:age
#> (Intercept)     1353968 -1353968 -34870.966   34870.966
#> sexmale        -1353968  2596387  34870.966  -67210.974
#> age              -34871    34871    899.896    -899.896
#> sexmale:age       34871   -67211   -899.896    1743.548
```

4.2.2 Estimated covariance matrix and standard errors

Example 4.1 (MLEs for birthweight data)**.** In model 3 above, $\hat{\mathcal{J}}(\beta)$ is:

If we take the square roots of the diagonals, we get the standard errors listed in the model output:

```
bw_lm2 |>
  vcov() |>
  diag() |>
  sqrt()
#> (Intercept)     sexmale         age sexmale:age
#>   1163.6015   1611.3309     29.9983     41.7558
```

```
bw_lm2 |>
  parameters() |>
  print_md()
```

Table 25: Estimated model for `birthweight` data with interaction term

Parameter	Coefficient	SE	95% CI	t(20)	p
(Intercept)	-2141.67	1163.60	(-4568.90, 285.56)	-1.84	0.081
sex (male)	872.99	1611.33	(-2488.18, 4234.17)	0.54	0.594
age	130.40	30.00	(67.82, 192.98)	4.35	$< .001$
sex (male) $\times$ age	-18.42	41.76	(-105.52, 68.68)	-0.44	0.664

So we can do confidence intervals, hypothesis tests, and p-values exactly as in the one-variable case we looked at previously.

4.2.3 Wald tests and confidence intervals

For Gaussian linear regression, the ordinary least squares (OLS) estimates $\hat{\beta}_k$ are exactly Gaussian when the error terms ϵ_i are Gaussian, for any sample size. See also the table of Gaussian vs. MLE-based tests[13].

Wald test statistic

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

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

Under H_0, $t_k \sim t_{n-p}$ exactly when errors are Gaussian.

Confidence intervals for regression coefficients

A 95% confidence interval for β_k is:

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

$$\hat{\beta}_k \pm t_{n-p}(0.975) \cdot \widehat{SE}(\hat{\beta}_k)$$

In R

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

```
bw_lm2 |>
  parameters() |>
  print_md(
    include_reference = TRUE
  )
```

Table 26: Wald tests and 95% CIs for `birthweight` linear regression

Parameter	Coefficient	SE	95% CI	t(20)	p
(Intercept)	-2141.67	1163.60	(-4568.90, 285.56)	-1.84	0.081
sex (female)	0.00				
sex (male)	872.99	1611.33	(-2488.18, 4234.17)	0.54	0.594
age	130.40	30.00	(67.82, 192.98)	4.35	$< .001$
sex (male) $\times$ age	-18.42	41.76	(-105.52, 68.68)	-0.44	0.664

To understand what's happening, let's replicate these results by hand for the interaction term.

P-values

```
bw_lm2 |>
  parameters(keep = "sexmale:age") |>
  print_md(
    include_reference = TRUE
  )
```

Parameter	Coefficient	SE	95% CI	t(20)	p
sex (male) $\times$ age	-18.42	41.76	(-105.52, 68.68)	-0.44	0.664

```
beta_hat <- coef(summary(bw_lm2))["sexmale:age", "Estimate"]
se_hat <- coef(summary(bw_lm2))["sexmale:age", "Std. Error"]
dfresid <- bw_lm2$df.residual
t_stat <- abs(beta_hat) / se_hat
pval_t <-
  pt(-t_stat, df = dfresid, lower.tail = TRUE) +
  pt(t_stat, df = dfresid, lower.tail = FALSE)
```

$$\begin{aligned}
&P\left(|\hat{\beta}_{AM}| > |-18.417241| \middle| H_0\right) \\
&= \Pr\left(\left|\frac{\hat{\beta}_{AM}}{\widehat{SE}(\hat{\beta}_{AM})}\right| > \left|\frac{-18.417241}{41.755817}\right| \middle| H_0\right) \\
&= \Pr\left(|T_{20}| > 0.44107 | H_0\right) \\
&= 0.663893
\end{aligned}$$

This matches the result in the table above.

Confidence intervals

```r
q_t_upper <- qt(
  p = 0.975,
  df = dfresid,
  lower.tail = TRUE
)

q_t_lower <- qt(
  p = 0.025,
  df = dfresid,
  lower.tail = TRUE
)

confint_radius_t <-
  se_hat * q_t_upper

confint_t <- beta_hat + c(-1, 1) * confint_radius_t

print(confint_t)
#> [1] -105.5184   68.6839
```

This also matches.

Gaussian approximations

For large samples, the t-distribution is well-approximated by the standard Gaussian:

```r
pval_z <- pnorm(abs(t_stat), lower.tail = FALSE) * 2

print(pval_z)
#> [1] 0.659162
```

```r
confint_radius_z <- se_hat * qnorm(0.975, lower.tail = TRUE)
confint_z <-
  beta_hat + c(-1, 1) * confint_radius_z
print(confint_z)
#> [1] -100.2571   63.4227
```

4.3 Inference for predicted means

Exercise 4.1. Given a maximum likelihood estimate $\hat{\tilde{\beta}}$ and a corresponding estimated covariance matrix $\hat{\Sigma} \overset{\text{def}}{=} \widehat{\text{Cov}}(\hat{\tilde{\beta}})$, calculate a 95% confidence interval for the predicted mean $\mu(\tilde{x}) = \text{E}\big[Y|\tilde{X} = \tilde{x}\big]$.

Solution 4.1.

By the Gauss-Markov theorem[14], the OLS estimate $\hat{\tilde{\beta}}$ is the best linear unbiased estimator of $\tilde{\beta}$. A 95% confidence interval for $\mu(\tilde{x})$ can be constructed directly on the original scale:

$$\hat{\mu}(\tilde{x}) \pm t_{n-p}(0.975) \cdot \widehat{\text{SE}}(\hat{\mu}(\tilde{x}))$$

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

Unlike in logistic regression, no transformation is needed; the confidence interval is constructed directly on the mean scale.

$$\mu(\tilde{x}) \in \Big(\hat{\mu}(\tilde{x}) \pm t_{n-p}(0.975) \cdot \widehat{\text{SE}}(\hat{\mu}(\tilde{x}))\Big)$$

[14] https://en.wikipedia.org/wiki/Gauss%E2%80%93Markov_theorem

Exercise 4.2.

How can we estimate the standard error of $\hat{\mu}(\tilde{x})$?

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

Solution 4.2.

$$\text{SE}(\hat{\mu}(\tilde{x})) = \sqrt{\text{Var}(\hat{\mu}(\tilde{x}))} \tag{12}$$

By the definition $\hat{\mu}(\tilde{x}) = \tilde{x}'\hat{\tilde{\beta}}$ and the variance of a linear combination[15]:

$$\begin{aligned} \text{Var}(\hat{\mu}(\tilde{x})) &= \text{Var}\left(\tilde{x}'\hat{\tilde{\beta}}\right) \\ &= \tilde{x}'\text{Cov}\left(\hat{\tilde{\beta}}\right)\tilde{x} \\ &= \tilde{x}^\top \Sigma \tilde{x} \end{aligned} \tag{13}$$

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

Expanding Equation 13 out of matrix-vector notation, we have:

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

Combining Equation 13 and the Gauss-Markov theorem:

Theorem 4.1 (Estimated variance and standard error of predicted mean).

$$\widehat{Var}(\hat{\mu}(\tilde{x})) = \tilde{x}^\top \hat{\Sigma} \tilde{x} \tag{14}$$

$$\widehat{SE}(\hat{\mu}(\tilde{x})) = \sqrt{\tilde{x}^\top \hat{\Sigma} \tilde{x}} \tag{15}$$

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

In R

In R, `predict()` with `se.fit = TRUE` computes the estimated mean $\hat{\mu}(\tilde{x}) = \tilde{x}'\hat{\tilde{\beta}}$ and its estimated standard error for each covariate pattern:

```
library(dplyr)
new_data <- tibble(
  age = c(36, 38, 40),
  sex = "male"
)

pred_mean <-
```

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

```
  bw_lm2 |>
  predict(
    newdata = new_data,
    se.fit = TRUE
  )

new_data |>
  mutate(
    mu_hat = pred_mean$fit,
    se = pred_mean$se.fit,
    ci_lower = mu_hat - qt(0.975, df = bw_lm2$df.residual) * se,
    ci_upper = mu_hat + qt(0.975, df = bw_lm2$df.residual) * se
  ) |>
  knitr::kable(digits = 3)
```

Table 27: Predicted means and 95% CI for `birthweight` linear regression

age	sex	mu_hat	se	ci_lower	ci_upper
36	male	2762.71	85.508	2584.34	2941.07
38	male	2986.67	53.030	2876.05	3097.29
40	male	3210.64	71.147	3062.23	3359.05

Alternatively, `predict()` with `interval = "confidence"` gives the same result:

```
bw_lm2 |>
  predict(
    newdata = new_data,
    interval = "confidence"
  ) |>
  cbind(new_data) |>
  knitr::kable(digits = 3)
```

Table 28: Predicted means and 95% CI using `interval = 'confidence'`

fit	lwr	upr	age	sex
2762.71	2584.34	2941.07	36	male
2986.67	2876.05	3097.29	38	male
3210.64	3062.23	3359.05	40	male

4.4 Inference for differences in means

Exercise 4.3. Given a maximum likelihood estimate $\hat{\tilde{\beta}}$ and a corresponding estimated covariance matrix $\hat{\Sigma} \overset{\text{def}}{=} \widehat{\text{Cov}}(\hat{\tilde{\beta}})$, calculate a 95% confidence interval for the difference in means comparing covariate patterns $\tilde{x}$ and $\tilde{x}^*$, $\mu(\tilde{x}) - \mu(\tilde{x}^*)$.

Solution 4.3.

The difference in means is a linear function of $\hat{\tilde{\beta}}$, so we can construct the confidence interval directly:

$$\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)} \pm t_{n-p}(0.975) \cdot \widehat{\text{SE}}\Big(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}\Big)$$

No transformation is needed (unlike for odds ratios in logistic regression).

$$\mu(\tilde{x}) - \mu(\tilde{x}^*) \in \left(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)} \pm t_{n-p}(0.975) \cdot \widehat{\mathrm{SE}}\left(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}\right)\right)$$

Exercise 4.4. Express the difference in means $\mu(\tilde{x}) - \mu(\tilde{x}^*)$ as a linear function of $\tilde{\beta}$.

Solution 4.4.

$$\begin{aligned} \mu(\tilde{x}) - \mu(\tilde{x}^*) &= \tilde{x}^\top \tilde{\beta} - (\tilde{x}^*)^\top \tilde{\beta} \\ &= (\tilde{x} - \tilde{x}^*)' \tilde{\beta} \\ &= \Delta\tilde{x}' \tilde{\beta} \end{aligned} \tag{16}$$

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

Exercise 4.5.

How can we estimate the standard error of $\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}$?

$$\widehat{\mathrm{SE}}\left(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}\right) = ?$$

Solution 4.5.

$$\mathrm{SE}\left(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}\right) = \sqrt{\mathrm{Var}\left(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}\right)} \tag{17}$$

By Solution 4.4 and the variance of a linear combination[16]:

$$\begin{aligned} \mathrm{Var}\left(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}\right) &= \mathrm{Var}\left((\Delta\tilde{x})'\hat{\tilde{\beta}}\right) \\ &= (\Delta\tilde{x})^\top \mathrm{Cov}\left(\hat{\tilde{\beta}}\right)(\Delta\tilde{x}) \\ &= (\Delta\tilde{x})^\top \Sigma (\Delta\tilde{x}) \end{aligned} \tag{18}$$

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

Expanding Equation 18 out of matrix-vector notation, we have:

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

Combining Equation 18 and the Gauss-Markov theorem:

Theorem 4.2 (Estimated variance and standard error of difference in means).

$$\widehat{Var}\left(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}\right) = \Delta\tilde{x}^\top \hat{\Sigma} (\Delta\tilde{x}) \tag{19}$$

$$\widehat{SE}\left(\widehat{\mu(\tilde{x}) - \mu(\tilde{x}^*)}\right) = \sqrt{\Delta\tilde{x}^\top \hat{\Sigma} (\Delta\tilde{x})} \tag{20}$$

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

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

Compare this result with the formula for inference for predicted means: the only change is to replace $\tilde{x}$ with $\Delta\tilde{x} = \tilde{x} - \tilde{x}^*$.

In R

In R, we can compute the CI for the difference in means by computing the predicted means for both covariate patterns and applying the variance formula directly:

```
library(dplyr)
new_data_pair <- tibble(
  sex = factor(c("female", "male"), levels = levels(bw$sex)),
  age = c(40, 40)
)

pred_pair <-
  bw_lm2 |>
  predict(
    newdata = new_data_pair,
    se.fit = TRUE
  )

design_mat <- model.matrix(delete.response(terms(bw_lm2)), new_data_pair)
delta_x <- design_mat[2, ] - design_mat[1, ]

sigma_hat <- vcov(bw_lm2)

diff_mean_hat <- diff(pred_pair$fit)
se_diff <- sqrt(t(delta_x) %*% sigma_hat %*% delta_x)
t_crit <- qt(0.975, df = bw_lm2$df.residual)

tibble(
  diff_mean = diff_mean_hat,
  se = as.numeric(se_diff),
  ci_lower = diff_mean_hat - t_crit * se,
  ci_upper = diff_mean_hat + t_crit * se
) |>
  knitr::kable(digits = 3)
```

Table 29: 95% CI for difference in birthweight means (male vs. female)

diff_mean	se	ci_lower	ci_upper
136.305	95.846	-63.626	336.236

4.5 Likelihood ratio statistics

```
logLik(bw_lm2)
#> 'log Lik.' -156.579 (df=5)
logLik(bw_lm1)
#> 'log Lik.' -156.695 (df=4)

log_LR <- (logLik(bw_lm2) - logLik(bw_lm1)) |> as.numeric()
delta_df <- (bw_lm1$df.residual - df.residual(bw_lm2))
```

```r
x_max <- 1
```

```r
d_log_LR <- function(x, df = delta_df) dchisq(x, df = df)

chisq_plot <-
  ggplot() +
  geom_function(fun = d_log_LR) +
  stat_function(
    fun = d_log_LR,
    xlim = c(log_LR, x_max),
    geom = "area",
    fill = "gray"
  ) +
  geom_segment(
    aes(
      x = log_LR,
      xend = log_LR,
      y = 0,
      yend = d_log_LR(log_LR)
    ),
    col = "red"
  ) +
  xlim(0.0001, x_max) +
  ylim(0, 4) +
  ylab("p(X=x)") +
  xlab("log(likelihood ratio) statistic [x]") +
  theme_classic()
chisq_plot |> print()
```

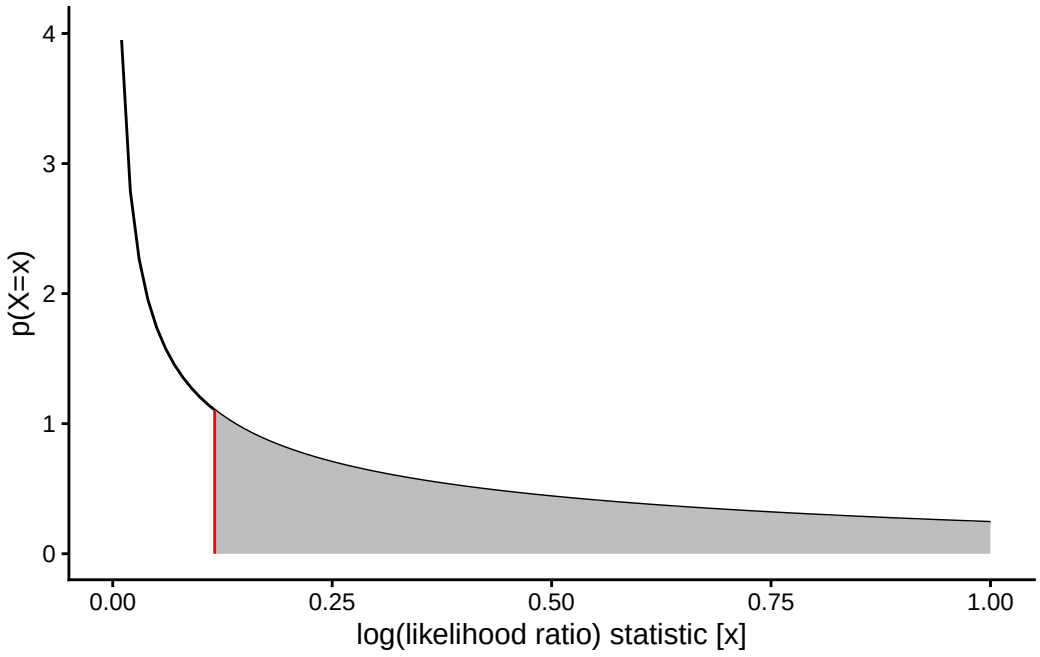


Figure 11: Chi-square distribution

Now we can get the p-value:

```
pchisq(
  q = 2 * log_LR,
  df = delta_df,
  lower = FALSE
) |>
  print()
#> [1] 0.629806
```

In practice you don't have to do this by hand; there are functions to do it for you:

```
# built in
library(lmtest)
lrtest(bw_lm2, bw_lm1)
#> # A tibble: 2 x 5
#>   `#Df` LogLik    Df  Chisq `Pr(>Chisq)`
#>   <dbl>  <dbl> <dbl>  <dbl>        <dbl>
#> 1     5  -157.    NA NA           NA
#> 2     4  -157.    -1  0.232        0.630
```

5 Prediction

5.1 Prediction for linear models

Definition 5.1 (Predicted value)**.** In a regression model $\mathrm{p}(y|\tilde{x})$, the **predicted value** of y given $\tilde{x}$ is the estimated mean of Y given $\tilde{X} = \tilde{x}$:

$$\hat{y} \overset{\text{def}}{=} \hat{\mathrm{E}}\big[Y|\tilde{X} = \tilde{x}\big]$$

For linear models, the predicted value can be straightforwardly calculated by multiplying each predictor value x_j by its corresponding coefficient β_j and adding up the results:

$$\begin{aligned}\hat{y} &= \hat{\mathrm{E}}\big[Y|\tilde{X} = \tilde{x}\big] \\ &= \tilde{x}'\hat{\beta} \\ &= \hat{\beta}_0 \cdot 1 + \hat{\beta}_1 x_1 + \ldots + \hat{\beta}_p x_p\end{aligned}$$

5.2 Example: prediction for the `birthweight` data

```
x <- c(1, 1, 40)
sum(x * coef(bw_lm1))
#> [1] 3225.49
```

R has built-in functions for prediction:

```
x <- tibble(age = 40, sex = "male")
bw_lm1 |> predict(newdata = x)
#>        1
#> 3225.49
```

If you don't provide `newdata`, R will use the covariate values from the original dataset:

```
predict(bw_lm1)
#>        1        2        3        4        5        6        7        8        9       10
#> 3225.49 3062.45 2983.70 2578.87 3225.49 3062.45 2621.02 2820.66 2741.91 3304.24
#>       11       12       13       14       15       16       17       18       19       20
```

```
#> 2862.81 2941.56 3346.38 3062.45 3225.49 2699.77 2862.81 2578.87 2983.70 2820.66
#>      21      22      23      24
#> 3225.49 2941.56 2983.70 3062.45
```

These special predictions are called the *fitted values* of the dataset:

Definition 5.2. For a given dataset $(\tilde{Y}, \mathbf{X})$ and corresponding fitted model $\mathrm{p}_{\hat{\beta}}(\tilde{y}|\mathbf{x})$, the **fitted value** of y_i is the predicted value of y when $\tilde{X} = \tilde{x}_i$ using the estimate parameters $\hat{\beta}$.

R has an extra function to get these values:

```
fitted(bw_lm1)
#>       1       2       3       4       5       6       7       8       9      10
#> 3225.49 3062.45 2983.70 2578.87 3225.49 3062.45 2621.02 2820.66 2741.91 3304.24
#>      11      12      13      14      15      16      17      18      19      20
#> 2862.81 2941.56 3346.38 3062.45 3225.49 2699.77 2862.81 2578.87 2983.70 2820.66
#>      21      22      23      24
#> 3225.49 2941.56 2983.70 3062.45
```

5.3 Confidence intervals

Use `predict(se.fit = TRUE)` to compute SEs for predicted values:

```
bw_lm1 |>
  predict(
    newdata = x,
    se.fit = TRUE
  )
#> $fit
#>       1
#> 3225.49
#>
#> $se.fit
#> [1] 61.4599
#>
#> $df
#> [1] 21
#>
#> $residual.scale
#> [1] 177.116
```

The output of `predict.lm(se.fit = TRUE)` is a `list()`; you can extract the elements with `$` or `magrittr::use_series()`:

```
library(magrittr)
bw_lm1 |>
  predict(
    newdata = x,
    se.fit = TRUE
  ) |>
  use_series(se.fit)
#> [1] 61.4599
```

We can construct **confidence intervals** for $\mathrm{E}[Y|X = x]$ using the usual formula:

$$\mu(\tilde{x}) \in (\hat{\mu}(\tilde{x}) \pm \zeta_\alpha)$$

$$\zeta_\alpha = t_{n-p}\left(1 - \frac{\alpha}{2}\right) * \widehat{\mathrm{se}}(\hat{\mu}(\tilde{x}))$$

$$\hat{\mu}(\tilde{x}) = \tilde{x} \cdot \hat{\beta}$$

$$\begin{aligned}
\text{se}(\hat{\mu}(\tilde{x})) &= \sqrt{\text{Var}(\hat{\mu}(\tilde{x}))} \\
\text{Var}(\hat{\mu}(\tilde{x})) &= \text{Var}\left(x'\hat{\beta}\right) \\
&= x'\text{Var}\left(\hat{\beta}\right)x \\
&= x'\sigma^2(\mathbf{X}'\mathbf{X})^{-1}x \\
&= \sigma^2 x'(\mathbf{X}'\mathbf{X})^{-1}x \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j \text{Cov}\left(\hat{\beta}_i, \hat{\beta}_j\right) \\
\widehat{\text{Var}}(\hat{\mu}(\tilde{x})) &= \hat{\sigma}^2 x'(\mathbf{X}'\mathbf{X})^{-1}x
\end{aligned}$$

```
bw_lm2 |> predict(
  newdata = x,
  interval = "confidence"
)
#>       fit     lwr     upr
#> 1 3210.64 3062.23 3359.05
```

```
library(sjPlot)
bw_lm2 |>
  plot_model(type = "pred", terms = c("age", "sex"), show.data = TRUE) +
  theme_sjplot() +
  theme(legend.position = "bottom")
```

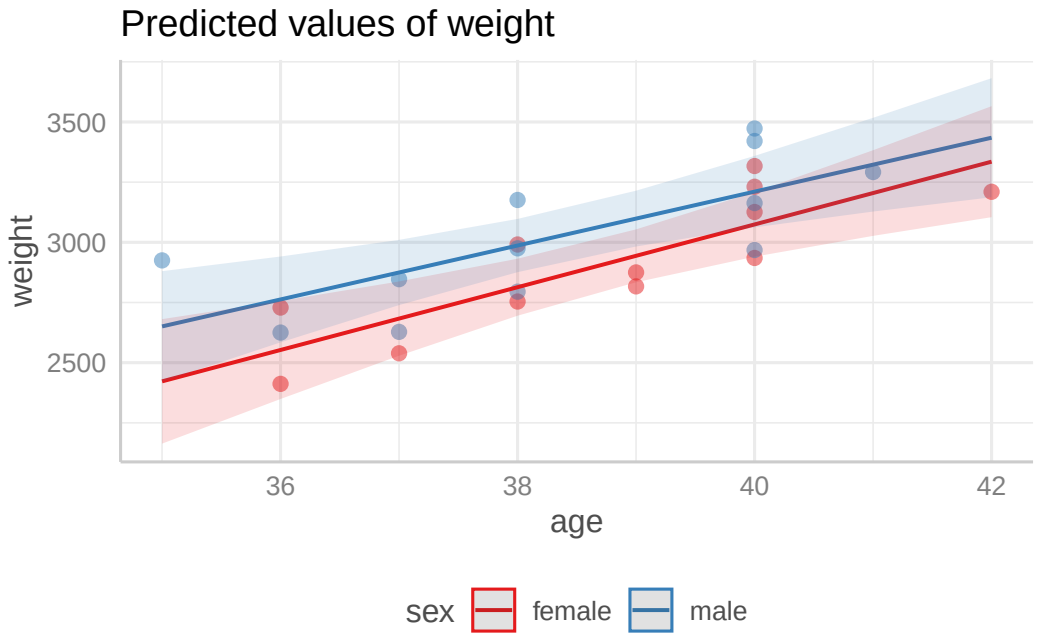


Figure 12: Predicted values and confidence bands for the `birthweight` model with interaction term

5.4 Prediction intervals

We can also construct **prediction intervals** for the value of a new observation Y^*, given a covariate pattern $\tilde{x}^*$.

A new observation Y^* at $\tilde{x}^*$ follows the same linear model as the training data:

$$Y^* = (\tilde{x}^*)^\top \tilde{\beta} + \varepsilon^*$$

where $\varepsilon^* \sim \mathrm{N}(0, \sigma^2)$ is independent of the training data (and therefore independent of $\hat{\beta}$).

The predicted value of Y^* is:

$$\hat{Y}^* \overset{\text{def}}{=} \hat{\mu}(\tilde{x}^*) = (\tilde{x}^*)^\top \hat{\beta}$$

We base the prediction interval on the **prediction error** $Y^* - \hat{Y}^*$:

$$\begin{aligned} Y^* - \hat{Y}^* &= (\tilde{x}^*)^\top \tilde{\beta} + \varepsilon^* - (\tilde{x}^*)^\top \hat{\beta} \\ &= \varepsilon^* - (\tilde{x}^*)^\top (\hat{\beta} - \tilde{\beta}) \end{aligned}$$

The prediction error is unbiased:

$$\begin{aligned} \mathrm{E}\left[Y^* - \hat{Y}^*\right] &= \mathrm{E}[\varepsilon^*] - (\tilde{x}^*)^\top \mathrm{E}\left[\hat{\beta} - \tilde{\beta}\right] \\ &= 0 - (\tilde{x}^*)^\top \cdot 0 \\ &= 0 \end{aligned}$$

The variance of the prediction error is:

$$\begin{aligned} \mathrm{Var}\left(Y^* - \hat{Y}^*\right) &= \mathrm{Var}\left(\varepsilon^* - (\tilde{x}^*)^\top (\hat{\beta} - \tilde{\beta})\right) \\ &= \mathrm{Var}(\varepsilon^*) + \mathrm{Var}\left((\tilde{x}^*)^\top \hat{\beta}\right) \quad (\text{since } \varepsilon^* \perp\!\!\!\perp \hat{\beta}) \\ &= \sigma^2 + (\tilde{x}^*)^\top \mathrm{Var}\left(\hat{\beta}\right) \tilde{x}^* \\ &= \sigma^2 + (\tilde{x}^*)^\top (\sigma^2 (\mathbf{X}'\mathbf{X})^{-1}) \tilde{x}^* \\ &= \sigma^2 + \sigma^2 (\tilde{x}^*)^\top (\mathbf{X}'\mathbf{X})^{-1} \tilde{x}^* \\ &= \sigma^2 \left(1 + (\tilde{x}^*)^\top (\mathbf{X}'\mathbf{X})^{-1} \tilde{x}^*\right) \end{aligned} \tag{21}$$

See Hogg et al. (2015) §7.6 (p. 340).

```
bw_lm2 |>
  predict(newdata = x, interval = "predict")
#>       fit     lwr     upr
#> 1 3210.64 2805.71 3615.57
```

If you don't specify `newdata`, you get a warning:

```
bw_lm2 |>
  predict(interval = "predict") |>
  head()
#> Warning in predict.lm(bw_lm2, interval = "predict"): predictions on current data refer to _future
#>       fit     lwr     upr
#> 1 2552.73 2124.50 2980.97
#> 2 2552.73 2124.50 2980.97
#> 3 2683.13 2275.99 3090.27
#> 4 2813.53 2418.60 3208.47
#> 5 2813.53 2418.60 3208.47
#> 6 2943.93 2551.48 3336.38
```

The warning from the last command is: "predictions on current data refer to *future* responses" (since you already know what happened to the current data, and thus don't need to predict it).

See `?predict.lm` for more.

```
library(rlang) # defines the `.data` pronoun
plot_PIs_and_CIs <- function(data, model = NULL) {
  if (is.null(model)) {
    rlang::abort("`model` must be supplied to `plot_PIs_and_CIs()`.")
  }

  if (!is.data.frame(data) && is.data.frame(model)) {
    rlang::warn(
      paste0(
        "`plot_PIs_and_CIs()` received `model` as the first argument ",
        "and `data` as the second. ",
        "Please update the call to use `data` first and `model` second."
      )
    )
    tmp <- data
    data <- model
    model <- tmp
  }

  cis <- model |>
    predict(newdata = data, interval = "confidence") |>
    suppressWarnings() |>
    tibble::as_tibble()
  names(cis) <- paste("ci", names(cis), sep = "_")

  preds <- model |>
    predict(newdata = data, interval = "predict") |>
    suppressWarnings() |>
    tibble::as_tibble()
  names(preds) <- paste("pred", names(preds), sep = "_")
  dplyr::bind_cols(data, cis, preds) |>
    ggplot2::ggplot() +
    ggplot2::aes(
      x = .data$age,
      y = .data$weight,
      col = .data$sex
    ) +
    ggplot2::geom_point() +
    ggplot2::theme(legend.position = "bottom") +
    ggplot2::geom_line(ggplot2::aes(y = .data$ci_fit)) +
    ggplot2::geom_ribbon(
      ggplot2::aes(
        ymin = .data$pred_lwr,
        ymax = .data$pred_upr
      ),
      alpha = 0.2
    ) +
    ggplot2::geom_ribbon(
      ggplot2::aes(
        ymin = .data$ci_lwr,
        ymax = .data$ci_upr
      ),
```

```
      alpha = 0.5
    ) +
    ggplot2::facet_wrap(~sex)
}
```

```
plot_PIs_and_CIs(bw, bw_lm2)
```

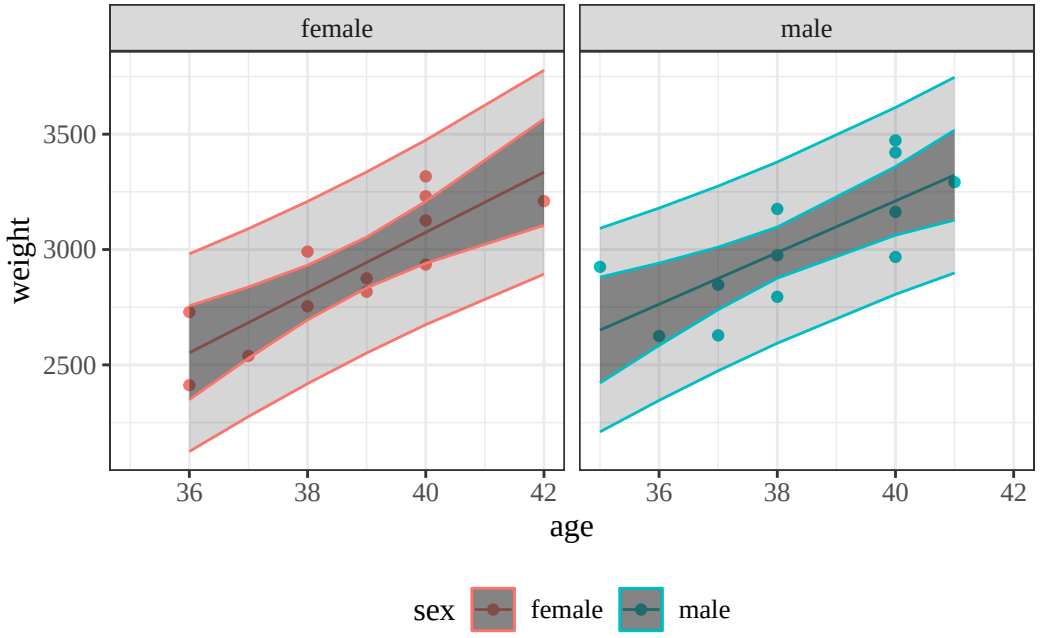


Figure 13: Confidence and prediction intervals for `birthweight` model 3

6 Assessing model fit

6.1 Goodness of fit

6.1.1 AIC and BIC

This section is adapted from Vittinghoff et al. (2012, sec. 4.5) and Kleinbaum et al. (2014, sec. 15).

When we use likelihood ratio tests, we are comparing how well different models fit the data.

Likelihood ratio tests require **nested** models: one must be a special case of the other.

AIC and BIC can be used to compare both nested and non-nested models.

6.1.2 Formulas

Definition 6.1 (Akaike Information Criterion (AIC))**.**

$$\text{AIC} = -2\ell(\hat{\theta}) + 2p$$

where $\ell(\hat{\theta})$ is the log-likelihood evaluated at the maximum-likelihood estimates $\hat{\theta}$, p is the number of estimated parameters (including $\hat{\sigma}^2$ for Gaussian models), and n is the number of observations.

Definition 6.2 (Bayesian Information Criterion (BIC))**.**

$$\text{BIC} = -2\ell(\hat{\theta}) + p\log(n)$$

where $\ell(\hat{\theta})$, p, and n are defined as in Definition 6.1.

6.1.3 Conceptual basis

Each criterion has two components:

- **Fit term** ($-2\ell(\hat{\theta})$): measures lack of fit — lower is better. A model with more parameters will always achieve a higher (or equal) log-likelihood on the observed data.
- **Penalty term** ($2p$ for AIC; $p\log(n)$ for BIC): penalizes model complexity to guard against overfitting.

Together, they balance **goodness of fit** against **parsimony**.

The AIC was introduced by Akaike (1974) and is grounded in information theory (specifically, the Kullback-Leibler divergence). The BIC was introduced by Schwarz (1978) as an approximation to the Bayes factor for model comparison.

6.1.4 AIC vs. BIC

Criterion	Penalty per parameter	Tends to select
AIC	2	larger models
BIC	$\log(n)$	smaller models

The BIC penalty exceeds the AIC penalty whenever $\log(n) > 2$, i.e., when $n > e^2 \approx 7.4$. In practice, BIC almost always penalizes additional parameters more heavily than AIC and therefore tends to select simpler (more parsimonious) models (Vittinghoff et al. 2012; Kleinbaum et al. 2014).

AIC in R

```
-2 * logLik(bw_lm2) |> as.numeric() +
  2 * (length(coef(bw_lm2)) + 1) # sigma counts as a parameter here
#> [1] 323.159

AIC(bw_lm2)
#> [1] 323.159
```

BIC in R

```
-2 * logLik(bw_lm2) |> as.numeric() +
  (length(coef(bw_lm2)) + 1) * log(nobs(bw_lm2))
#> [1] 329.049

BIC(bw_lm2)
#> [1] 329.049
```

6.1.5 Interpretation

- **Lower values are better.** There are no hypothesis tests or p-values associated with these criteria.
- To compare models, calculate the criterion for each model and choose the model with the **smallest value**.

Table 30: Unique covariate combinations in the `birthweight` data, with replicate counts

```
bw_X_unique
#> # A tibble: 12 x 3
#>    sex      age     n
#>    <fct>  <dbl> <int>
#>  1 female    36     2
#>  2 female    37     1
#>  3 female    38     2
#>  4 female    39     2
#>  5 female    40     4
#>  6 female    42     1
#>  7 male      35     1
#>  8 male      36     1
#>  9 male      37     2
#> 10 male      38     3
#> 11 male      40     4
#> 12 male      41     1
```

- Differences of less than 2 units are generally considered negligible; differences greater than 10 are considered strong evidence in favor of the lower-criterion model.
- BIC tends to favor simpler models than AIC, especially when the sample size is large.

6.1.6 (Residual) Deviance

Let q be the number of distinct covariate combinations in a data set.

```
bw_X_unique <-
  bw |>
  count(sex, age)

n_unique_bw <- nrow(bw_X_unique)
```

For example, in the `birthweight` data, there are $q = 12$ unique patterns (Table 30).

Definition 6.3 (Replicates)**.** If a given covariate pattern has more than one observation in a dataset, those observations are called **replicates**.

Example 6.1 (Replicates in the `birthweight` data)**.** In the `birthweight` dataset, there are 2 replicates of the combination "female, age 36" (Table 30).

Exercise 6.1 (Replicates in the `birthweight` data)**.** Which covariate pattern(s) in the `birthweight` data has the most replicates?

Solution 6.1 (Replicates in the `birthweight` data). Two covariate patterns are tied for most replicates: males at age 40 weeks and females at age 40 weeks. 40 weeks is the usual length for human pregnancy (Polin et al. (2011)), so this result makes sense.

```
bw_X_unique |> dplyr::filter(n == max(n))
#> # A tibble: 2 x 3
#>   sex      age     n
#>   <fct>  <dbl> <int>
#> 1 female    40     4
#> 2 male      40     4
```

Saturated models

The most complicated model we could fit would have one parameter (a mean) for each covariate pattern, plus a variance parameter:

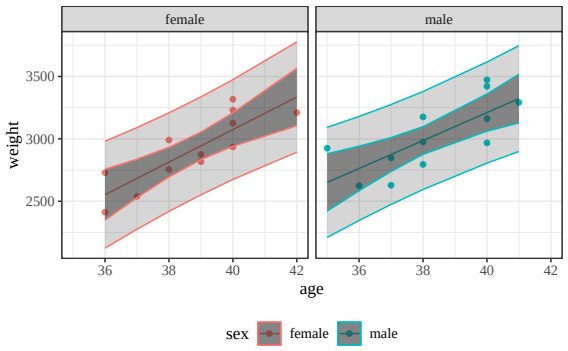
```
lm_max <-
  bw |>
  mutate(age = factor(age)) |>
  lm(
    formula = weight ~ sex:age - 1,
    data = _
  )

lm_max |>
  parameters() |>
  print_md()
```

Table 31: Saturated model for the `birthweight` data

Parameter	Coefficient	SE	95% CI	t(12)	p
sex (male) × age35	2925.00	187.92	(2515.55, 3334.45)	15.56	< .001
sex (female) × age36	2570.50	132.88	(2280.98, 2860.02)	19.34	< .001
sex (male) × age36	2625.00	187.92	(2215.55, 3034.45)	13.97	< .001
sex (female) × age37	2539.00	187.92	(2129.55, 2948.45)	13.51	< .001
sex (male) × age37	2737.50	132.88	(2447.98, 3027.02)	20.60	< .001
sex (female) × age38	2872.50	132.88	(2582.98, 3162.02)	21.62	< .001
sex (male) × age38	2982.00	108.50	(2745.60, 3218.40)	27.48	< .001
sex (female) × age39	2846.00	132.88	(2556.48, 3135.52)	21.42	< .001
sex (female) × age40	3152.25	93.96	(2947.52, 3356.98)	33.55	< .001
sex (male) × age40	3256.25	93.96	(3051.52, 3460.98)	34.66	< .001
sex (male) × age41	3292.00	187.92	(2882.55, 3701.45)	17.52	< .001
sex (female) × age42	3210.00	187.92	(2800.55, 3619.45)	17.08	< .001

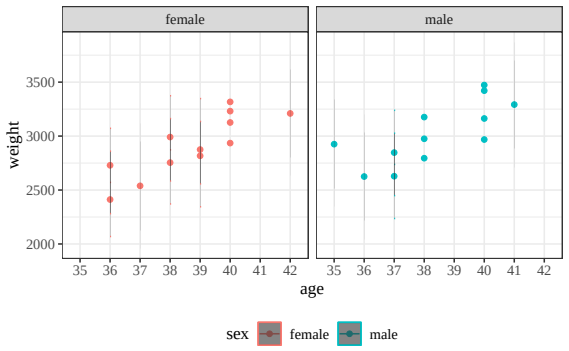
We call this model the **full**, **maximal**, or **saturated** model for this dataset.

```
plot_PIs_and_CIs(bw, bw_lm2)
```



(a) Model 3 (linear with age:sex interaction)

```
plot_PIs_and_CIs(bw |> mutate(age = factor(age)), lm_max)
```



(b) Saturated model

Figure 14: Model 3 and saturated model for `birthweight` data, with confidence and prediction intervals

We can calculate the log-likelihood of this model as usual:

```
logLik(lm_max)
#> 'log Lik.' -151.402 (df=13)
```

We can compare this model to our other models using chi-square tests, as usual:

```
lrtest(lm_max, bw_lm2)
#> # A tibble: 2 x 5
#>   `#Df` LogLik    Df Chisq `Pr(>Chisq)`
#>   <dbl>  <dbl> <dbl> <dbl>        <dbl>
#> 1    13  -151.    NA  NA         NA
#> 2     5  -157.    -8  10.4        0.241
```

The likelihood ratio statistic for this test is

$$\lambda = 2 * (\ell_{\text{full}} - \ell) = 10.355374$$

where:

- ℓ_{full} is the log-likelihood of the full model: -151.401601
- ℓ is the log-likelihood of our comparison model (two slopes, two intercepts): -156.579288

This statistic is called the **deviance** or **residual deviance** for our two-slopes and two-intercepts model; it tells us how much the likelihood of that model deviates from the likelihood of the maximal model.

The corresponding p-value tells us whether there we have enough evidence to detect that our two-slopes, two-intercepts model is a worse fit for the data than the maximal model; in other words, it tells us if there's evidence that we missed any important patterns. (Remember, a nonsignificant p-value could mean that we didn't miss anything and a more complicated model is unnecessary, or it could mean we just don't have enough data to tell the difference between these models.)

6.1.7 Null Deviance

Similarly, the *least* complicated model we could fit would have only one mean parameter, an intercept:

$$\mathrm{E}[Y|X = x] = \beta_0$$

We can fit this model in R like so:

```
lm0 <- lm(weight ~ 1, data = bw)

lm0 |>
  parameters() |>
  print_md()
```

Parameter	Coefficient	SE	95% CI	t(23)	p
(Intercept)	2967.67	57.58	(2848.56, 3086.77)	51.54	$< .001$

```
plot_PIs_and_CIs(bw, lm0)
```

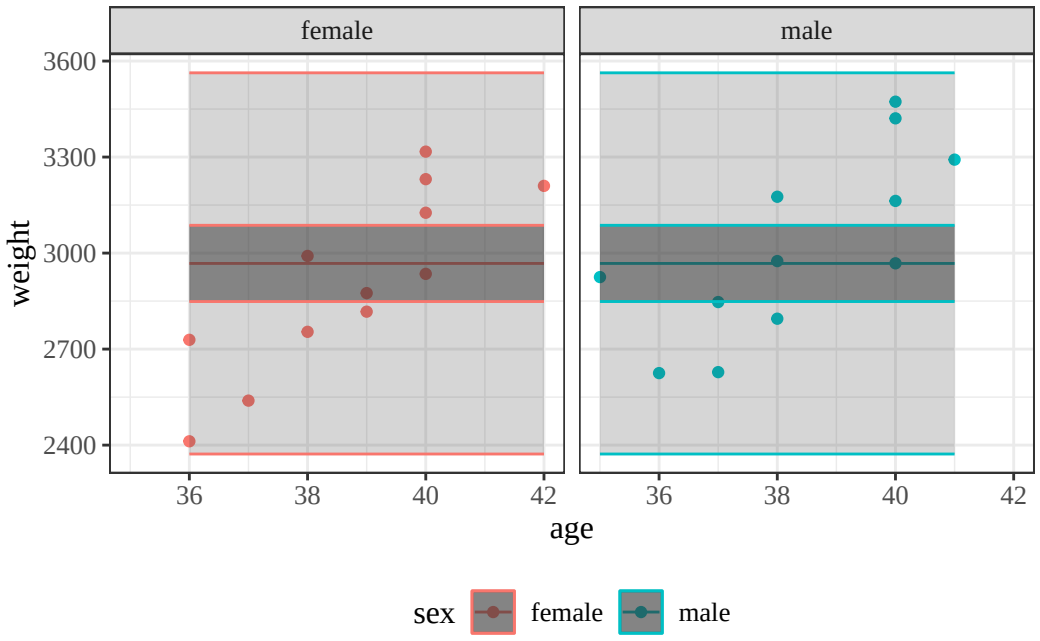


Figure 15: Null model for birthweight data, with 95% confidence and prediction intervals.

This model also has a likelihood:

```
logLik(lm0)
#> 'log Lik.' -168.955 (df=2)
```

And we can compare it to more complicated models using a likelihood ratio test:

```
lrtest(bw_lm2, lm0)
#> # A tibble: 2 x 5
#>   `#Df` LogLik    Df Chisq `Pr(>Chisq)`
#>   <dbl>  <dbl> <dbl> <dbl>        <dbl>
#> 1     5  -157.    NA  NA     NA
#> 2     2  -169.    -3  24.8    0.0000174
```

The likelihood ratio statistic for the test comparing the null model to the maximal model is

$$\lambda = 2 * (\ell_{\text{full}} - \ell_0) = 35.106732$$

where:

- ℓ_0 is the log-likelihood of the null model: -168.954967
- ℓ_{full} is the log-likelihood of the maximal model: -151.401601

In R, this test is:

```
lrtest(lm_max, lm0)
#> # A tibble: 2 x 5
#>   `#Df` LogLik    Df Chisq `Pr(>Chisq)`
#>   <dbl>  <dbl> <dbl> <dbl>        <dbl>
#> 1    13  -151.    NA  NA      NA
#> 2     2  -169.   -11  35.1     0.000238
```

This log-likelihood ratio statistic is called the **null deviance**. It tells us whether we have enough data to detect a difference between the null and full models.

6.2 Gaussian Deviance vs. GLM Deviance

The residual deviance is a general concept that applies to all GLMs, including Gaussian linear regression. For any GLM, the residual deviance is:

$$D = 2(\ell_{\text{sat}} - \ell(\hat{\beta})) \tag{22}$$

where ℓ_{sat} is the log-likelihood of the saturated model and $\ell(\hat{\beta})$ is the log-likelihood of the fitted model. However, this formula simplifies differently depending on the distribution family, and the resulting test statistics have different null distributions.

6.2.1 Gaussian linear regression deviance

From Equation 8, the Gaussian log-likelihood is:

$$\ell(\hat{\beta}, \hat{\sigma}^2) = -\frac{n}{2}\log(2\pi\hat{\sigma}^2) - \frac{1}{2\hat{\sigma}^2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

The saturated model has one free mean parameter per distinct covariate pattern. When there are no replicates (each covariate pattern appears exactly once), it sets $\hat{\mu}_i = y_i$ for every observation, so its residual sum of squares is zero:

$$\ell_{\text{sat}}(\hat{\sigma}^2) = -\frac{n}{2}\log(2\pi\hat{\sigma}^2)$$

Substituting into Equation 22, the Gaussian deviance simplifies to the **residual sum of squares** (RSS), scaled by $\hat{\sigma}^2$:

$$D = 2(\ell_{\text{sat}} - \ell(\hat{\beta})) = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\hat{\sigma}^2} = \frac{\text{RSS}}{\hat{\sigma}^2}$$

Because σ^2 is unknown and must be estimated, comparing deviances between two nested Gaussian models uses an **F-test**, which is exact under Gaussian assumptions. Substituting $D = \text{RSS}/\hat{\sigma}^2$, the $\hat{\sigma}^2$ factors cancel:

$$F = \frac{(D_1 - D_2)/(p_2 - p_1)}{D_2/(n - p_2)} = \frac{(\text{RSS}_1 - \text{RSS}_2)/(p_2 - p_1)}{\text{RSS}_2/(n - p_2)} \sim F_{p_2 - p_1,\, n - p_2}$$

In R, `deviance()` applied to an `lm` object returns **RSS** (the unscaled deviance):

```
deviance(bw_lm2)
#> [1] 652425
sum(residuals(bw_lm2)^2)
#> [1] 652425
```

The two expressions above return the same value.

The Gaussian linear regression model can equivalently be fit as a GLM with `family = gaussian`, which also returns RSS as the deviance:

```
bw_glm2 <- glm(
  weight ~ sex + age + sex:age,
  data = bw,
  family = gaussian
)

deviance(bw_lm2)
#> [1] 652425
deviance(bw_glm2)
#> [1] 652425
```

`deviance(bw_lm2)` and `deviance(bw_glm2)` return the same value, confirming that Gaussian linear regression is a special case of the GLM framework where the deviance equals RSS.

6.2.2 Non-Gaussian GLM deviance

For non-Gaussian GLMs, the deviance does **not** simplify to RSS. The formula depends on the distribution family:

Poisson:

$$D = 2\sum_{i=1}^{n}\left[y_i \log\left(\frac{y_i}{\hat{\mu}_i}\right) - (y_i - \hat{\mu}_i)\right]$$

Binomial:

$$D = 2\sum_{i=1}^{n}\left[y_i \log\left(\frac{y_i}{\hat{\pi}_i}\right) + (n_i - y_i)\log\left(\frac{n_i - y_i}{n_i - \hat{\pi}_i}\right)\right]$$

For Poisson and Binomial models, the dispersion parameter $\phi = 1$ is **fixed** rather than estimated. Consequently, the difference in deviances between two nested models follows an approximate χ^2 distribution:

$$D_1 - D_2 \dot{\sim} \chi^2_{p_2 - p_1}$$

This asymptotic result replaces the exact F-test used for Gaussian models.

6.2.3 Saturated vs. fully parametrized models with replicates

When some covariate patterns appear more than once (i.e., when there are **replicates**), it is important to distinguish between two special models:

- The **saturated model** has one free mean parameter per **distinct covariate pattern** (q parameters, where $q \leq n$ is the number of unique patterns).
- The **fully parametrized model** has one free mean parameter per **observation** (n parameters).

When there are no replicates ($q = n$), these two coincide. When there are replicates ($q < n$), the saturated model constrains all observations sharing a covariate pattern to have the same mean, but places no constraint on means across different patterns. See Kleinbaum and Klein (2010) for further discussion of this distinction.

Deviance is always measured relative to the **saturated model**, not the fully parametrized model.

Gaussian deviance with replicates

When covariate pattern k has n_k replicates with sample mean $\bar{y}_k$, the saturated model fits $\hat{\mu}_k = \bar{y}_k$ for each pattern k, so its residual sum of squares equals the **within-group (pure error) SS**:

$$\text{RSS}_{\text{sat}} = \sum_{k=1}^{q}\sum_{i:\tilde{x}_i = \tilde{x}_k}(y_i - \bar{y}_k)^2$$

This is nonzero whenever any covariate pattern has replicates with different response values. The Gaussian deviance relative to the saturated model is therefore:

$$D = 2(\ell_{\text{sat}} - \ell(\hat{\beta})) = \frac{\text{RSS} - \text{RSS}_{\text{sat}}}{\hat{\sigma}^2}$$

> **Note**
>
> R's `deviance()` applied to an `lm` object returns the **total fitted-model RSS**, not the deviance relative to the saturated model. To compute the deviance relative to the saturated model, subtract the saturated model's RSS: `deviance(lm_fit) - deviance(lm_saturated)`.

For the `birthweight` data, we can verify this directly using `bw_lm2` (the interaction model) and `lm_max` (the saturated model):

```
deviance(bw_lm2)                      # total RSS of fitted model
#> [1] 652425
deviance(lm_max)                      # within-group (pure error) SS
#> [1] 423783
deviance(bw_lm2) - deviance(lm_max)   # lack-of-fit SS (deviance vs. saturated)
#> [1] 228642
```

The lack-of-fit SS (`deviance(bw_lm2) - deviance(lm_max)`) measures how much additional unexplained variation remains after accounting for pure measurement error within covariate patterns.

GLM deviance with replicates

For a Binomial GLM fit to data **grouped by covariate pattern** (with y_k events and n_k observations for pattern k), the saturated model sets $\hat{\pi}_k^{\text{sat}} = y_k/n_k$ for each pattern k. R's `deviance()` correctly computes $2(\ell_{\text{sat}} - \ell(\hat{\beta}))$ using this grouping:

$$D = 2\sum_{k=1}^{q}\left[y_k \log\left(\frac{y_k/n_k}{\hat{\pi}_k}\right) + (n_k - y_k)\log\left(\frac{1-y_k/n_k}{1-\hat{\pi}_k}\right)\right]$$

By convention, terms with $y_k = 0$ or $y_k = n_k$ contribute zero to the sum, since $0\log(0) = 0$ in the limit.

When binomial data is **ungrouped** (individual Bernoulli observations, $n_i = 1$), R uses the **fully parametrized** model as its reference — assigning $\hat{\pi}_i = y_i \in \{0, 1\}$ to each individual observation. Since each predicted probability is exactly 0 or 1, every Bernoulli likelihood contribution equals 1, and hence $\ell_{\text{fp}} = 0$. Thus R's `deviance()` returns $-2\ell(\hat{\beta})$.

We can verify this directly: observations are ungrouped Bernoulli with repeated covariate patterns ($x \in \{0, 1\}$ appears three times each).

```
set.seed(42)
x_ug <- rep(0:1, each = 3)
y_ug <- c(0L, 1L, 0L, 1L, 1L, 0L)
fit_ug <- glm(y_ug ~ x_ug, family = binomial)
deviance(fit_ug)                      # R's deviance
#> [1] 7.63817
-2 * as.numeric(logLik(fit_ug))       # -2 * log-likelihood (using ell_fp = 0)
#> [1] 7.63817
```

The two values are equal, confirming that R uses $\ell_{\text{fp}} = 0$ as its reference when data are ungrouped.

> **Note**
>
> This reference model is the **fully parametrized** model (one parameter per observation), not the **saturated** model (one parameter per distinct covariate pattern). They coincide only when there are no repeated covariate patterns ($q = n$). When patterns do repeat ($q < n$), the saturated model sets $\hat{\pi}_k = y_k/n_k$ per pattern, giving $\ell_{\text{sat}} < 0$.
> `deviance()` for ungrouped data **cannot** be used as a goodness-of-fit test against the χ^2 distribution when $q < n$. The correct GOF statistic is $2(\ell_{\text{sat}} - \ell(\hat{\beta}))$, but R's `deviance()` for ungrouped data returns $-2\ell(\hat{\beta})$ (using $\ell_{\text{fp}} = 0$). These two quantities differ by $-2\ell_{\text{sat}} > 0$

whenever $q < n$. Even if each covariate pattern has many replicates (large n_k), R's ungrouped deviance is the wrong statistic to compare against $\chi^2(q-p)$. To obtain a valid GOF test when patterns repeat, fit the model using **grouped** data (one row per pattern with y_k and n_k), so that R uses the saturated model as its reference.
For further discussion, see Dunn and Smyth (2018, chap. 9) and this Stats Stack Exchange thread[a].

[a] https://stats.stackexchange.com/questions/626597/is-there-a-justification-for-the-bernoulli-deviance-in-the-r-stats-package

6.2.4 Summary

Feature	Gaussian linear regression	Non-Gaussian GLMs (e.g., Poisson, Binomial)
Deviance formula	$(\text{RSS} - \text{RSS}_{\text{sat}})/\hat{\sigma}^2$	$2(\ell_{\text{sat}} - \ell(\hat{\beta}))$
`deviance()` in R	Returns total RSS	Returns $2(\ell_{\text{sat}} - \ell(\hat{\beta}))$
Saturated model reference	Per covariate pattern	Per covariate pattern (grouped) or per observation (ungrouped)
Dispersion ϕ	Unknown; estimated as $s^2 = \text{RSS}/(n-p)$	Fixed ($\phi = 1$)
Test for nested models	F-test (exact)	χ^2-test (asymptotic)

6.3 Diagnostics

Tip

This section is adapted from Dobson and Barnett (2018, secs. 6.2–6.3) and Dunn and Smyth (2018) Chapter 3[a].

[a] https://link.springer.com/chapter/10.1007/978-1-4419-0118-7_3

6.3.1 Assumptions in linear regression models

$$Y_i|\tilde{X}_i \sim_{\perp\!\!\!\perp} \text{N}(\mu_i, \sigma^2)$$
$$\mu_i = \tilde{x} \cdot \tilde{\beta}$$

1. Normality

The model assumes that the distribution conditional on a given X value is Gaussian.

2. Correct Functional Form of Conditional Mean Structure (Linear Component)

The model assumes that the conditional means have the structure:

$$\text{E}[Y|\tilde{X} = \tilde{x}] = \tilde{x}'\tilde{\beta}$$

3. Homoskedasticity

The model assumes that variance σ^2 is constant (with respect to $\tilde{x}$).

4. Independence

The model assumes that the observations are statistically independent.

6.3.2 Direct visualization

The most direct way to examine the fit of a model is to compare it to the raw observed data.

```r
bw <-
  bw |>
  mutate(
    predlm2 = predict(bw_lm2)
  ) |>
  arrange(sex, age)

plot1_interact <-
  plot1 %+% bw +
  geom_line(aes(y = predlm2))

print(plot1_interact)
```

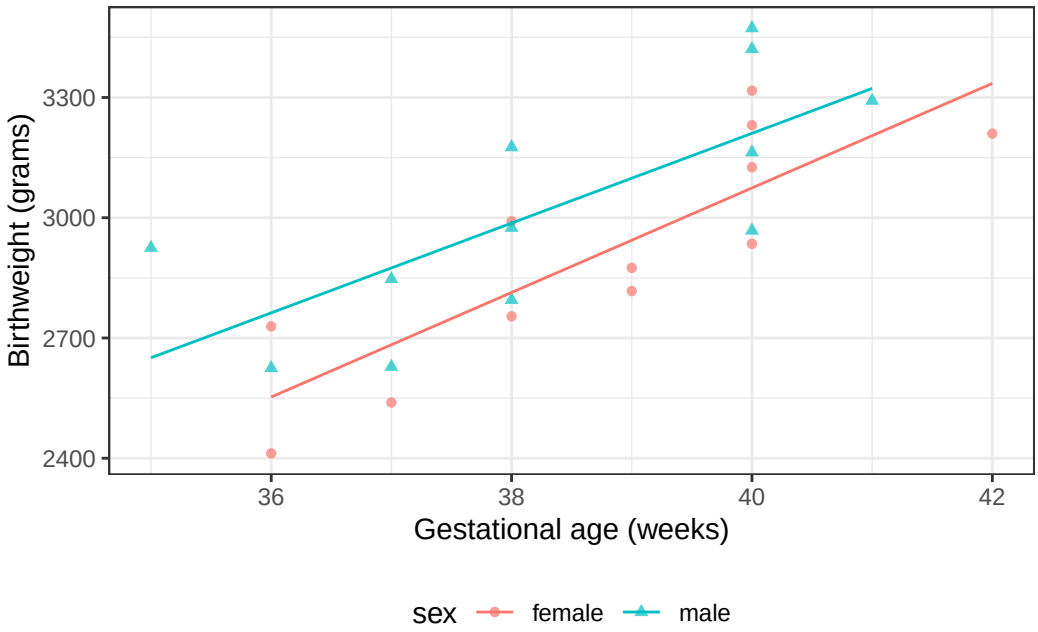


Figure 16: Birthweight model with interaction term

It's not easy to assess these assumptions from this model. If there are multiple continuous covariates, it becomes even harder to visualize the raw data.

Fitted model for `hers` data

Consider the `hers` data from Vittinghoff et al. (2012).

The "heart and estrogen/progestin study" (HERS) was a clinical trial of hormone therapy for prevention of recurrent heart attacks and death among 2,763 post-menopausal women with existing coronary heart disease (CHD) (Hulley et al. 1998).

Suppose we consider models with and without intercept terms (i.e., possibly forcing the intercept to go through 0):

```r
hers_lm_with_int <- lm(
  na.action = na.exclude,
  LDL ~ smoking * age, data = hers
)
```

Table 32: `hers` data

```
hers <- fs::path_package("rme", "extdata/hersdata.dta") |>
  haven::read_dta()
hers
#> # A tibble: 2,763 x 37
#>    HT             age raceth  nonwhite smoking drinkany exercise physact globrat
#>    <dbl+lbl>    <dbl> <dbl+l> <dbl+lb> <dbl+l> <dbl+lb> <dbl+lb> <dbl+l> <dbl+l>
#>  1 0 [placebo]     70 2 [Afr~ 1 [yes]  0 [no]  0 [no]   0 [no]   5 [muc~ 3 [goo~
#>  2 0 [placebo]     62 2 [Afr~ 1 [yes]  0 [no]  0 [no]   0 [no]   1 [muc~ 3 [goo~
#>  3 1 [hormone ~    69 1 [Whi~ 0 [no]   0 [no]  0 [no]   0 [no]   3 [abo~ 3 [goo~
#>  4 0 [placebo]     64 1 [Whi~ 0 [no]   1 [yes] 1 [yes]  0 [no]   1 [muc~ 3 [goo~
#>  5 0 [placebo]     65 1 [Whi~ 0 [no]   0 [no]  0 [no]   0 [no]   2 [som~ 3 [goo~
#>  6 1 [hormone ~    68 2 [Afr~ 1 [yes]  0 [no]  1 [yes]  0 [no]   3 [abo~ 3 [goo~
#>  7 0 [placebo]     70 1 [Whi~ 0 [no]   0 [no]  0 [no]   0 [no]   3 [abo~ 2 [fai~
#>  8 1 [hormone ~    69 1 [Whi~ 0 [no]   0 [no]  0 [no]   1 [yes]  5 [muc~ 4 [ver~
#>  9 1 [hormone ~    61 1 [Whi~ 0 [no]   0 [no]  1 [yes]  1 [yes]  3 [abo~ 4 [ver~
#> 10 1 [hormone ~    62 1 [Whi~ 0 [no]   1 [yes] 1 [yes]  0 [no]   2 [som~ 3 [goo~
#> # i 2,753 more rows
#> # i 28 more variables: poorfair <dbl+lbl>, medcond <dbl>, htnmeds <dbl+lbl>,
#> #   statins <dbl+lbl>, diabetes <dbl+lbl>, dmpills <dbl+lbl>,
#> #   insulin <dbl+lbl>, weight <dbl>, BMI <dbl>, waist <dbl>, WHR <dbl>,
#> #   glucose <dbl>, weight1 <dbl>, BMI1 <dbl>, waist1 <dbl>, WHR1 <dbl>,
#> #   glucose1 <dbl>, tchol <dbl>, LDL <dbl>, HDL <dbl>, TG <dbl>, tchol1 <dbl>,
#> #   LDL1 <dbl>, HDL1 <dbl>, TG1 <dbl>, SBP <dbl>, DBP <dbl>, age10 <dbl>
```

```
library(equatiomatic)
equatiomatic::extract_eq(hers_lm_with_int)
```

$$\text{LDL} = \alpha + \beta_1(\text{smoking}) + \beta_2(\text{age}) + \beta_3(\text{smoking} \times \text{age}) + \epsilon \tag{23}$$

```
hers_lm_no_int <- lm(
  na.action = na.exclude,
  LDL ~ age + smoking:age - 1, data = hers
)

library(equatiomatic)
equatiomatic::extract_eq(hers_lm_no_int)
```

$$\text{LDL} = \beta_1(\text{age}) + \beta_2(\text{age} \times \text{age}_{\text{smoking}}) + \epsilon \tag{24}$$

Table 33: `hers` data models with and without intercepts

(a) With intercept

```
library(gtsummary)
hers_lm_with_int |>
  tbl_regression(intercept = TRUE)
```

Characteristic	Beta	95% CI	p-value
(Intercept)	154	138, 170	<0.001
current smoker	54	15, 94	0.007
age in years	-0.14	-0.38, 0.09	0.2
current smoker * age in years	-0.79	-1.4, -0.17	0.012

Abbreviation: CI = Confidence Interval

(b) No intercept

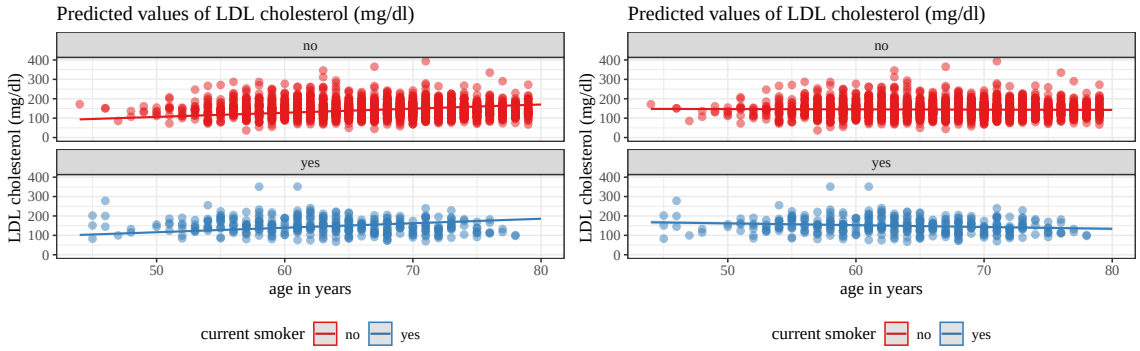
```
hers_lm_no_int |>
  tbl_regression(intercept = TRUE)
```

Characteristic	Beta	95% CI	p-value
age in years	2.1	2.1, 2.2	<0.001
current smoker	0.19	0.12, 0.26	<0.001
age in years * current smoker			

Abbreviation: CI = Confidence Interval

```
library(sjPlot)

hers_plot1 <- hers_lm_no_int |>
  sjPlot::plot_model(
    type = "pred",
    terms = c("age", "smoking"),
    show.data = TRUE
  ) +
  facet_wrap(~group_col, ncol = 1) +
  expand_limits(y = 0) +
  theme(legend.position = "bottom")

hers_plot1
```

```
library(sjPlot)

hers_plot2 <- hers_lm_with_int |>
  sjPlot::plot_model(
    type = "pred",
    terms = c("age", "smoking"),
    show.data = TRUE
  ) +
  facet_wrap(~group_col, ncol = 1) +
  expand_limits(y = 0) +
  theme(legend.position = "bottom")

hers_plot2
```



(a) No intercept

(b) With intercept

Figure 17: `hers` data models with and without intercepts

6.3.3 Residuals

Maybe we can transform the data and model in some way to make it easier to inspect.

Definition 6.4 (Residual noise/deviation from the population mean)**.** The **residual noise** in a probabilistic model $p(Y)$, also known as the **residual deviation of an observation from its population mean** or **residual** for short, is the difference between an observed value y and its population mean:

$$\varepsilon(y) \stackrel{\text{def}}{=} y - \mathrm{E}[Y] \tag{25}$$

We use the same notation for residual noise that we used for errors[17].

$\mathrm{E}[Y]$ can be viewed as an estimate of Y, before y is observed. Conversely, each observation y can be viewed as an estimate of $\mathrm{E}[Y]$ (albeit an imprecise one, individually, since $n = 1$).

We can rearrange Equation 25 to view y as the sum of its mean plus the residual noise:

$$y = \mathrm{E}[Y] + \varepsilon(y)$$

Theorem 6.1 (Residuals in Gaussian models)**.** *If Y has a Gaussian distribution, then $\varepsilon(Y)$ also has a Gaussian distribution, and vice versa.*

Proof. Left to the reader. □

Definition 6.5 (Residuals of a fitted model value)**.** The **residual of a fitted value** $\hat{y}$ (shorthand: "residual") is its error[18] relative to the observed data:

$$\begin{aligned} e(\hat{y}) &\stackrel{\text{def}}{=} \varepsilon(\hat{y}) \\ &= y - \hat{y} \end{aligned}$$

Example 6.2 (residuals in `birthweight` data)**.**

[17] estimation.qmd#def-error
[18] estimation.qmd#def-error

```
plot1_interact +
  facet_wrap(~sex) +
  geom_segment(
    aes(
      x = age,
      y = predlm2,
      xend = age,
      yend = weight,
      col = sex,
      group = id
    ),
    linetype = "dotted"
  )
```

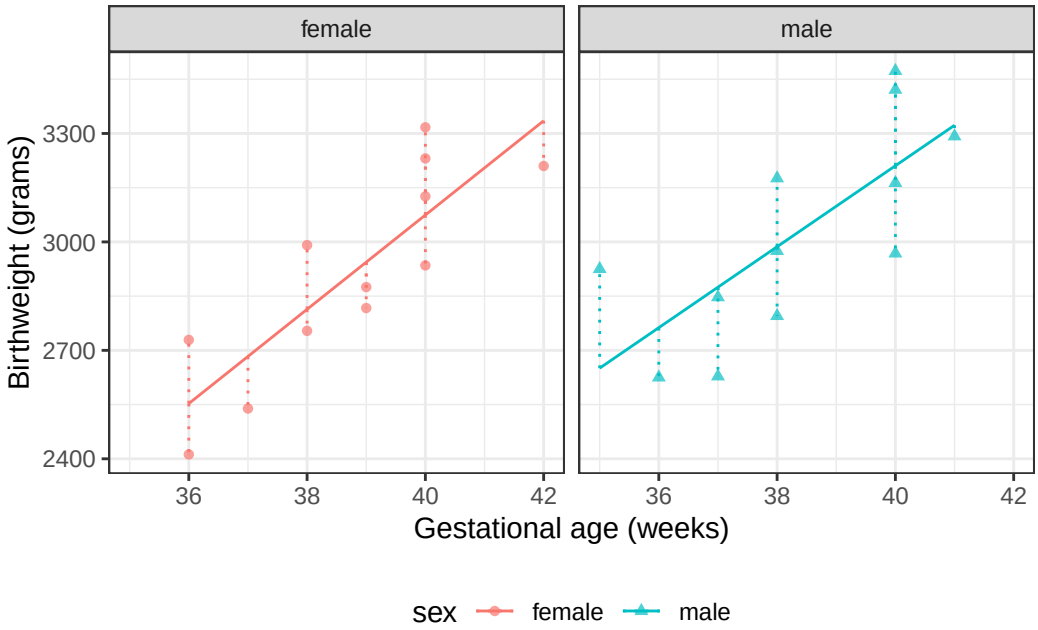


Figure 18: Fitted values and residuals for interaction model for `birthweight` data

---

Residuals of fitted values vs residual noise

$e(\hat{y})$ can be seen as the maximum likelihood estimate of the residual noise:

$$\begin{aligned} e(\hat{y}) &= y - \hat{y} \\ &= \hat{\varepsilon}_{ML} \end{aligned}$$

General characteristics of residuals

Theorem 6.2. *If $\hat{E}[Y]$ is an unbiased*[19] *estimator of the mean $E[Y]$, then:*

$$E[e(y)] = 0 \tag{26}$$

$$Var(e(y)) \approx \sigma^2 \tag{27}$$

---

[19] estimation.qmd#sec-unbiased-estimators

Proof.

Equation 26:

$$\begin{aligned} \mathrm{E}[e(y)] &= \mathrm{E}[y - \hat{y}] \\ &= \mathrm{E}[y] - \mathrm{E}[\hat{y}] \\ &= \mathrm{E}[y] - \mathrm{E}[y] \\ &= 0 \end{aligned}$$

Equation 27:

$$\begin{aligned} \mathrm{Var}(e(y)) &= \mathrm{Var}(y - \hat{y}) \\ &= \mathrm{Var}(y) + \mathrm{Var}(\hat{y}) - 2\mathrm{Cov}(y, \hat{y}) \\ &\approx \mathrm{Var}(y) + 0 - 2 \cdot 0 \\ &= \mathrm{Var}(y) \\ &= \sigma^2 \end{aligned}$$

□

Characteristics of residuals in Gaussian models

With enough data and a correct model, the residuals will be approximately Gaussian distributed, with variance σ^2, which we can estimate using $\hat{\sigma}^2$; that is:

$$e_i \sim_{\text{iid}} N(0, \hat{\sigma}^2)$$

Computing residuals in R

R provides a function for residuals:

```
resid(bw_lm2)
#>         1         2         3         4         5         6         7         8
#>  176.2667 -140.7333 -144.1333  -59.5333  177.4667 -126.9333  -68.9333  242.6667
#>         9        10        11        12        13        14        15        16
#> -139.3333   51.6667  156.6667 -125.1333  274.2759 -137.7069  -27.6897 -246.6897
#>        17        18        19        20        21        22        23        24
#> -191.6724  189.3276  -11.6724 -242.6379  -47.6379  262.3621  210.3621  -30.6207
```

Exercise 6.2. Check R's output by computing the residuals directly.

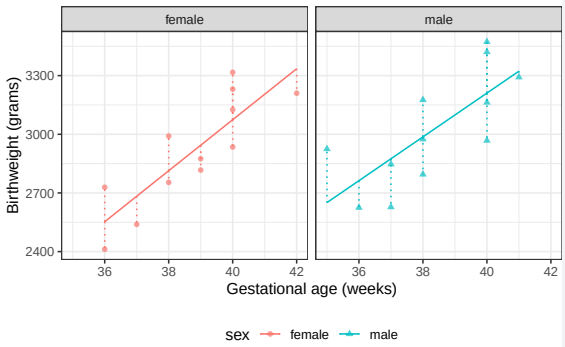
Solution.

```
bw$weight - fitted(bw_lm2)
#>         1         2         3         4         5         6         7         8
#>  176.2667 -140.7333 -144.1333  -59.5333  177.4667 -126.9333  -68.9333  242.6667
#>         9        10        11        12        13        14        15        16
#> -139.3333   51.6667  156.6667 -125.1333  274.2759 -137.7069  -27.6897 -246.6897
#>        17        18        19        20        21        22        23        24
#> -191.6724  189.3276  -11.6724 -242.6379  -47.6379  262.3621  210.3621  -30.6207
```

This matches R's output!

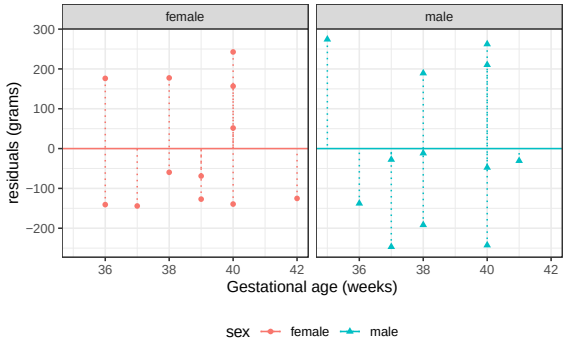
Graphing the residuals

```
plot1_interact +
  facet_wrap(~sex) +
  geom_segment(
    aes(
      x = age,
      y = predlm2,
      xend = age,
      yend = weight,
      col = sex,
      group = id
    ),
    linetype = "dotted"
  )
```



(a) fitted values

```
bw <- bw |>
  mutate(
    resids_intxn =
      weight - fitted(bw_lm2)
  )

plot_bw_resid <-
  bw |>
  ggplot(aes(
    x = age,
    y = resids_intxn,
    linetype = sex,
    shape = sex,
    col = sex
  )) +
  theme_bw() +
  xlab("Gestational age (weeks)") +
  ylab("residuals (grams)") +
  theme(legend.position = "bottom") +
  geom_hline(aes(
    yintercept = 0,
    col = sex
  )) +
  geom_segment(
    aes(yend = 0),
    linetype = "dotted"
  ) +
  geom_point()
# expand_limits(y = 0, x = 0) +
geom_point(alpha = .7)
#> geom_point: na.rm = FALSE
#> stat_identity: na.rm = FALSE
#> position_identity
print(plot_bw_resid + facet_wrap(~sex))
```



(b) Residuals

Figure 19: Fitted values and residuals for interaction model for `birthweight` data

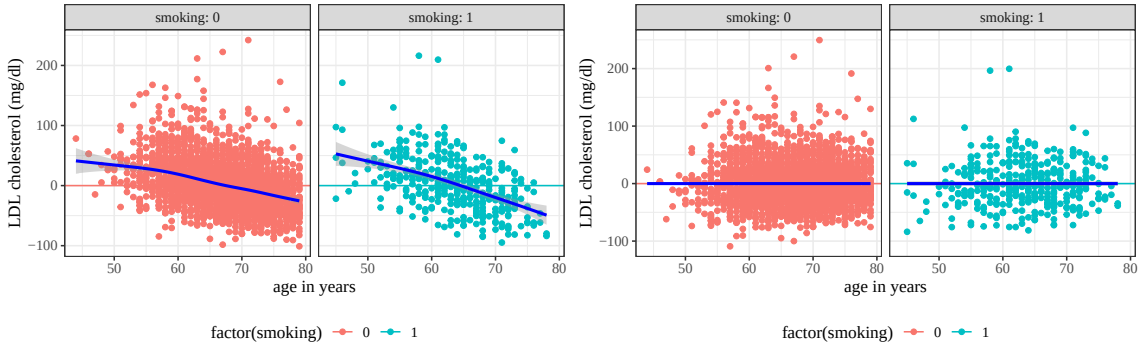
---

Residuals versus predictors

```
hers <- hers |>
  mutate(
    resids_no_intcpt =
      LDL - fitted(hers_lm_no_int),
    resids_with_intcpt =
      LDL - fitted(hers_lm_with_int)
  )
```

```
hers |>
  arrange(age) |>
  ggplot() +
  aes(x = age, y = resids_no_intcpt, col
  geom_point() +
  geom_hline(aes(yintercept = 0, col = fa
  facet_wrap(~smoking, labeller = "label_
  theme(legend.position = "bottom") +
  geom_smooth(col = "blue")
```

```
hers |>
  arrange(age) |>
  ggplot() +
  aes(x = age, y = resids_with_intcpt, col = factor(smoking
  geom_point() +
  geom_hline(aes(yintercept = 0, col = factor(smoking))) +
  facet_wrap(~smoking, labeller = "label_both") +
  theme(legend.position = "bottom") +
  geom_smooth(col = "blue")
```



(a) no intercept

(b) with intercept

Figure 20: Residuals of `hers` data vs predictors

Residuals versus fitted values

If the model contains multiple continuous covariates, how do we check for errors in the mean structure assumption?

```
library(ggfortify)
hers_lm_no_int |>
  update(na.action = na.omit) |>
  autoplot(
    which = 1,
    ncol = 1,
    smooth.colour = NA
  ) +
  geom_hline(yintercept = 0, col = "red")
```

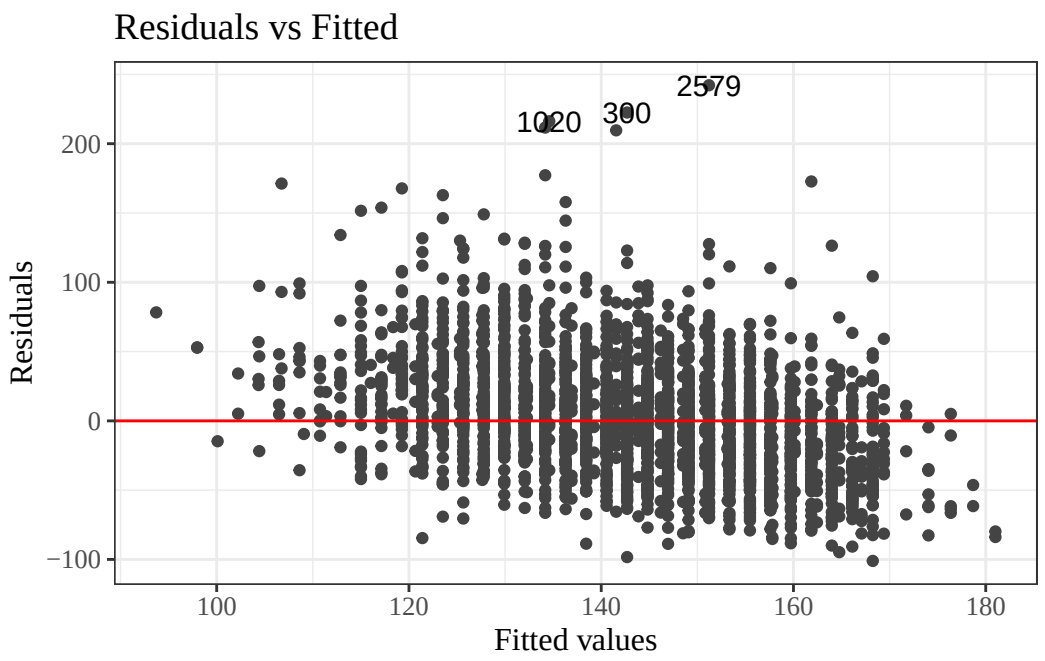


Figure 21: Residuals of interaction model for `hers` data

We can add a LOESS smooth to visualize where the residual mean is nonzero:

```
library(ggfortify)
hers_lm_no_int |>
  update(na.action = na.omit) |>
  autoplot(
    which = 1,
    ncol = 1
  ) +
  geom_hline(yintercept = 0, col = "red")
```

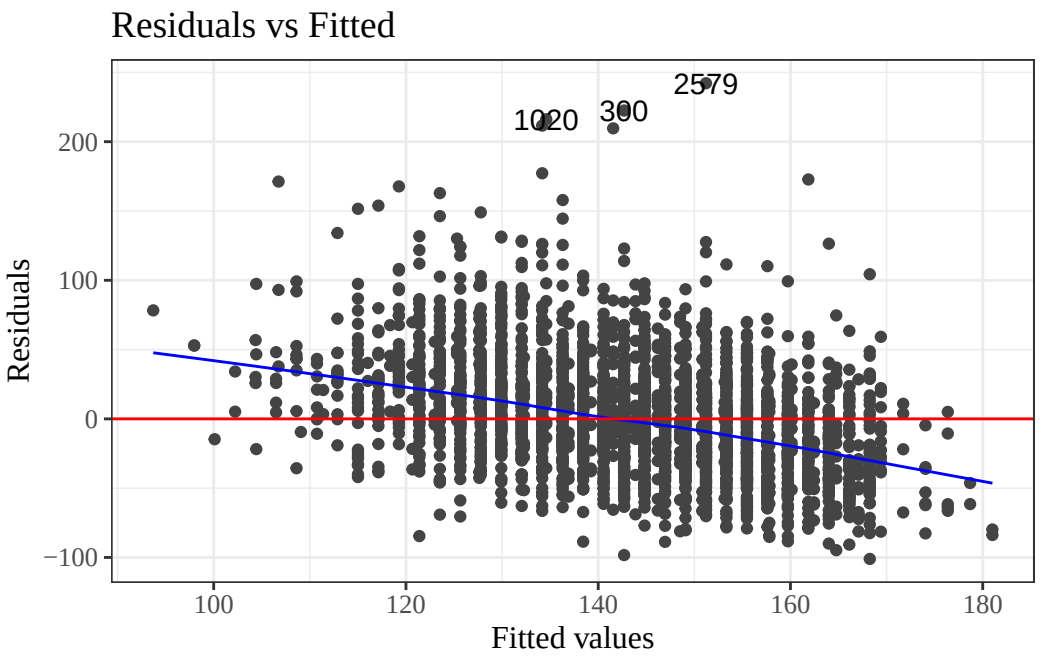
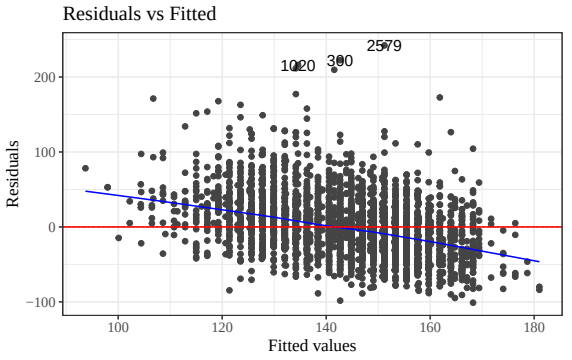


Figure 22: Residuals of interaction model for `hers` data, no intercept term

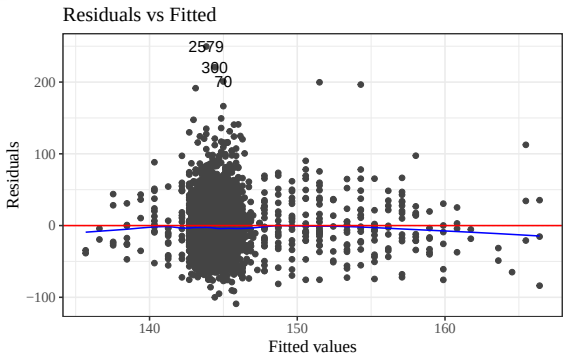
---

```
library(ggfortify)
hers_lm_no_int |>
  update(na.action = na.omit) |>
  autoplot(
    which = 1,
    ncol = 1
  ) +
  geom_hline(yintercept = 0, col = "red")
```



(a) no intercept term

```
hers_lm_with_int |>
  update(na.action = na.omit) |>
  autoplot(
    which = 1,
    ncol = 1
  ) +
  geom_hline(yintercept = 0, col = "red")
```



(b) with intercept term

Figure 23: Residuals of interaction model for `hers` data, with and without intercept term

---

Definition 6.6 (Standardized residuals)**.**

$$r_i = \frac{e_i}{\widehat{SD}(e_i)}$$

Hence, with enough data and a correct model, the standardized residuals will be approximately standard Gaussian; that is,

$$r_i \sim_{\text{iid}} N(0,1)$$

6.3.4 Marginal distributions of residuals

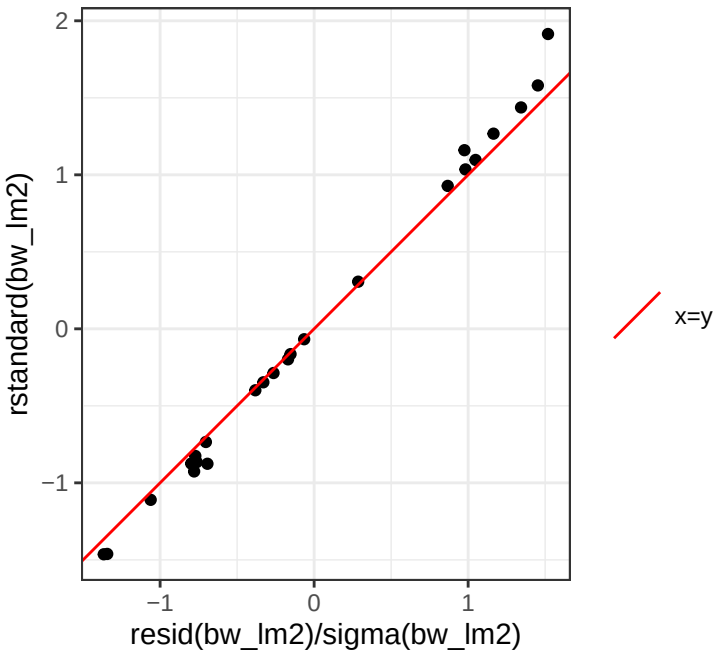
To look for problems with our model, we can check whether the residuals e_i and standardized residuals r_i look like they have the distributions that they are supposed to have, according to the model.

Standardized residuals in R

```
rstandard(bw_lm2)
#>          1          2          3          4          5          6          7
#>  1.1598166 -0.9260109 -0.8747917 -0.3472255  1.0350665 -0.7347315 -0.3990086
#>          8          9         10         11         12         13         14
#>  1.4375164 -0.8253872  0.3060646  0.9280669 -0.8761592  1.9142780 -0.8655921
#>         15         16         17         18         19         20         21
#> -0.1642993 -1.4637574 -1.1101599  1.0965787 -0.0676062 -1.4615865 -0.2869582
#>         22         23         24
#>  1.5803994  1.2671652 -0.1980543
resid(bw_lm2) / sigma(bw_lm2)
#>          1          2          3          4          5          6          7
#>  0.9759331 -0.7791962 -0.7980209 -0.3296173  0.9825771 -0.7027900 -0.3816622
#>          8          9         10         11         12         13         14
#>  1.3435690 -0.7714449  0.2860621  0.8674141 -0.6928239  1.5185792 -0.7624398
#>         15         16         17         18         19         20         21
#> -0.1533089 -1.3658431 -1.0612299  1.0482473 -0.0646265 -1.3434099 -0.2637562
#>         22         23         24
#>  1.4526163  1.1647086 -0.1695371
```

These are not quite the same, because R is doing something more complicated and precise to get the standard errors. Let's not worry about those details for now; the difference is pretty small in this case:

```
rstandard_compare_plot <-
  tibble(
    x = resid(bw_lm2) / sigma(bw_lm2),
    y = rstandard(bw_lm2)
  ) |>
  ggplot(aes(x = x, y = y)) +
  geom_point() +
  theme_bw() +
  coord_equal() +
  xlab("resid(bw_lm2)/sigma(bw_lm2)") +
  ylab("rstandard(bw_lm2)") +
  geom_abline(
    aes(
      intercept = 0,
      slope = 1,
      col = "x=y"
    )
  ) +
  labs(colour = "") +
  scale_colour_manual(values = "red")

print(rstandard_compare_plot)
```



Let's add these residuals to the `tibble` of our dataset:

```
bw <-
  bw |>
  mutate(
    fitted_lm2 = fitted(bw_lm2),
    resid_lm2 = resid(bw_lm2),
    resid_lm2_alt = weight - fitted_lm2,
    std_resid_lm2 = rstandard(bw_lm2),
    std_resid_lm2_alt = resid_lm2 / sigma(bw_lm2)
  )

bw |>
  select(
    sex,
    age,
    weight,
    fitted_lm2,
    resid_lm2,
    std_resid_lm2
  )
#> # A tibble: 24 x 6
#>    sex      age weight fitted_lm2 resid_lm2 std_resid_lm2
#>    <fct>  <dbl>  <dbl>      <dbl>     <dbl>         <dbl>
#>  1 female    36   2729      2553.     176.          1.16
#>  2 female    36   2412      2553.    -141.         -0.926
#>  3 female    37   2539      2683.    -144.         -0.875
#>  4 female    38   2754      2814.     -59.5        -0.347
#>  5 female    38   2991      2814.     177.          1.04
#>  6 female    39   2817      2944.    -127.         -0.735
#>  7 female    39   2875      2944.     -68.9        -0.399
#>  8 female    40   3317      3074.     243.          1.44
#>  9 female    40   2935      3074.    -139.         -0.825
#> 10 female    40   3126      3074.      51.7         0.306
#> # i 14 more rows
```

Now let's build histograms:

```
resid_marginal_hist <-
  bw |>
  ggplot(aes(x = resid_lm2)) +
  geom_histogram()

print(resid_marginal_hist)
```

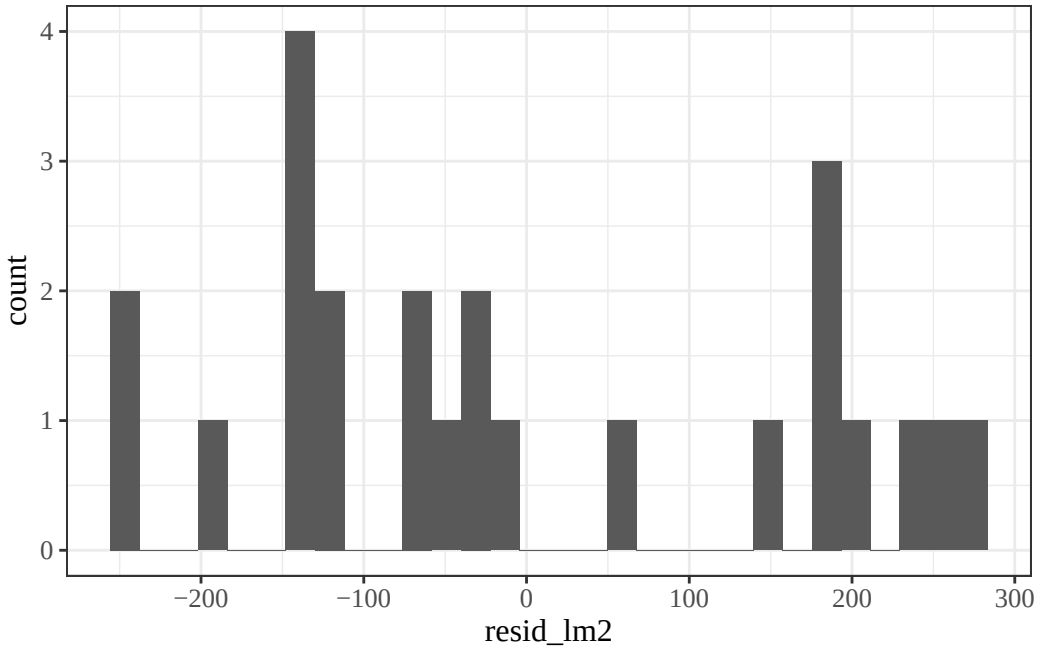


Figure 24: Marginal distribution of (nonstandardized) residuals

Hard to tell with this small amount of data, but I'm a bit concerned that the histogram doesn't show a bell-curve shape.

```
std_resid_marginal_hist <-
  bw |>
  ggplot(aes(x = std_resid_lm2)) +
  geom_histogram()

print(std_resid_marginal_hist)
```

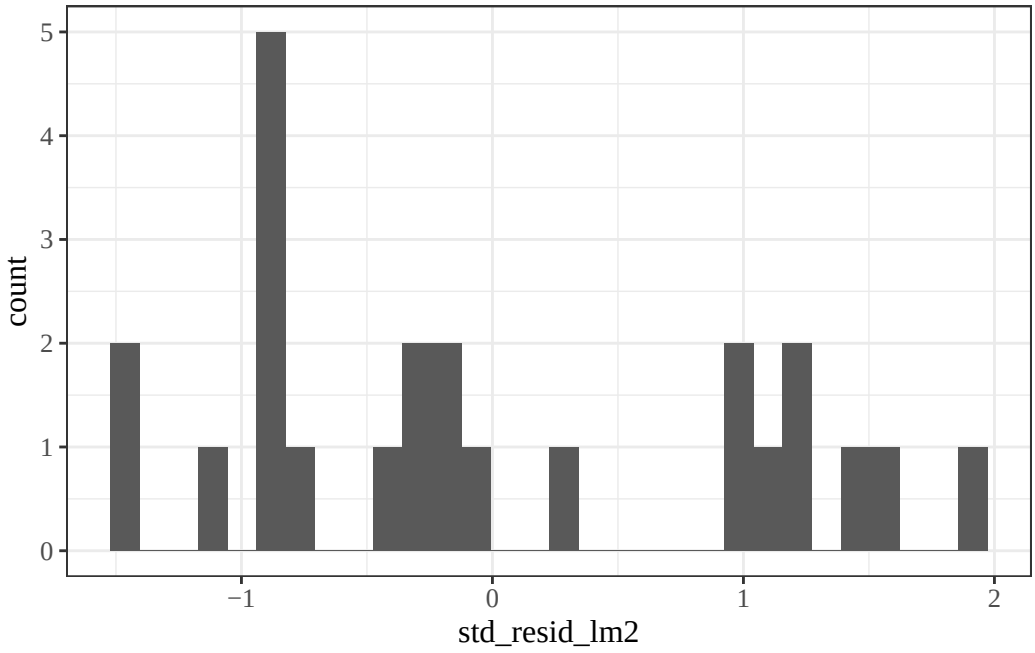


Figure 25: Marginal distribution of standardized residuals

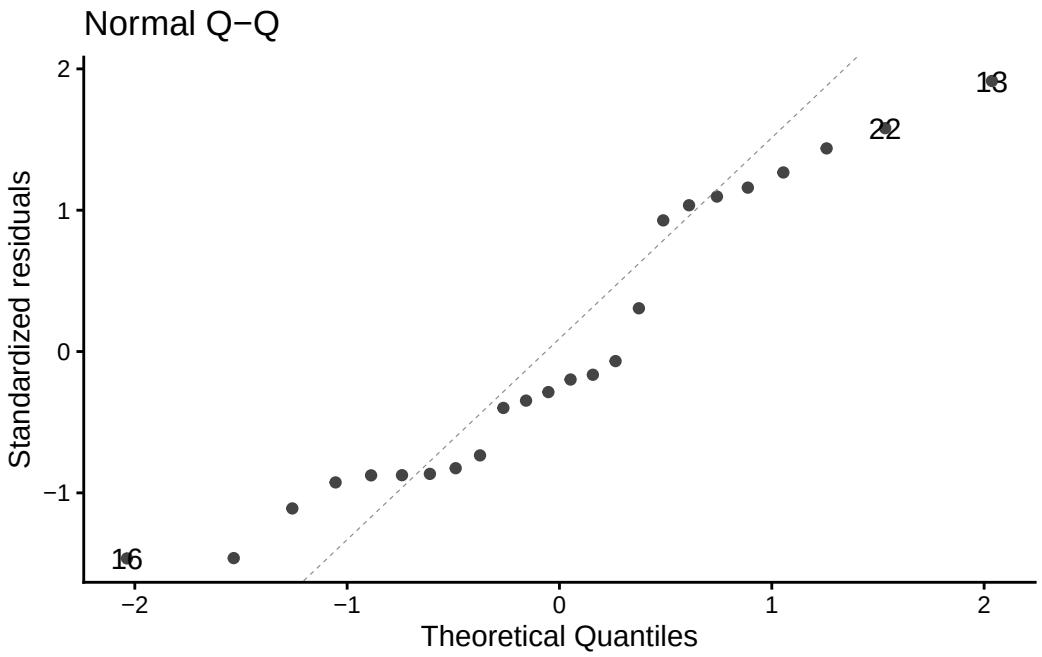
This looks similar, although the scale of the x-axis got narrower, because we divided by $\hat{\sigma}$ (roughly speaking).

Still hard to tell if the distribution is Gaussian.

6.3.5 QQ plot of standardized residuals

Another way to assess normality is the QQ plot of the standardized residuals versus normal quantiles:

```
library(ggfortify)
# needed to make ggplot2::autoplot() work for `lm` objects

qqplot_lm2_auto <-
  bw_lm2 |>
  autoplot(
    which = 2, # options are 1:6; can do multiple at once
    ncol = 1
  ) +
  theme_classic()

print(qqplot_lm2_auto)
```



If the Gaussian model were correct, these points should follow the dotted line.

Fig 2.4 panel (c) in Dobson and Barnett (2018) is a little different; they didn't specify how they produced it, but other statistical analysis systems do things differently from R.

See also Dunn and Smyth (2018) §3.5.4[20].

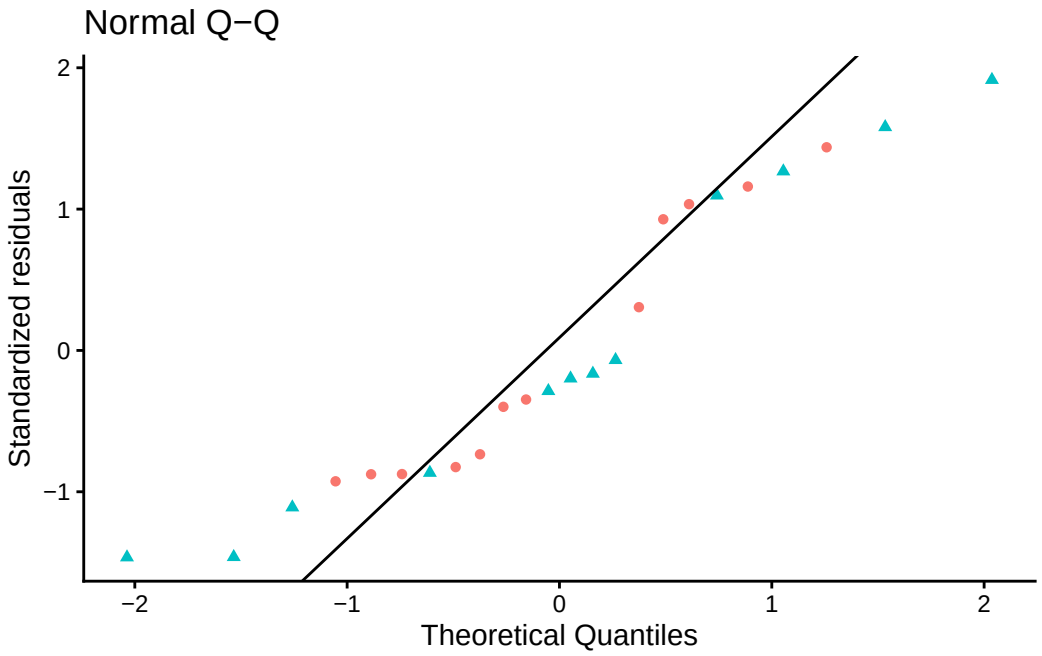
QQ plot - how it's built

Let's construct it by hand:

```
bw <- bw |>
  mutate(
    p = (rank(std_resid_lm2) - 1 / 2) / n(), # "Blom's method"
    expected_quantiles_lm2 = qnorm(p)
  )

qqplot_lm2 <-
  bw |>
  ggplot(
    aes(
      x = expected_quantiles_lm2,
      y = std_resid_lm2,
      col = sex,
      shape = sex
    )
  ) +
  geom_point() +
  theme_classic() +
  theme(legend.position = "none") + # removing the plot legend
  ggtitle("Normal Q-Q") +
  xlab("Theoretical Quantiles") +
  ylab("Standardized residuals")
```

[20] https://link.springer.com/chapter/10.1007/978-1-4419-0118-7_3#Sec14:~:text=3.5.4%20Q%E2%80%93Q%20Plots%20and%20Normality

```r
# find the expected line:

ps <- c(.25, .75) # reference probabilities
a <- quantile(rstandard(bw_lm2), ps) # empirical quantiles
b <- qnorm(ps) # theoretical quantiles

qq_slope <- diff(a) / diff(b)
qq_intcpt <- a[1] - b[1] * qq_slope

qqplot_lm2 <-
  qqplot_lm2 +
  geom_abline(slope = qq_slope, intercept = qq_intcpt)

print(qqplot_lm2)
```



6.3.6 Conditional distributions of residuals

If our Gaussian linear regression model is correct, the residuals e_i and standardized residuals r_i should have:

- an approximately Gaussian distribution, with:
- a mean of 0
- a constant variance

This should be true **for every** value of x.

If we didn't correctly guess the functional form of the linear component of the mean,

$$\mathrm{E}[Y|X = x] = \beta_0 + \beta_1 X_1 + ... + \beta_p X_p$$

Then the residuals might have nonzero mean.

Regardless of whether we guessed the mean function correctly, ther the variance of the residuals might differ between values of x.

Residuals versus fitted values

To look for these issues, we can plot the residuals e_i against the fitted values $\hat{y}_i$ (Figure 26).

```
autoplot(bw_lm2, which = 1, ncol = 1) |> print()
```

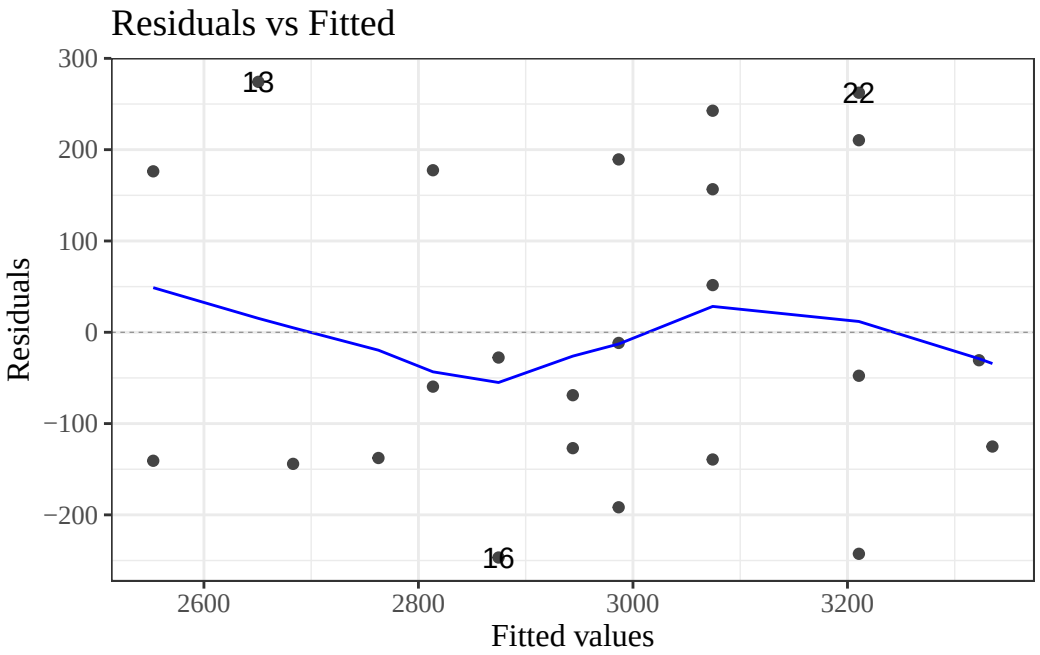


Figure 26: `birthweight` model (Equation 3): residuals versus fitted values

If the model is correct, the blue line should stay flat and close to 0, and the cloud of dots should have the same vertical spread regardless of the fitted value.

If not, we probably need to change the functional form of linear component of the mean,

$$\mathrm{E}[Y|X = x] = \beta_0 + \beta_1 X_1 + ... + \beta_p X_p$$

Example: PLOS Medicine title length data

(Adapted from Dobson and Barnett (2018), §6.7.1)

```
data(PLOS, package = "dobson")
library(ggplot2)
fig1 =
  PLOS |>
  ggplot(
    aes(x = authors,
        y = nchar)
  ) +
  geom_point() +
  theme(legend.position = "bottom") +
  labs(col = "") +
  guides(col=guide_legend(ncol=3))
fig1
```

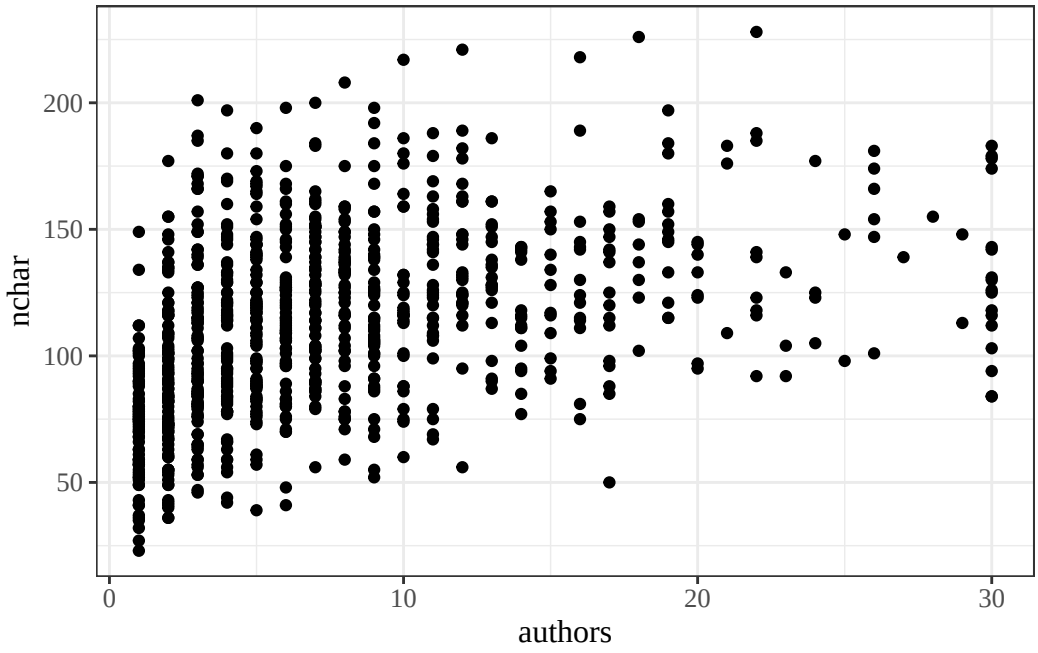


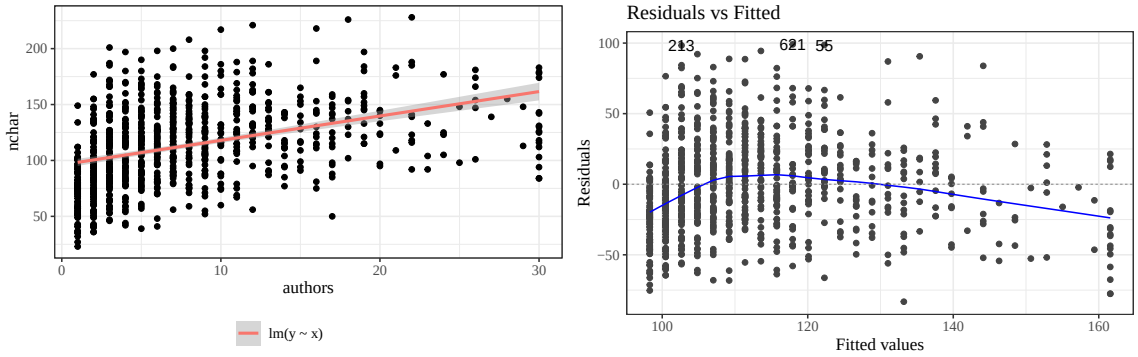
Figure 27: Number of authors versus title length in *PLOS Medicine* articles

---

Linear fit

```
lm_PLOS_linear = lm(
  formula = nchar ~ authors,
  data = PLOS)
```

```
fig2 = fig1 +
  geom_smooth(
    method = "lm",
               fullrange = TRUE,
               aes(col = "lm(y ~ x)"))
fig2

library(ggfortify)
autoplot(lm_PLOS_linear, which = 1, ncol = 1)
```



(a) Data and fit

(b) Residuals vs fitted

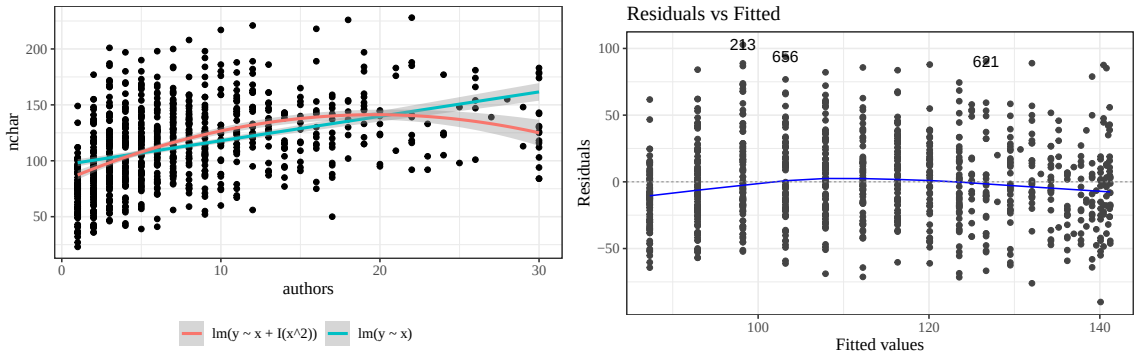
Figure 28: Number of authors versus title length in *PLOS Medicine*, with linear model fit

---

Quadratic fit

```
lm_PLOS_quad = lm(
  formula = nchar ~ authors + I(authors^2),
  data = PLOS)
```

```
fig3 =
  fig2 +
geom_smooth(
    method = "lm",
    fullrange = TRUE,
    formula = y ~ x + I(x ^ 2),
    aes(col = "lm(y ~ x + I(x^2))")
  )
fig3

autoplot(lm_PLOS_quad, which = 1, ncol = 1)
```



(a) Data and fit

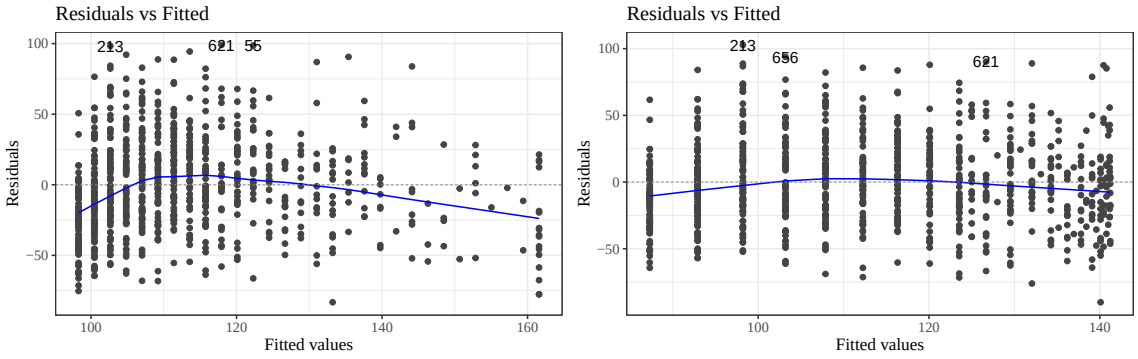
(b) Residuals vs fitted

Figure 29: Number of authors versus title length in *PLOS Medicine*, with quadratic model fit

---

Linear versus quadratic fits

```
library(ggfortify)
autoplot(lm_PLOS_linear, which = 1, ncol = 1)

autoplot(lm_PLOS_quad, which = 1, ncol = 1)
```



(a) Linear

(b) Quadratic

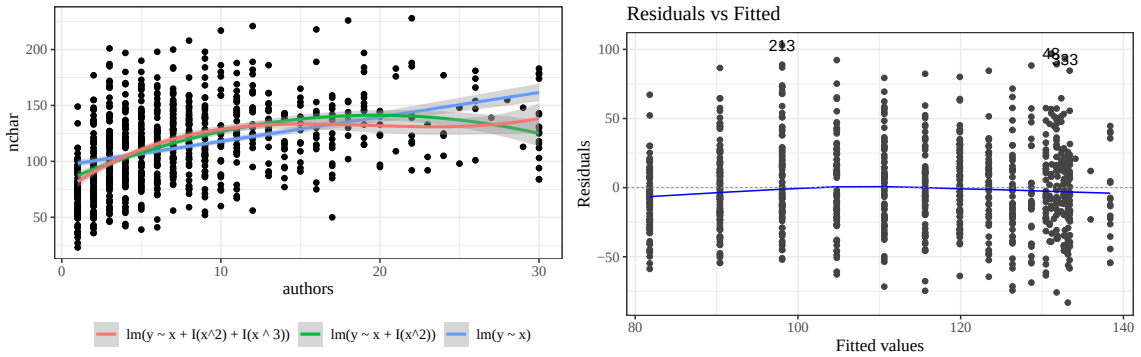
Figure 30: Residuals versus fitted plot for linear and quadratic fits to `PLOS` data

---

Cubic fit

```
lm_PLOS_cub = lm(
  formula = nchar ~ authors + I(authors^2) + I(authors^3),
  data = PLOS)
```

```
fig4 =
  fig3 +
geom_smooth(
    method = "lm",
    fullrange = TRUE,
    formula = y ~ x + I(x ^ 2) + I(x ^ 3),
    aes(col = "lm(y ~ x + I(x^2) + I(x ^ 3))")
  )
fig4

autoplot(lm_PLOS_cub, which = 1, ncol = 1)
```



(a) Data and fit

(b) Residuals vs fitted

Figure 31: Number of authors versus title length in *PLOS Medicine*, with cubic model fit

---

Logarithmic fit

```
lm_PLOS_log = lm(nchar ~ log(authors), data = PLOS)
```

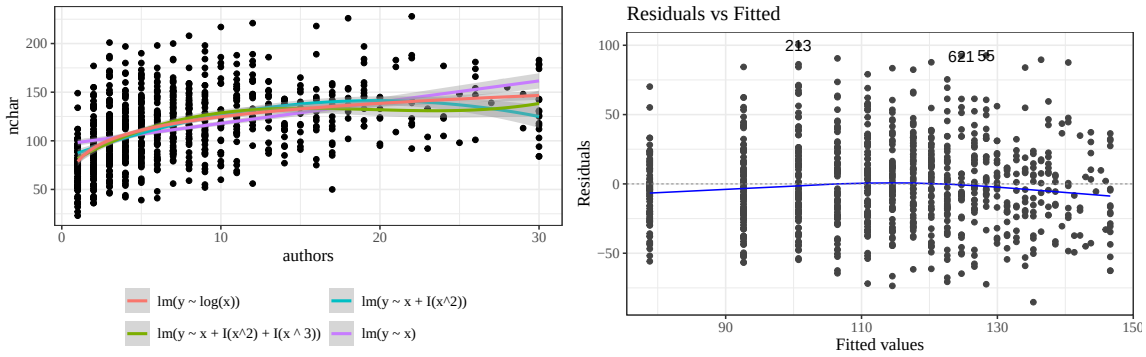
```
fig5 = fig4 +
  geom_smooth(
    method = "lm",
    fullrange = TRUE,
    formula = y ~ log(x),
    aes(col = "lm(y ~ log(x))")
  )
fig5

autoplot(lm_PLOS_log, which = 1, ncol = 1)
```

Table 34: linear vs quadratic

```
anova(lm_PLOS_linear, lm_PLOS_quad)
#> # A tibble: 2 x 6
#>   Res.Df     RSS    Df `Sum of Sq`     F  `Pr(>F)`
#>    <dbl>   <dbl> <dbl>       <dbl> <dbl>     <dbl>
#> 1    876 947502.    NA          NA    NA   NA
#> 2    875 880950.     1      66552.  66.1  1.46e-15
```

Table 35: quadratic vs cubic

```
anova(lm_PLOS_quad, lm_PLOS_cub)
#> # A tibble: 2 x 6
#>   Res.Df     RSS    Df `Sum of Sq`     F  `Pr(>F)`
#>    <dbl>   <dbl> <dbl>       <dbl> <dbl>     <dbl>
#> 1    875 880950.    NA          NA    NA   NA
#> 2    874 865933.     1      15018.  15.2  0.000106
```



(a) Data and fit

(b) Residuals vs fitted

Figure 32: logarithmic fit

Model selection

AIC/BIC

```
AIC(lm_PLOS_quad)
#> [1] 8567.61
AIC(lm_PLOS_cub)
#> [1] 8554.51
```

```
AIC(lm_PLOS_cub)
#> [1] 8554.51
AIC(lm_PLOS_log)
#> [1] 8543.63
```

```
BIC(lm_PLOS_cub)
#> [1] 8578.4
BIC(lm_PLOS_log)
#> [1] 8557.97
```

Extrapolation is dangerous

```
fig_all = fig5 +
  xlim(0, 60)
fig_all
```

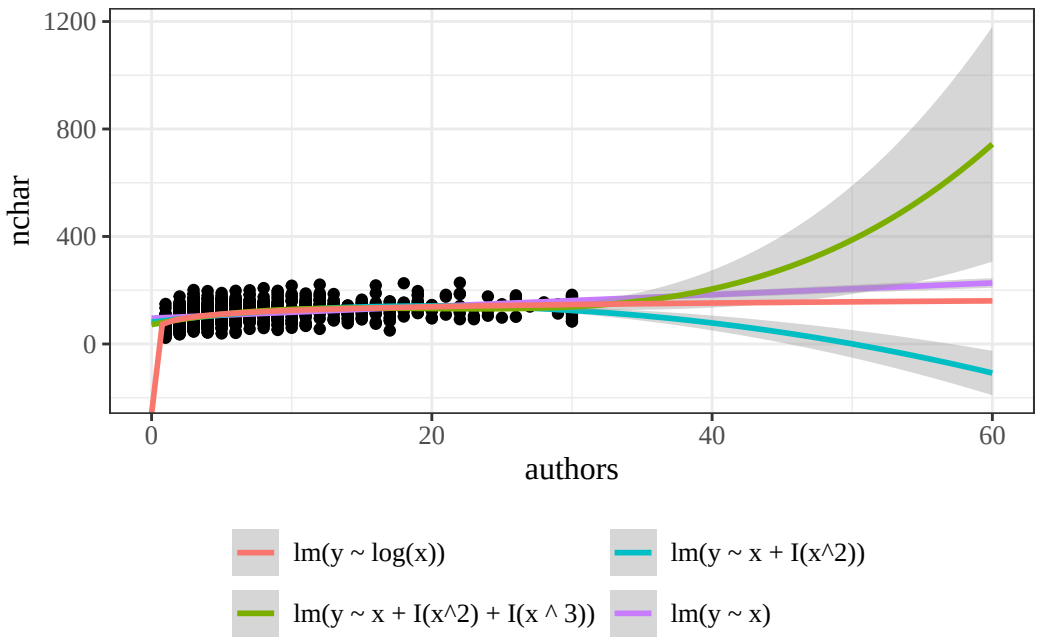


Figure 33: Number of authors versus title length in *PLOS Medicine*

Scale-location plot

We can also plot the square roots of the absolute values of the standardized residuals against the fitted values (Figure 34).

```
autoplot(bw_lm2, which = 3, ncol = 1) |> print()
```

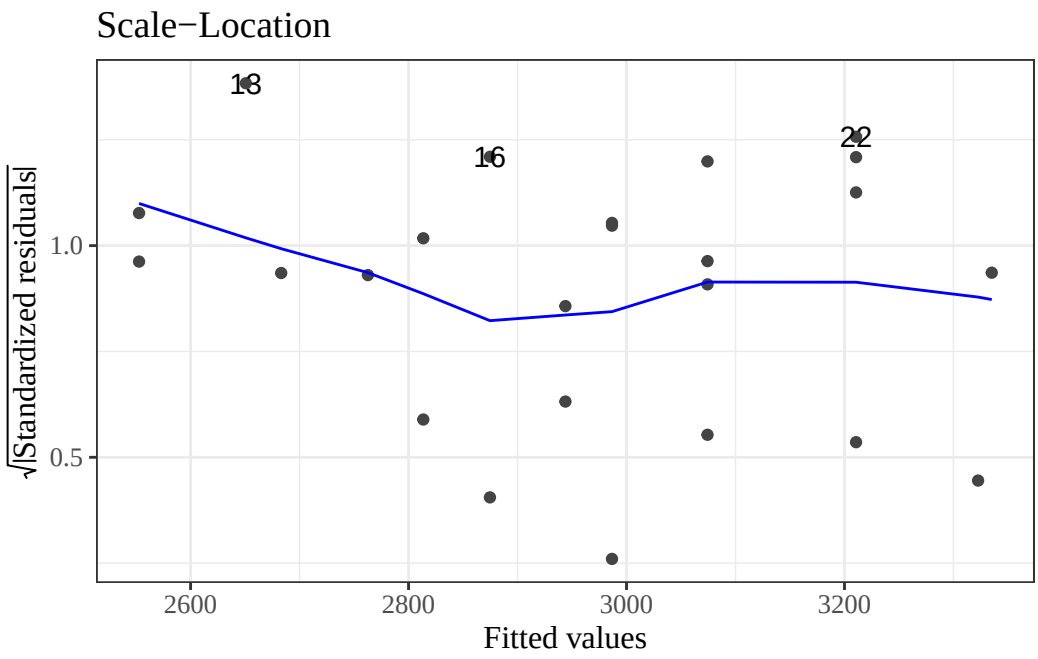


Figure 34: Scale-location plot of `birthweight` data

Here, the blue line doesn't need to be near 0, but it should be flat. If not, the residual variance σ^2 might not be constant, and we might need to transform our outcome Y (or use a model that allows non-constant variance).

Residuals versus leverage

We can also plot our standardized residuals against "leverage", which roughly speaking is a measure of how unusual each x_i value is. Very unusual x_i values can have extreme effects on the model fit, so we might want to remove those observations as outliers, particularly if they have large residuals.

```
autoplot(bw_lm2, which = 5, ncol = 1) |> print()
```

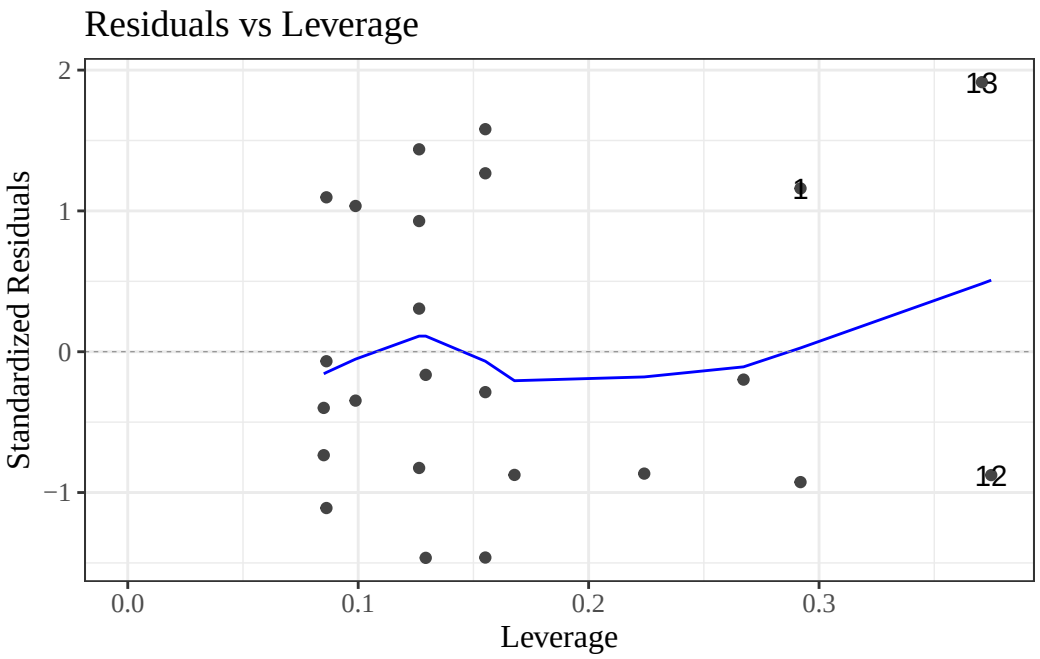


Figure 35: `birthweight` model with interactions (Equation 3): residuals versus leverage

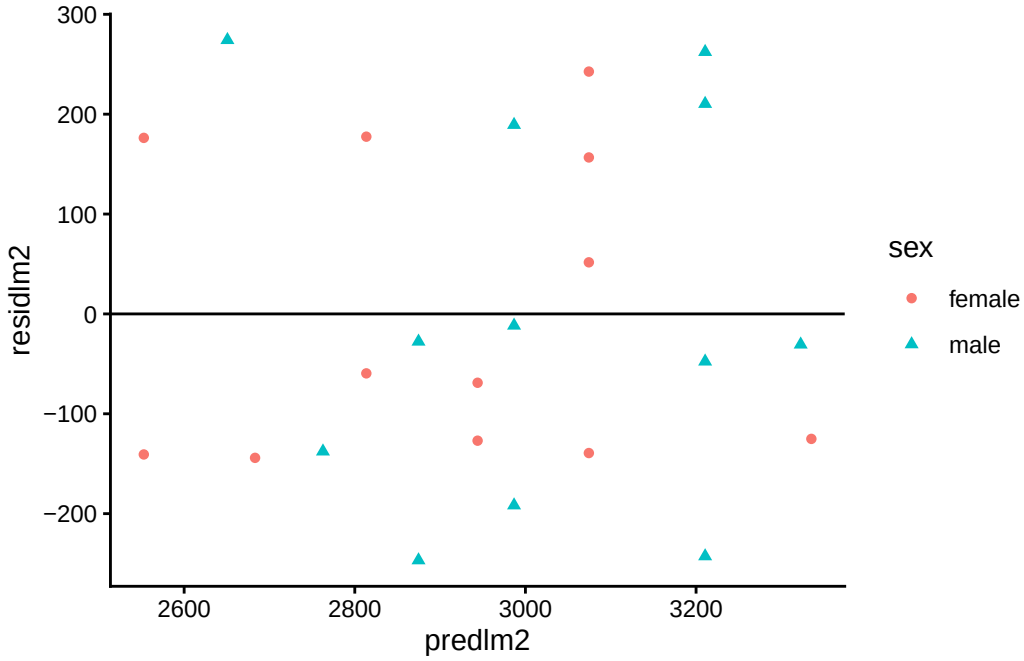
The blue line should be relatively flat and close to 0 here.

6.3.7 Diagnostics constructed by hand

```
bw <-
  bw |>
  mutate(
    predlm2 = predict(bw_lm2),
    residlm2 = weight - predlm2,
    std_resid = residlm2 / sigma(bw_lm2),
    # std_resid_builtin = rstandard(bw_lm2), # uses leverage
    sqrt_abs_std_resid = std_resid |> abs() |> sqrt()
  )
```

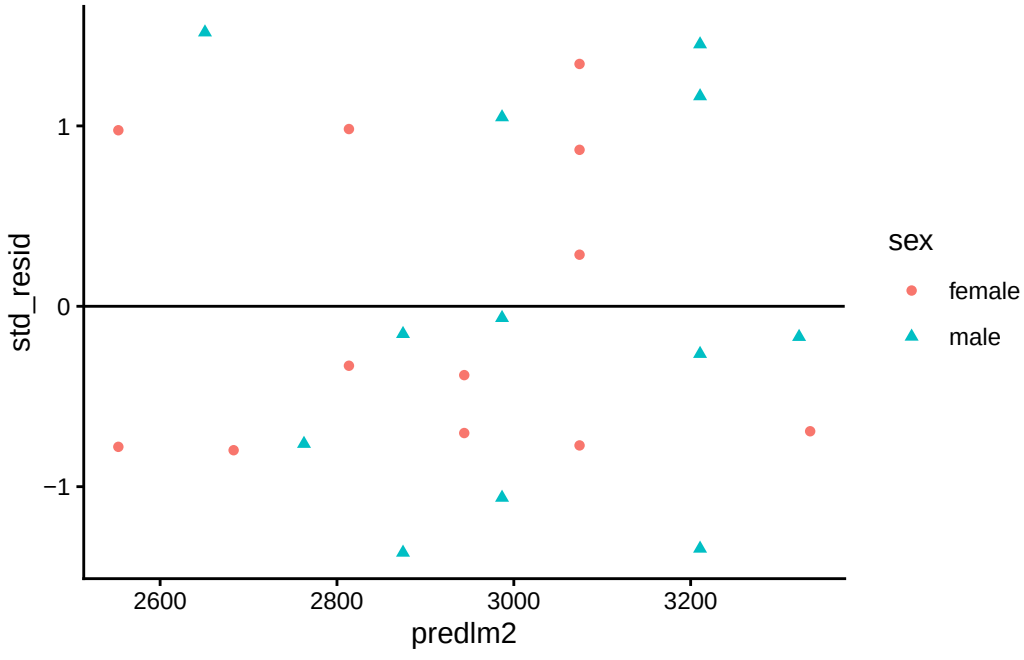
Residuals vs fitted

```
resid_vs_fit <- bw |>
  ggplot(
    aes(x = predlm2, y = residlm2, col = sex, shape = sex)
  ) +
  geom_point() +
  theme_classic() +
  geom_hline(yintercept = 0)

print(resid_vs_fit)
```



Standardized residuals vs fitted

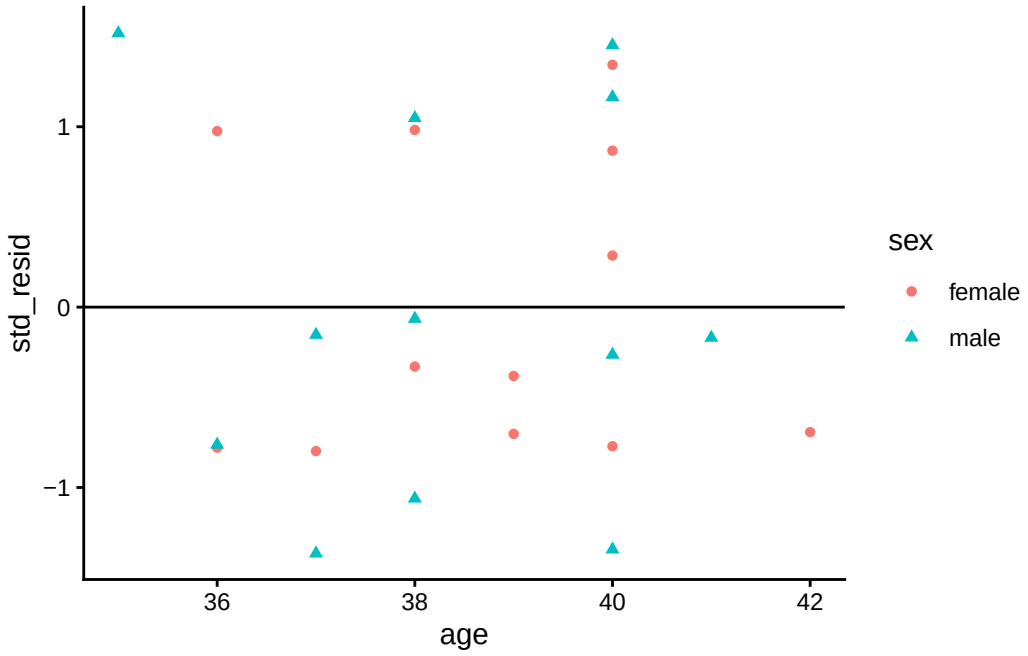
```
bw |>
  ggplot(
    aes(x = predlm2, y = std_resid, col = sex, shape = sex)
  ) +
  geom_point() +
  theme_classic() +
  geom_hline(yintercept = 0)
```



Standardized residuals vs gestational age

```
bw |>
  ggplot(
```

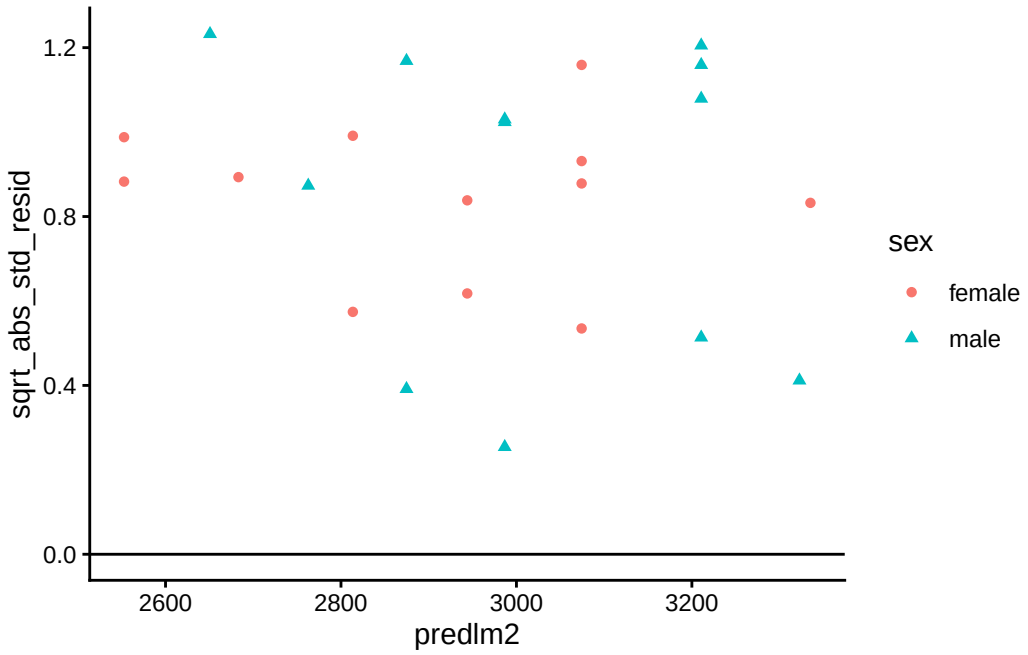
```
    aes(x = age, y = std_resid, col = sex, shape = sex)
  ) +
  geom_point() +
  theme_classic() +
  geom_hline(yintercept = 0)
```



`sqrt(abs(rstandard()))` vs fitted

Compare with `autoplot(bw_lm2, 3)`

```
bw |>
  ggplot(
    aes(x = predlm2, y = sqrt_abs_std_resid, col = sex, shape = sex)
  ) +
  geom_point() +
  theme_classic() +
  geom_hline(yintercept = 0)
```



6.4 Model selection

(adapted from Dobson and Barnett (2018) §6.3.3; for more information on prediction, see James et al. (2013) and Harrell (2015)).

If we have a lot of covariates in our dataset, we might want to choose a small subset to use in our model.

There are a few possible metrics to consider for choosing a "best" model.

6.4.1 Mean squared error

We might want to minimize the **mean squared error**, $\mathrm{E}[(y-\hat{y})^2]$, for new observations that weren't in our data set when we fit the model.

Unfortunately,

$$\frac{1}{n}\sum_{i=1}^{n}(y_i-\hat{y}_i)^2$$

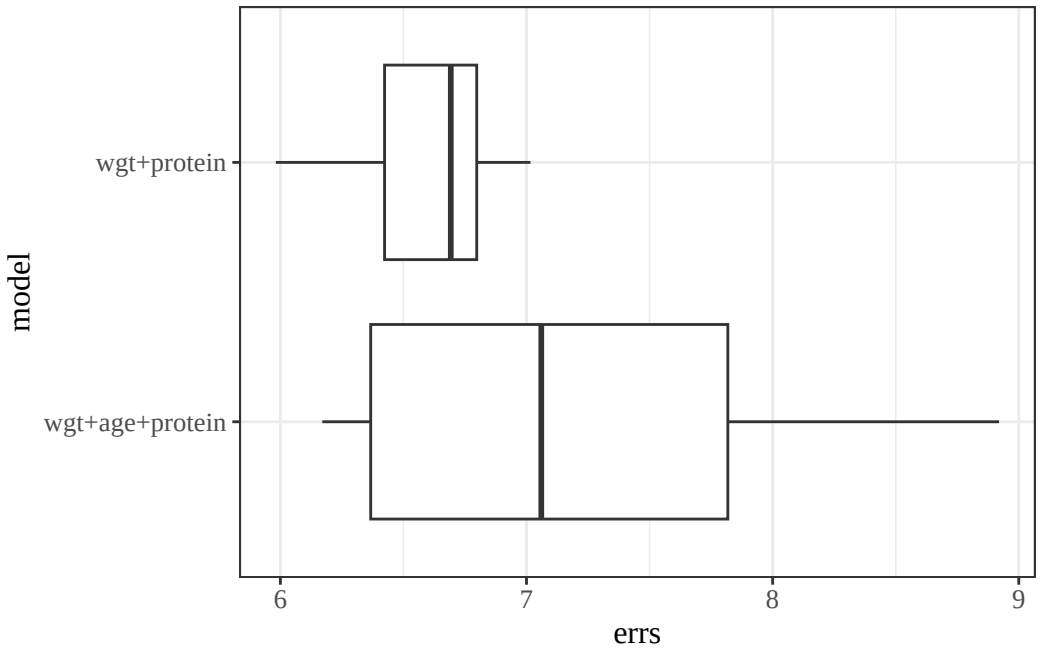
gives a biased estimate of $\mathrm{E}[(y-\hat{y})^2]$ for new data. If we want an unbiased estimate, we will have to be clever.

Cross-validation

```
data("carbohydrate", package = "dobson")
library(cvTools)
full_model <- lm(carbohydrate ~ ., data = carbohydrate)
cv_full <-
  full_model |> cvFit(
    data = carbohydrate, K = 5, R = 10,
    y = carbohydrate$carbohydrate
  )

reduced_model <- full_model |> update(formula = ~ . - age)

cv_reduced <-
  reduced_model |> cvFit(
```

```
    data = carbohydrate, K = 5, R = 10,
    y = carbohydrate$carbohydrate
  )
```

```
results_reduced <-
  tibble(
    model = "wgt+protein",
    errs = cv_reduced$reps[]
  )
results_full <-
  tibble(
    model = "wgt+age+protein",
    errs = cv_full$reps[]
  )

cv_results <-
  bind_rows(results_reduced, results_full)

cv_results |>
  ggplot(aes(y = model, x = errs)) +
  geom_boxplot()
```



---

comparing metrics

```
compare_results <- tribble(
  ~model, ~cvRMSE, ~r.squared, ~adj.r.squared, ~trainRMSE, ~loglik,
  "full",
  cv_full$cv,
  summary(full_model)$r.squared,
  summary(full_model)$adj.r.squared,
  sigma(full_model),
  logLik(full_model) |> as.numeric(),
  "reduced",
```

```
  cv_reduced$cv,
  summary(reduced_model)$r.squared,
  summary(reduced_model)$adj.r.squared,
  sigma(reduced_model),
  logLik(reduced_model) |> as.numeric()
)

compare_results
#> # A tibble: 2 x 6
#>   model   cvRMSE r.squared adj.r.squared trainRMSE loglik
#>   <chr>    <dbl>     <dbl>         <dbl>     <dbl>  <dbl>
#> 1 full      7.17     0.481         0.383      5.96  -61.8
#> 2 reduced   6.60     0.445         0.380      5.97  -62.5
```

```
anova(full_model, reduced_model)
#> # A tibble: 2 x 6
#>   Res.Df   RSS    Df `Sum of Sq`     F `Pr(>F)`
#>    <dbl> <dbl> <dbl>       <dbl> <dbl>    <dbl>
#> 1     16  568.    NA        NA    NA      NA
#> 2     17  606.    -1       -38.4  1.08    0.314
```

---

stepwise regression

> ⚠ Caution about stepwise selection
>
> Stepwise regression has several known problems:
> - It tends to select too many variables (overfitting)
> - P-values and confidence intervals are biased after selection
> - It ignores model uncertainty
> - Results can be unstable across different samples
>
> Consider using cross-validation, penalized methods (like Lasso), or subject-matter knowledge instead. See Harrell (2015) and Heinze et al. (2018) for more discussion.

```
library(olsrr)
olsrr:::ols_step_both_aic(full_model)
#>
#>
#>                               Stepwise Summary
#> -------------------------------------------------------------------------
#> Step    Variable         AIC        SBC       SBIC       R2       Adj. R2
#> -------------------------------------------------------------------------
#>  0      Base Model     140.773    142.764    83.068    0.00000    0.00000
#>  1      protein (+)    137.950    140.937    80.438    0.21427    0.17061
#>  2      weight (+)     132.981    136.964    77.191    0.44544    0.38020
#> -------------------------------------------------------------------------
#>
#> Final Model Output
#> ------------------
#>
#>                           Model Summary
#> ---------------------------------------------------------------
#> R                        0.667       RMSE                 5.505
#> R-Squared                0.445       MSE                 30.301
#> Adj. R-Squared           0.380       Coef. Var           15.879
```

```
#> Pred R-Squared          0.236       AIC                132.981
#> MAE                    4.593       SBC                136.964
#> ----------------------------------------------------------------
#>  RMSE: Root Mean Square Error
#>  MSE: Mean Square Error
#>  MAE: Mean Absolute Error
#>  AIC: Akaike Information Criteria
#>  SBC: Schwarz Bayesian Criteria
#>
#>                                ANOVA
#> -------------------------------------------------------------------
#>                 Sum of
#>                Squares        DF    Mean Square      F        Sig.
#> -------------------------------------------------------------------
#> Regression     486.778         2        243.389    6.827    0.0067
#> Residual       606.022        17         35.648
#> Total         1092.800        19
#> -------------------------------------------------------------------
#>
#>                                  Parameter Estimates
#> ----------------------------------------------------------------------------------------
#>       model      Beta    Std. Error    Std. Beta      t        Sig      lower     upper
#> ----------------------------------------------------------------------------------------
#> (Intercept)    33.130        12.572                2.635    0.017     6.607    59.654
#>     protein     1.824         0.623        0.534    2.927    0.009     0.509     3.139
#>      weight    -0.222         0.083       -0.486   -2.662    0.016    -0.397    -0.046
#> ----------------------------------------------------------------------------------------
```

Lasso

$$\arg\max_{\theta} \left\{ \ell(\theta) - \lambda \sum_{j=1}^{p} |\beta_j| \right\}$$

```
library(glmnet)
y <- carbohydrate$carbohydrate
x <- carbohydrate |>
  select(age, weight, protein) |>
  as.matrix()
fit <- glmnet(x, y)
```

```
autoplot(fit, xvar = "lambda")
```

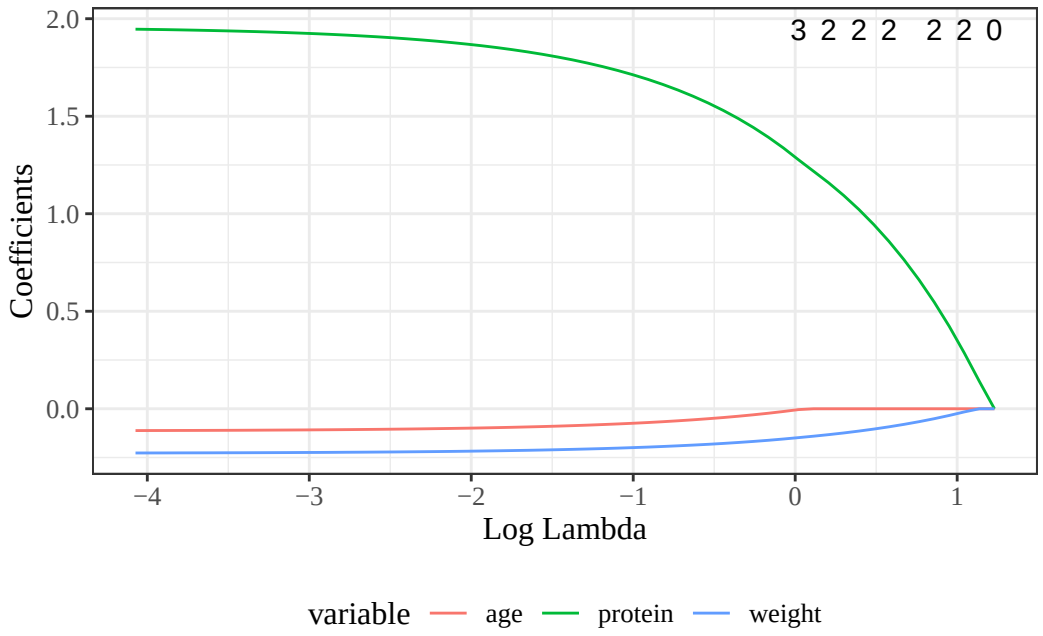
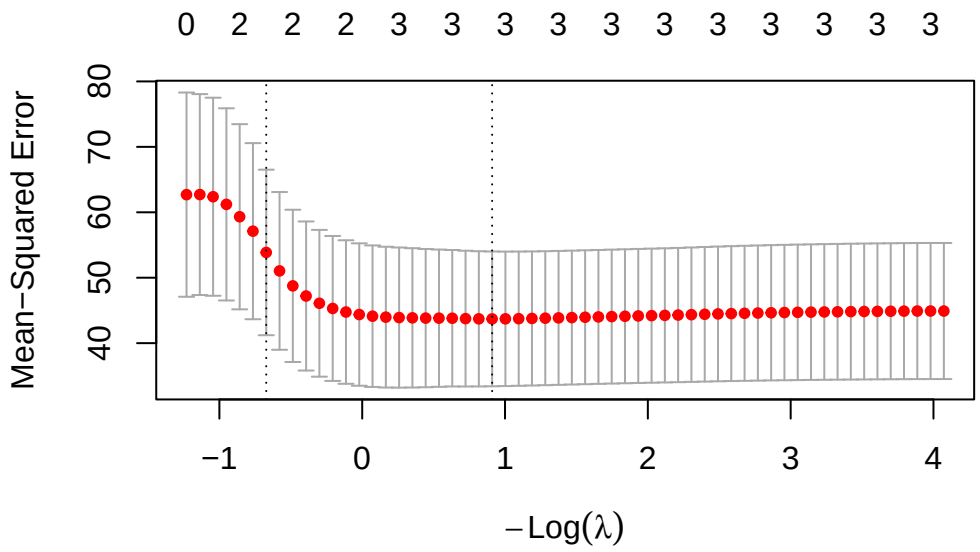


Figure 36: Lasso selection

```
cvfit <- cv.glmnet(x, y)
plot(cvfit)
```



```
coef(cvfit, s = "lambda.1se")
#> 4 x 1 sparse Matrix of class "dgCMatrix"
#>             lambda.1se
#> (Intercept) 34.3091615
#> age          .
#> weight      -0.0800142
```

```
#> protein      0.7640510
```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