Chapter 3 - Linear Model Estimation

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To open this information in an interactive Colab notebook, click the Open in Colab graphic below.

```
if(!require(palmerpenguins, quietly = TRUE)) {
  install.packages("palmerpenguins", repos = "https://cran.rstudio.com/")
  library(palmerpenguins)
}
if(!require(ggplot2, quietly = TRUE)) {
  install.packages("ggplot2", repos = "https://cran.rstudio.com/")
  library(ggplot2)
}
```

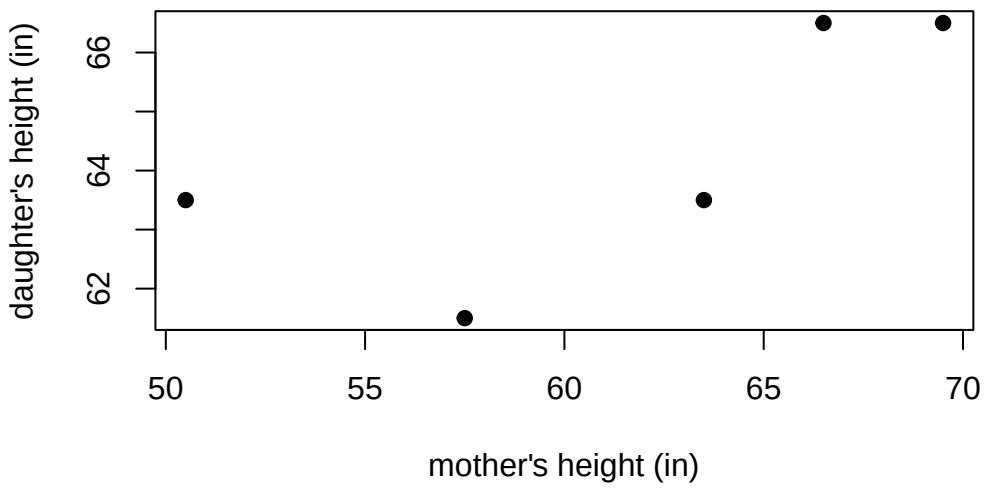
A simple motivating example

Suppose you observe data related to the heights of 5 mothers and their adult daughters. The data are in the table below.

observation	mother	daughter
1	57.5	61.5
2	60.5	63.5
3	63.5	63.5
4	66.5	66.5
5	69.5	66.5

Would it be reasonable to use a mother's height to predict the height of her adult daughter? Consider the plot below.

```r
x <- c(57.5, 50.5, 63.5, 66.5, 69.5) # mothers' heights
y <- c(61.5, 63.5, 63.5, 66.5, 66.5) # daughters' heights
plot(y ~ x, pch = 19, xlab = "mother's height (in)", ylab = "daughter's height (in)")
```



What is regression?

A **regression analysis** is the process of building a model describing the typical relationship between a set of observed variables.

- A regression analysis builds the model using observed values of the variables for n subjects sampled from a population.
- In our example, we want to build a **regression** model for the height of adult daughters using their height of their mothers.

Response versus predictor variables

The variables in a regression analysis may be divided into two types:

- The response variable.
- The predictor variables.

The outcome variable we are trying to predict is known as the **response variable**.

- Response variables are also known as **outcome**, **output**, or **dependent** variables.
- The response variable is denoted by Y.
- Y_i denotes the value of Y for observation i.

The variables available to model the response variable are known as **predictors variables**:

- They are also called **explanatory**, **regressor**, **input**, **dependent** variables or simply as **features**.
- Following the convention of Weisberg (2014), we use the term **regressor** to refer to the variables used in our regression model, whether that is the original predictor variable, some transformation of a predictor, some combination of predictors, etc.
- Every predictor can be a regressor but not all regressors are a predictor.
- The regressor variables are denoted as $X_1, X_2, \ldots, X_{p-1}$.
- $x_{i,j}$ denotes the value of X_j for observation i
- If there is only a single regressor in the model, we can denote the single regressor as X and the observed values of X as $x_1, x_2, \ldots, x_n$.

For the height data, the 5 pairs of observed data are denoted

$$(x_1, Y_1), (x_2, Y_2), \ldots, (x_5, Y_5),$$

with (x_i, Y_i) denoting the data for observation i.

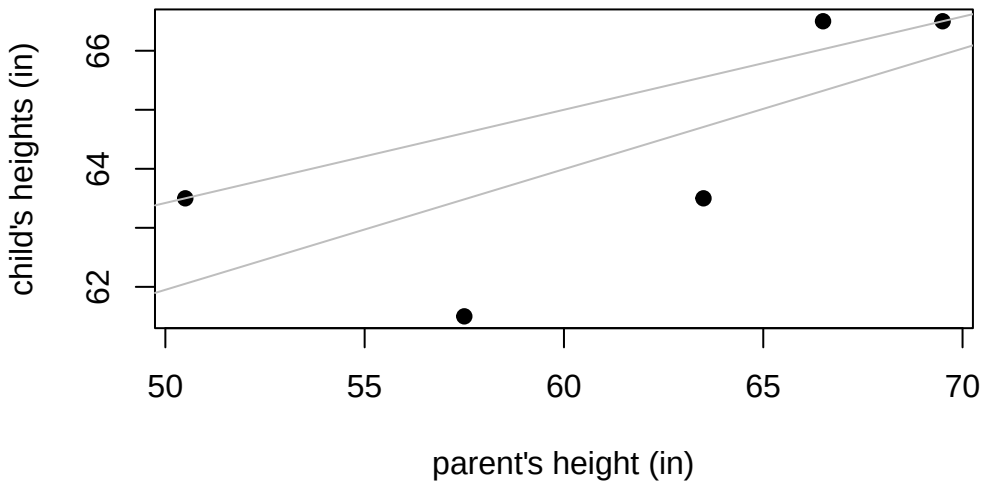
- x_i denotes the mother's height for observation i.
- Y_i denotes the daughter's height for observation i.

Selecting the best model

Suppose we want to find the straight line that best fits the plot of mother and daughter heights.

How do we determine the "best fitting" model?

Consider these potential "best fitting" lines that are drawn on the scatter plot of the height data. Which one is best?



Estimation of the simple linear regression model

Parameter estimation is the process of using observed data to estimate values for the regression coefficients.

There are many different methods of parameter estimation in statistics:

- Method-of-moments.
- Maximum likelihood.
- Bayesian.
- Etc.

The most common parameter estimation method for linear models is the **least squares method**, which is commonly called **Ordinary Least Squares (OLS)** estimation.

OLS estimation estimates the regression coefficients with the values that minimize the residual sum of squares (RSS), which we will define shortly.

Defining a simple linear regression model

The regression model for Y as a function of X, denoted $E(Y \mid X)$, is the expected value of Y conditional on the regressor X.

The **simple linear regression model** for a response variable assumes the mean of Y conditional on a single regressor X is

$$E(Y \mid X) = \beta_0 + \beta_1 X.$$

The response variable Y is modeled as

$$\begin{aligned} Y &= E(Y \mid X) + \epsilon \\ &= \beta_0 + \beta_1 X + \epsilon, \end{aligned}$$

where ϵ is known as the model error.

The error term ϵ is literally the deviation of the response variable from its mean.

- We typically assume that conditional on the regressor variable, the error term has mean 0 and variance σ^2.
- This is written as $E(\epsilon \mid X) = 0$ and $\text{var}(\epsilon \mid X) = \sigma^2$.

The observed data are modeled as

$$\begin{aligned} Y_i &= \beta_0 + \beta_1 x_i + \epsilon \\ &= E(Y \mid X = x_i) + \epsilon_i, \end{aligned}$$

for $i = 1, 2, ..., n$, where ϵ_i denotes the error for observation i.

Important terminology

The **estimated regression model** is defined as

$$\hat{E}(Y|X) = \hat{\beta}_0 + \hat{\beta}_1 X,$$

where $\hat{\beta}_j$ denotes the estimated value of β_j for $j = 0, 1$.

The ith **fitted value** is defined as

$$\hat{Y}_i = \hat{E}(Y|X = x_i) = \hat{\beta}_0 + \hat{\beta}_1 x_i.$$

- The ith fitted value is the estimated mean of Y when the regressor $X = x_i$.

The ith **residual** is defined as

$$\hat{\epsilon}_i = Y_i - \hat{Y}_i.$$

- The ith residual is the difference between the response and estimated mean response of observation i.

The **residual sum of squares (RSS)** of a regression model is the sum of its squared residuals. The RSS for a simple linear regression model, as a function of the estimated regression coefficients $\hat{\beta}_0$ and $\hat{\beta}_1$, is defined as

$$RSS(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=1}^{n} \hat{\epsilon}_i^2.$$

Using the various objects defined above, there are many equivalent expressions for the RSS.

$$\begin{aligned} RSS(\hat{\beta}_0, \hat{\beta}_1) &= \sum_{i=1}^{n} \hat{\epsilon}_i^2 \\ &= \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 \\ &= \sum_{i=1}^{n} (Y_i - \hat{E}(Y|X = x_i))^2 \\ &= \sum_{i=1}^{n} (Y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i))^2. \end{aligned}$$

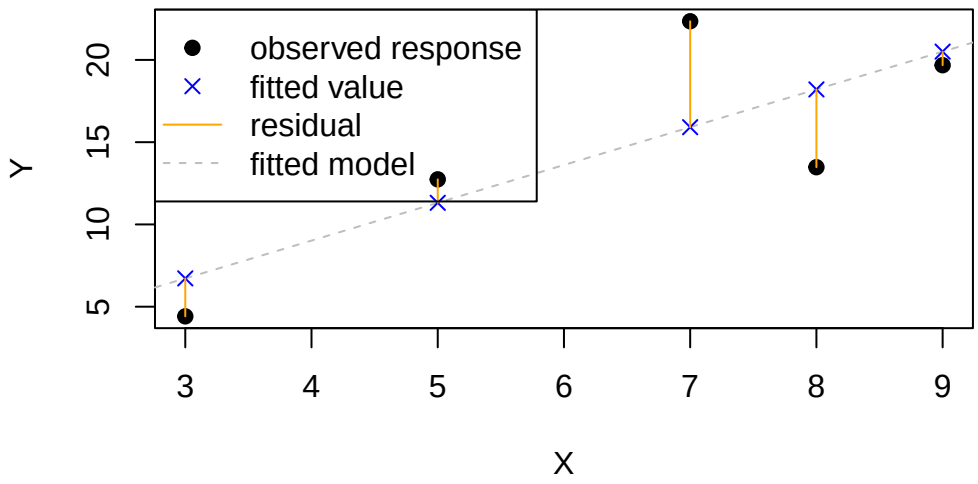
The **fitted model** is the estimated model that minimizes the RSS, and is written as

$$\hat{Y} = \hat{E}(Y|X) = \hat{\beta}_0 + \hat{\beta}_1 X.$$

- $\hat{Y}$ is used for brevity.
- $\hat{E}(Y|X)$ is used for clarity.

In a simple linear regression context, the fitted model is known as the **line of best fit**.

Visualizing terms



In the graphic above, we visualize the response values, fitted values, residuals, and fitted model in a simple linear regression context. Note that:

- The fitted model is shown as the dashed grey line and minimizes the RSS.
- The response values, shown as black dots, are the observed values of Y.
- The fitted values, shown as blue x's, are the values returned by evaluating the fitted model at the observed regressor values.
- The residuals, shown as solid orange lines, indicate the distance and direction between the observed responses and their corresponding fitted value. If the response is larger than the fitted value then the residual is positive, otherwise it is negative.
- The RSS is the sum of the squared vertical distances between the response and fitted values.

OLS estimators of the simple linear regression parameters

The estimators of β_0 and β_1 that minimize the RSS for a simple linear regression model can be obtained analytically using basic calculus (as long as $x_1, \ldots, x_n$ are not all equal to the same number).

Define:

- $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$.

- $\bar{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i$.

The OLS estimators of the simple linear regression coefficients that minimize the RSS are

$$\begin{aligned}\hat{\beta}_1 &= \frac{\sum_{i=1}^{n} x_i Y_i - \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} Y_i\right)}{\sum_{i=1}^{n} x_i^2 - \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right)^2} \\ &= \frac{\sum_{i=1}^{n}(x_i - \bar{x})(Y_i - \bar{Y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^{n}(x_i - \bar{x})Y_i}{\sum_{i=1}^{n}(x_i - \bar{x})x_i}\end{aligned}$$

and

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x}.$$

The most common estimator of the error variance is

$$\hat{\sigma}^2 = \frac{RSS}{\mathrm{df}_{RSS}}.$$

- df_{RSS} is the **degrees of freedom** of the RSS.
- For simple linear regression, $\mathrm{df}_{RSS} = n - 2$.

Penguins simple linear regression example

The `penguins` data set provides data related to various penguin species measured in the Palmer Archipelago (Antarctica), originally provided by Gorman et al. (2014). We start by loading the data into memory.

```
data(penguins, package = "palmerpenguins")
head(penguins)
```

```
# A tibble: 6 x 8
  species island    bill_length_mm bill_depth_mm flipper_l~1 body_~2 sex    year
  <fct>   <fct>              <dbl>         <dbl>       <int>   <int> <fct> <int>
1 Adelie  Torgersen           39.1          18.7         181    3750 male   2007
2 Adelie  Torgersen           39.5          17.4         186    3800 fema~  2007
3 Adelie  Torgersen           40.3          18           195    3250 fema~  2007
4 Adelie  Torgersen           NA            NA            NA      NA <NA>   2007
```

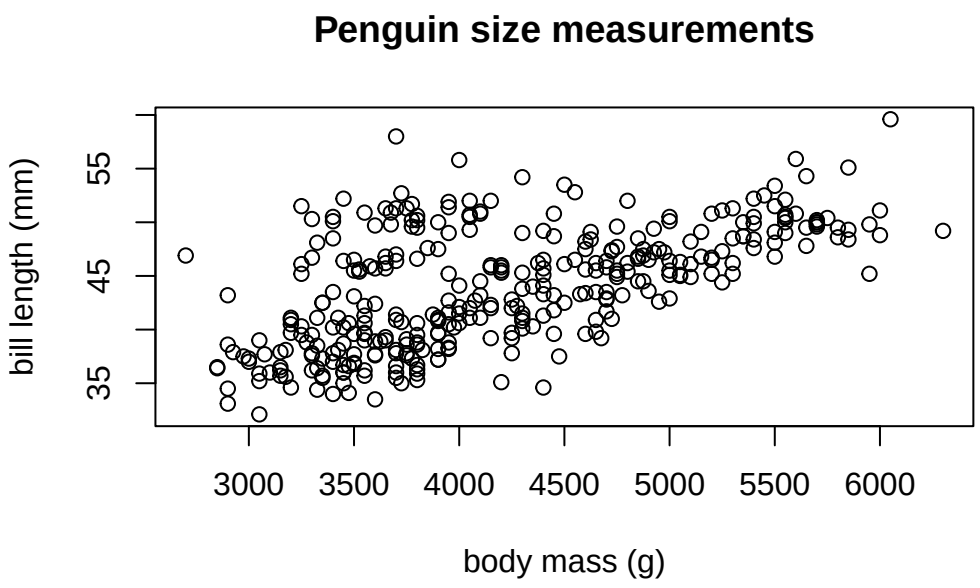
```
5 Adelie  Torgersen           36.7          19.3         193    3450 fema~  2007
6 Adelie  Torgersen           39.3          20.6         190    3650 male   2007
# ... with abbreviated variable names 1: flipper_length_mm, 2: body_mass_g
```

The data set includes 344 observations of 8 variables. The variables are:

- `species`: a `factor` indicating the penguin species.
- `island`: a `factor` indicating the island the penguin was observed.
- `bill_length_mm`: a `numeric` variable indicating the bill length in millimeters.
- `bill_depth_mm`: a `numeric` variable indicating the bill depth in millimeters.
- `flipper_length_mm`: an `integer` variable indicating the flipper length in millimeters
- `body_mass_g`: an `integer` variable indicating the body mass in grams.
- `sex`: a `factor` indicating the penguin sex (`female`, `male`).
- `year`: an integer denoting the study year the penguin was observed (2007, 2008, or 2009).

We begin by creating a scatter plot of `bill_length_mm` versus `body_mass_g`.

```
plot(bill_length_mm ~ body_mass_g, data = penguins,
     ylab = "bill length (mm)", xlab = "body mass (g)",
     main = "Penguin size measurements")
```



Questions:

- Is there a positive/negative association between body mass and bill length?
- Is the relationship approximately linear?

We will build a simple linear regression model that regresses `bill_length_mm` on `body_mass_g`.

We want to estimate the parameters of the model

$$E(\texttt{bill\_length\_mm} \mid \texttt{body\_mass\_g}) = \beta_0 + \beta_1 \, \texttt{body\_mass\_g}.$$

The `lm` function uses OLS estimation to fit a linear model to data. The function has two main arguments:

- `data`: the data frame in which the model variables are stored. This can be omitted if the variables are already stored in memory.
- `formula`: a Wilkinson and Rogers (1973) style formula describing the linear regression model. For complete details, run `?stats:formula` in the Console. If `y` is the response variable and `x` is an available numeric predictor, then `formula = y ~ x` tells `lm` to fit the simple linear regression model $E(Y|X) = \beta_0 + \beta_1 X$.

```
lmod <- lm(bill_length_mm ~ body_mass_g, data = penguins) # fit model
class(lmod) # class of lmod
```

```
[1] "lm"
```

The `summary` function is commonly used to summarize the results of our fitted model.

When an `lm` object is supplied to the `summary` function, it returns:

- `Call`: the function call used to fit the model.
- `Residuals`: A 5-number summary of the $\hat{\epsilon}_1, \ldots, \hat{\epsilon}_n$.
- `Coefficients`: A table that lists:
  - The regressors in the fitted model.
  - `Estimate`: the estimated coefficient for each regressor.
  - `Std. Error`: the *estimated* standard error of the estimated coefficients.
  - `t value`: the computed test statistic associated with testing $H_0 : \beta_j = 0$ versus $H_a : \beta_j \neq 0$ for each regression coefficient in the model.
  - `Pr(>|t|)`: the associated p-value of each test.
- Various summary statistics:
  - `Residual standard error` is the value of $\hat{\sigma}$, the estimate of the error standard deviation. The degrees of freedom is df_{RSS}, the number of observations minus the number of estimated coefficients in the model.

- `Multiple R-squared` is an estimate of model fit.
- `Adjusted R-squared` is a modified version of `Multiple R-squared`.
- `F-statistic` is the test statistic for the test that compares the model with an only an intercept to the fitted model. The `DF` (degrees of freedom) values relate to the statistic under the null hypothesis, and the `p-value` is the p-value for the test.

We use the `summary` function on `lmod` to produce the output below.

```
# summarize results stored in lmod
summary(lmod)
```

```
Call:
lm(formula = bill_length_mm ~ body_mass_g, data = penguins)

Residuals:
     Min       1Q   Median       3Q      Max
-10.1251  -3.0434  -0.8089   2.0711  16.1109

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 2.690e+01  1.269e+00   21.19   <2e-16 ***
body_mass_g 4.051e-03  2.967e-04   13.65   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.394 on 340 degrees of freedom
  (2 observations deleted due to missingness)
Multiple R-squared:  0.3542,    Adjusted R-squared:  0.3523
F-statistic: 186.4 on 1 and 340 DF,  p-value: < 2.2e-16
```

Using the output above, we see that the estimated parameters are $\hat{\beta}_0 = 26.9$ and $\hat{\beta}_1 = 0.004$.

Our fitted model is

$$\widehat{\texttt{bill\_length\_mm}} = 26.9 + 0.004\,\texttt{body\_mass\_g}.$$

In the context of a simple linear regression model:

- The intercept term is the expected response when the value of the regressor is zero.
- The slope is the expected change in the response when the regressor increases by 1 unit.

Thus, based on the model we fit to the `penguins` data, we can make the following interpretations:

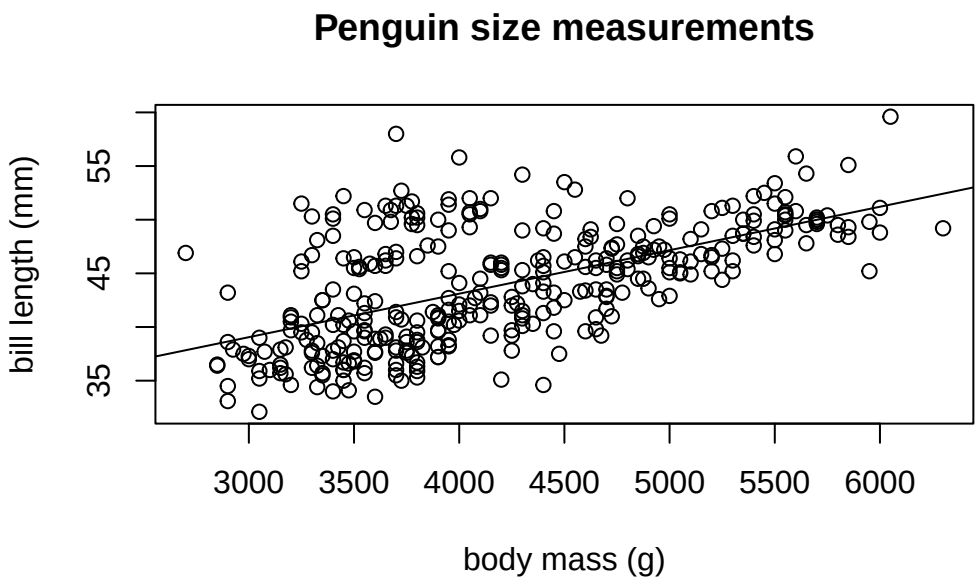
- $\widehat{\beta}_1$: If a penguin has a body mass 1 gram larger than another penguin, we expect the larger penguin's bill length to be 0.004 millimeters longer.
- $\widehat{\beta}_0$: A penguin with a body mass of 0 grams is expected to have a bill length of 26.9 millimeters.

Question:

- Does the intercept term make sense physically?

The `abline` function can be used to automatically overlay the fitted model on the observed data.

```
plot(bill_length_mm ~ body_mass_g,
     data = penguins, main = "Penguin size measurements",
     ylab = "bill length (mm)", xlab = "body mass (g)")
# draw fitted line of plot
abline(lmod)
```



R provides many additional methods (generic functions that do something specific when applied to a certain type of object) for `lm` objects. Commonly used ones include:

```r
(coeffs <- coef(lmod)) # extract, assign, and print coefficients
```

```
 (Intercept)  body_mass_g
26.898872424  0.004051417
```

```r
ehat <- residuals(lmod) # extract and assign residuals
head(ehat) # first few residuals
```

```
        1         2         3         5         6         7
-2.9916846 -2.7942554  0.2340237 -4.1762596 -2.3865430 -2.6852575
```

```r
yhat <- fitted(lmod) # extract and assign fitted values
head(yhat) # first few fitted values
```

```
       1        2        3        5        6        7
42.09168 42.29426 40.06598 40.87626 41.68654 41.58526
```

```r
yhat2 <- predict(lmod) # compute and assign fitted values
head(yhat2) # first few fitted values
```

```
       1        2        3        5        6        7
42.09168 42.29426 40.06598 40.87626 41.68654 41.58526
```

```r
(rss <- deviance(lmod)) # extract, assign, and print rss
```

```
[1] 6564.494
```

```r
(dfr <- df.residual(lmod)) # extract residual df
```

```
[1] 340
```

```r
(sigmasqhat <- sigma(lmod)^2) # estimated error variance
```

```
[1] 19.30734
```

Question:

- What is the RSS of the fitted model?

Defining a linear model

Defining terms (again)

- Y denotes the response variable.
  - The response variable is treated as a random variable.
  - We will observe realizations of this random variable for each observation in our data set.
- X denotes a single regressor variable. $X_1, X_2, \ldots, X_{p-1}$ denote distinct regressor variables if we are performing regression with multiple regressor variables.
  - The regressor variables are treated as non-random variables.
  - The observed values of the regressor variables are treated as fixed, known values.
- $\mathbb{X} = \{X_0, X_1, \ldots, X_{p-1}\}$ denotes the collection of all regressors.
  - X_0 is usually the constant regressor 1, which is needed to include an intercept in the regression model.
- β_0, β_1, ..., β_{p-1} denote **regression coefficients**.
  - Regression coefficients are statistical parameters that we will estimate from our data.
  - The regression coefficients are treated as fixed, non-random but unknown values.
  - Regression coefficients are not observable.
- ϵ denotes model **error**.
  - The model error is more accurately described as random variation of each observation from the regression model.
  - The error is treated as a random variable.
  - The error is assumed to have mean 0 for all values of the regressors, i.e., $E(\epsilon \mid \mathbb{X}) = 0$.
  - The variance of the errors is assumed to be a constant value for all values of the regressors, i.e.,$\text{var}(\epsilon \mid \mathbb{X}) = \sigma^2$.
  - The error is never observable (except in the context of a simulation study where the experimenter literally defines the true model).

Standard definition of linear model

In general, a linear regression model can have an arbitrary number of regressors.

A **multiple linear regression** model has two or more regressors.

A **linear model** for Y is defined by the equation

$$\begin{aligned} Y &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{p-1} X_{p-1} + \epsilon \\ &= E(Y \mid \mathbb{X}) + \epsilon. \end{aligned}$$

Notice:

- The response value equals the expected response for that combination of regressor values plus some error.
- $E(Y \mid \mathbb{X}) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{p-1} X_{p-1}$.

A linear regression model can be written as

$$E(Y \mid \mathbb{X}) = \sum_{j=0}^{p-1} c_j \beta_j.$$

- $c_0, c_1, \ldots, c_{p-1}$ are known functions of the regressor variables.
- e.g., $c_1 = X_1 X_2 X_3$, $c_3 = X_2^2$, $c_8 = \ln(X_1)/X_2^2$, etc.

Alternatively, if $g_0, \ldots, g_{p-1}$ are functions of $\mathbb{X}$, then a linear regression model can be written as

$$E(Y \mid \mathbb{X}) = \sum_{j=0}^{p-1} g_j(\mathbb{X}) \beta_j.$$

Examples of a linear model

A model is linear because of its *form* not the shape it produces.

Some examples of linear regression models are:

- $E(Y|X) = \beta_0$.
- $E(Y|X) = \beta_0 + +\beta_1 X + \beta_2 X^2$.
- $E(Y|X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$.
- $E(Y|X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$.
- $E(Y|X_1, X_2) = \beta_0 + \beta_1 \ln(X_1) + \beta_2 X_2^{-1}$.
- $E(\ln(Y)|X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$.

- $E(Y^{-1}|X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$.

Some examples of non-linear regression models are:

- $E(Y|X) = \beta_0 + e^{\beta_1 X}$.
- $E(Y|X) = \beta_0 + \beta_1 X/(\beta_2 + X)$.

Estimation of the multiple linear regression model

We want to estimate the parameters of the model

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_{p-1} X_{p-1} + \epsilon.$$

The system of equations relating the responses, the regressors, and the errors for all n observations can be written as

$$Y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \cdots + \beta_{p-1} x_{i,p-1} + \epsilon_i, \quad i = 1, 2, \ldots, n.$$

Using matrix notation to represent a linear model

We can simplify the linear model system of equations using using matrix notation.

We use the following notation:

- $\mathbf{y} = [Y_1, Y_2, \ldots, Y_n]$ denotes the column vector containing the n observed response values.
- $\mathbf{X}$ denotes the matrix containing a column of 1s and the observed regressor values for $X_1, X_2, \ldots, X_{p-1}$. This may be written as

$$\mathbf{X} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \cdots & x_{1,p-1} \\ 1 & x_{2,1} & x_{2,2} & \cdots & x_{2,p-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n,1} & x_{n,2} & \cdots & x_{n,p-1} \end{bmatrix}.$$

- $\beta = [\beta_0, \beta_1, \ldots, \beta_{p-1}]$ denotes the column vector containing the p regression coefficients.
- $\epsilon = [\epsilon_1, \epsilon_2, \ldots, \epsilon_n]$ denotes the column vector contained the n errors.

The system of equations defining the linear model in can be written as

$$\mathbf{y} = \mathbf{X}\beta + \epsilon.$$

Matrix definitions of residuals, fitted values, and RSS* for multiple linear regression

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The vector of estimated values for the coefficients contained in β is denoted

$$\hat{\beta} = [\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_{p-1}].$$

The vector of regressor values for the ith observation is denoted

$$\mathbf{x}_i = [1, x_{i,1}, \dots, x_{i,p-1}].$$

Question:

- Why do we include a 1 in our vector?

The ith **fitted value** in the context of multiple linear regression is defined as

$$\begin{aligned}\hat{Y}_i &= \hat{E}(Y \mid \mathbb{X} = \mathbf{x}_i) \\ &= \hat{\beta}_0 + \hat{\beta}_1 x_{i,1} + \cdots + \hat{\beta}_{p-1} x_{i,p-1} \\ &= \mathbf{x}_i^T \hat{\beta}.\end{aligned}$$

The notation "$\mathbb{X} = \mathbf{x}_i$" is a concise way of saying "$X_0 = 1, X_1 = x_{i,1}, \dots, X_{p-1} = x_{i,p-1}$".

The column vector of fitted values is defined as

$$\begin{aligned}\hat{\mathbf{y}} &= [\hat{Y}_1, \dots, \hat{Y}_n] \\ &= \mathbf{X}\hat{\beta}.\end{aligned}$$

The ith **residual** in the context of multiple linear regression can be written as

$$\hat{\epsilon}_i = Y_i - \hat{Y}_i = Y_i - \mathbf{x}_i^T \hat{\beta},$$

The column vector of residuals is defined as

$$\hat{\epsilon} = [\hat{\epsilon}_1, ..., \hat{\epsilon}_n].$$

Equivalent expressions for the residual vector are

$$\hat{\epsilon} = \mathbf{y} - \hat{\mathbf{y}} = \mathbf{y} - \mathbf{X}\hat{\beta}.$$

The RSS for a multiple linear regression model, as a function of the estimated regression coefficients, is

$$\begin{aligned} RSS(\hat{\beta}) &= \sum_{i=1}^{n} \hat{\epsilon}_i^2 \\ &= \hat{\epsilon}^T \hat{\epsilon} \qquad\qquad (\#eq : def - rss - matrix) \\ &= (\mathbf{y} - \hat{\mathbf{y}})^T (\mathbf{y} - \hat{\mathbf{y}}) \\ &= (\mathbf{y} - \mathbf{X}\hat{\beta})^T (\mathbf{y} - \hat{\beta}). \end{aligned}$$

OLS estimator in matrix form

The OLS estimator of the regression coefficient vector, β, is

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}.(\#eq : betahat)$$

This solution for $\hat{\beta}$ assumes $\mathbf{X}$ has full-rank ($n > p$ and none of the columns of $\mathbf{X}$ are linear combinations of other columns in $\mathbf{X}$).

The general estimator of the σ^2 in the context of multiple linear regression is

$$\hat{\sigma}^2 = \frac{RSS}{n-p},$$

Penguins multiple linear regression example

We will fit a multiple linear regression model regressing `bill_length_mm` on `body_mass_g` and `flipper_length_mm`, and will once again do so using the `lm` function.

Formula notation

Before we do that, we provide some additional discussion of the of the `formula` argument of the `lm` function. This will be very important as we discuss more complicated models. Assume `y` is the response variable and `x`, `x1`, `x2`, `x3` are available numeric predictors. Then:

- `y ~ x` describes the simple linear regression model $E(Y|X) = \beta_0 + \beta_1 X$.
- `y ~ x1 + x2` describes the multiple linear regression model $E(Y|X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$.
- `y ~ x1 + x2 + x1:x2` and `y ~ x1 * x2` describe the multiple linear regression model $E(Y|X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$.
- `y ~ -1 + x1 + x2` describe a multiple linear regression model without an intercept, in this case, $E(Y|X_1, X_2) = \beta_1 X_1 + \beta_2 X_2$. The `-1` tells R not to include an intercept in the fitted model.
- `y ~ x + I(x^2)` describe the multiple linear regression model $E(Y|X) = \beta_0 + \beta_1 X + \beta_2 X^2$. The `I()` function is a special function that tells R to create a regressor based on the syntax inside the `()` and include that regressor in the model.

Fitting a model

We fit the linear model regressing `bill_length_mm` on `body_mass_g` and `flipper_length_mm` and extract some statistics.

```
# fit model
mlmod <- lm(bill_length_mm ~ body_mass_g + flipper_length_mm, data = penguins)
# extract estimated coefficients
coef(mlmod)
```

```
    (Intercept)       body_mass_g flipper_length_mm
-3.4366939266      0.0006622186      0.2218654584
```

```r
# extract RSS
deviance(mlmod)
```

```
[1] 5764.585
```

The fitted model is

$$\widehat{\texttt{bill\_length\_mm}} = -3.44 + 0.0007\,\texttt{body\_mass\_g} + 0.22\,\texttt{flipper\_length\_mm}.$$

- **Question:** What is the RSS? How does it compare to the simple linear regression model we used before?

Types of linear models

- **Simple**: a model with an intercept and a single regressor.
- **Multiple**: a model with 2 or more regressors.
- **Polynomial**: a model with squared, cubic, quartic predictors, etc.
  - E.g, $E(Y \mid X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3$ is a 4th-degree polynomial.
- **First-order**: a model in which each predictor is used to create no more than one regressor.
- **Main effect**: a model in which none of the regressors are functions of more than one predictor. A predictor can be used more than once, but each regressor is only a function of one predictor.
  - E.g., if X_1 and X_2 are different predictors, then the regression model $E(Y \mid X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_2$ would be a main effect model, but not a first-order model since X_1 was used to create two regressors.
- **Interaction**: a model in which some of the regressors are functions of more than 1 predictor.
  - E.g., if X_1 and X_2 are different predictors, then the regression model $E(Y \mid X_1, X_2) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$ is a very simple interaction model since the third regressor is the product of X_1 and X_2.
- **Analysis of variance (ANOVA)**: a model for which all predictors used in the model are categorical.
- **Analysis of covariance (ANCOVA)**: a model that uses at least one numeric predictor and at least one categorical predictor.
- **Generalized (GLM)**: a "generalized" linear regression model in which the responses do not come from a normal distribution.

Categorical predictors

Categorical predictors can greatly improve the explanatory power or predictive capability of a fitted model when different patterns exist for different levels of the variables.

We discuss two basic linear regression models that have categorical predictors:

- **Parallel lines regression model**: a main effect regression model that has a single numeric regressor and a single categorical predictor.
  - The model produces parallel lines for each level of the categorical variable.
- **Separate lines regression model**, which adds an interaction term between the numeric regressor and categorical predictor of the parallel lines regression model.
  - The model produces separate lines for each level of the categorical variable.

Indicator variables

In order to compute $\widehat{\beta}$ both $\mathbf{X}$ and $\mathbf{y}$ must contain numeric values.

How can we use a categorical predictor in our regression model when its values are not numeric?

We must transform the categorical predictor into one or more **indicator** or **dummy variables**.

An **indicator function** is a function that takes the value 1 if a certain property is true and 0 otherwise.

An **indicator variable** is the variable that results from applying an indicator function to each observation of a variable. Many notations exist for indicator functions. We use the notation,

$$I_S(x) = \begin{cases} 1 & \text{if } x \in S \\ 0 & \text{if } x \notin S \end{cases}.$$

- This function returns 1 if x is in the set S and 0 otherwise.

Let C denote a categorical predictor with levels L_1 and L_2.

- C stands for "categorical".
- L stands for "level".
- c_i denotes the value of C for observation i.

Let D_j denote the indicator (dummy) variable for factor level L_j of C.

- The value of D_j for observation i is denoted $d_{i,j}$, with

$$d_{i,j} = I_{\{L_j\}}(c_i).$$

- $d_{i,j}$ is 1 if c_i has factor level L_j and 0 otherwise.

Parallel and separate lines models

Assume we want to build a linear regression model using a single numeric regressor X and a two-level categorical predictor C.

The standard simple linear regression model is

$$E(Y \mid X) = \beta_0 + \beta_1 X.$$

The parallel lines regression model is

$$E(Y \mid X, C) = \beta_0 + \beta_1 X + \beta_2 D_2.$$

Since $D_2 = 0$ when $C = L_1$ and $D_2 = 1$ when $C = L_2$,this model simplifies to

$$E(Y \mid X, C) = \begin{cases} \beta_0 + \beta_1 X & \text{if } C = L_1 \\ (\beta_0 + \beta_2) + \beta_1 X & \text{if } C = L_2. \end{cases}$$

- **Question:** What will the vertical distance between the lines be?

The separate lines regression model is

$$E(Y \mid X, C) = \beta_0 + \beta_1 X + \beta_2 D_2 + \beta_3 X D_2.$$

This model simplifies to

$$E(Y \mid X, C) = \begin{cases} \beta_0 + \beta_1 X & \text{if } C = L_1 \\ (\beta_0 + \beta_2) + (\beta_1 + \beta_3) X & \text{if } C = L_2. \end{cases}$$

More complex models with categorical predictors

If you had a categorical predictor C with K levels $L_1, L_2, \ldots, L_K$:

- We can add indicator variables $D_2, D_3, \ldots, L_K$ to a simple linear regression model to create a parallel lines model for each level of C.
- We can add regressors $D_2, D_3, \ldots, D_K, XD_2, XD_3, \ldots, XD_K$ to a simple linear regression model to create a separate lines model for each level of C.

It is easy to imagine using multiple categorical predictors in a model, interacting one or more categorical predictors with one or more numeric regressors in model, etc.

These models can be fit easily using R but are more difficult to interpret.

Avoiding collinearity

Why didn't we add D_1 to the parallel lines model? Or D_1 and D_1X to the separate lines model?

- We don't *need* to add them.
  - If an observation doesn't have level L_2 ($D_2 = 0$), then it must have level L_1.
- To avoid linear dependencies in the columns of the regressor matrix $\mathbf{X}$!

Consider a categorical variable C with two only levels L_1 and L_2.

- Let $\mathbf{d}_1 = [d_{1,1}, d_{2,1}, \ldots, d_{n,1}]$ denote the column vector of observed values for indicator variable D_1.
- Let $\mathbf{d}_2$ be the column vector for D_2.
- Then $\mathbf{d}_1 + \mathbf{d}_2$ is an $n \times 1$ vector of 1s.
- D_1 and D_2 will be linearly dependent with the intercept column of our $\mathbf{X}$ matrix, which creates estimation problems.

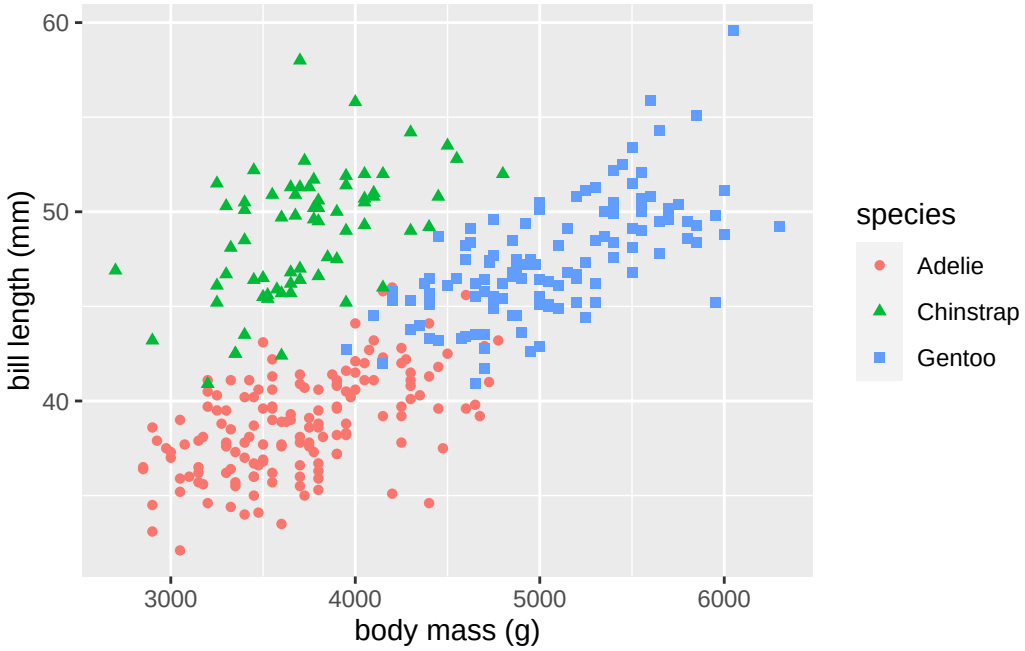
For a categorical predictor with K levels, we only need indicator variables for $K - 1$ levels of the categorical predictor.

- The level without an indicator variable in the regression model is known as the **reference level**.
- R automatically chooses the first level of a categorical (`factor`) variable to be the reference level, so we adopt that convention.

Penguins example with categorical predictor

We display the grouped scatter plot of `bill_length_mm` versus `body_mass_g` that distinguishes the `species` of each observation.

```
library(ggplot2) # load package
# create grouped scatterplot
ggplot(data = penguins) +
  geom_point(aes(x = body_mass_g, y = bill_length_mm, shape = species, color = species)) +
  xlab("body mass (g)") + ylab("bill length (mm)")
```



Question:

- Does the relationship between bill length and body mass change depending on the species of penguin?

How do you use a categorical variable in R's `lm` function?

- Each categorical variables should be a `factor`.
- The `lm` function will automatically convert a `factor` variable to the correct number of indicator variables when you include the `factor` variable in your `formula` argument.
- To add a main effect term for a categorical predictor, we simply add the term to our `lm` formula.

- To create an interaction term, we use `:` between the interacting variables.
  - E.g., if `c` is a `factor` variable and `x` is a `numeric` variable, you can use the notation `c:x` in your `formula` to get all the interactions between `c` and `x`.

Our categorical predictor `species` has the levels `Adelie`, `Chinstrap`, and `Gentoo`.

- The first level of species is `Adelie`, so R will treat that level as the reference level.
- R will automatically create indicator variables for the levels `Chinstrap` and `Gentoo`.

Let D_C denote the indicator variable for the `Chinstrap` level and D_G denote the indicator variable for the `Gentoo` level.

Fitting a parallel lines model

We fit the parallel lines regression model

$$E(\texttt{bill\_length\_mm} \mid \texttt{body\_mass\_g}, \texttt{species}) = \beta_0 + \beta_1 \texttt{body\_mass\_g} + \beta_2 D_C + \beta_3 D_G.$$

```
# fit parallel lines model
lmodp <- lm(bill_length_mm ~ body_mass_g + species, data = penguins)
# extract coefficients
coef(lmodp)
```

```
      (Intercept)       body_mass_g speciesChinstrap    speciesGentoo
24.919470977      0.003748497       9.920884113       3.557977539
```

The fitted parallel lines model is

$$\begin{aligned}&\hat{E}(\texttt{bill\_length\_mm} \mid \texttt{body\_mass\_g}, \texttt{species})\\ &= 24.92 + 0.004\texttt{body\_mass\_g} + 9.92 D_C + 3.56 D_G.\end{aligned}$$

Note that D_C is `speciesChinstrap` and D_G is `speciesGentoo`.

When an observation has `species` level `Adelie`, then the model simplifies to

$$\begin{aligned}&\hat{E}(\texttt{bill\_length\_mm} \mid \texttt{body\_mass\_g}, \texttt{species} = \texttt{Adelie})\\ &= 24.92 + 0.004\texttt{body\_mass\_g} + 9.92 \cdot 0 + 3.56 \cdot 0\\ &= 24.92 + 0.004\texttt{body\_mass\_g}.\end{aligned}$$

When an observation has `species` level `Chinstrap`, then the model simplifies to

$$\begin{aligned}
&\hat{E}(\texttt{bill_length_mm} \mid \texttt{body_mass_g}, \texttt{species} = \texttt{Chinstrap}) \\
&= 24.92 + 0.004\texttt{body_mass_g} + 9.92 \cdot 1 + 3.56 \cdot 0 \\
&= 34.84 + 0.004\texttt{body_mass_g}.
\end{aligned}$$

When an observation has `species` level `Gentoo`, then the model simplifies to

$$\begin{aligned}
&\hat{E}(\texttt{bill_length_mm} \mid \texttt{body_mass_g}, \texttt{species} = \texttt{Gentoo}) \\
&= 24.92 + 0.004\texttt{body_mass_g} + 9.92 \cdot 0 + 3.56 \cdot 1 \\
&= 28.48 + 0.004\texttt{body_mass_g}.
\end{aligned}$$

We add our fitted lines for each `species` to our scatter plot.

Let's try adding our fitted values to the `penguins` data frame.

- We use the `predict` function to obtained the fitted values of our fitted model.
- We use the `transform` function to add those values as the `pl_fitted` variable in the `penguins` data frame.

```
penguins <-
  penguins |>
  transform(pl_fitted = predict(lmodp))
```

```
Error in data.frame(structure(list(species = structure(c(1L, 1L, 1L, 1L, : arguments imply di
```

- **Question:** Why are we getting this error?

To handle this error, we refit our model while setting the `na.action` argument to `na.exclude`. As stated Details section of the documentation for the `lm` function (run `?lm` in the Console):

> ... when `na.exclude` is used the residuals and predictions are padded to the correct length by inserting `NA`s for cases omitted by `na.exclude`.

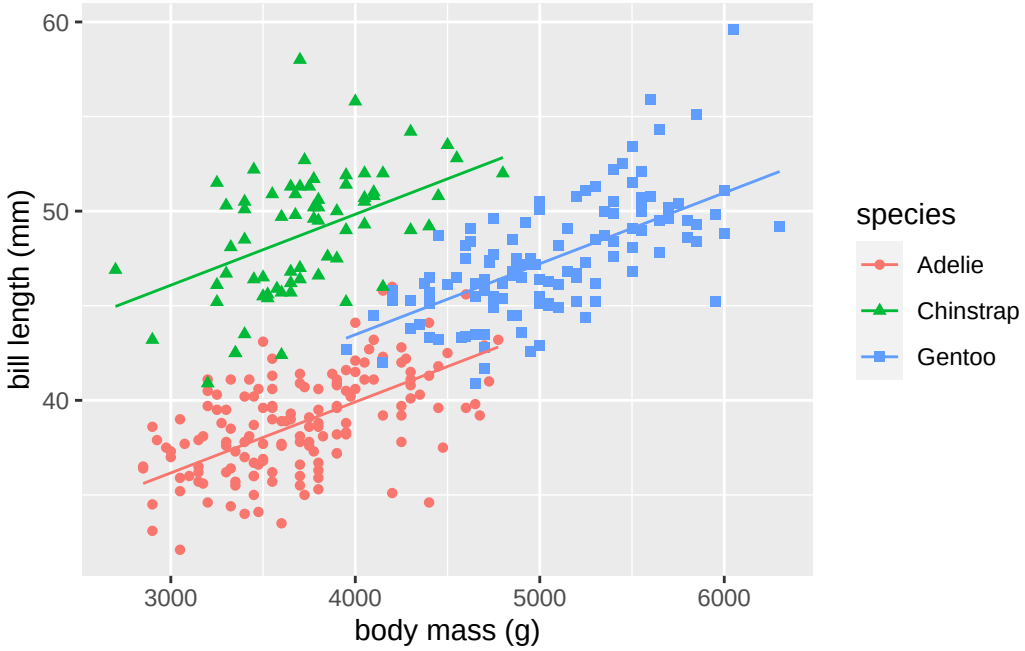
We refit the parallel lines model below with `na.action = na.exclude` and then repeat what we did before.

```
# refit parallel lines model with new na.action behavior
lmodp <- lm(bill_length_mm ~ body_mass_g + species,
            data = penguins, na.action = na.exclude)
# add fitted values to penguins data frame
penguins <-
```

```
  penguins |>
  transform(pl_fitted = predict(lmodp))
```

We now use the `geom_line` function to add the fitted lines for each `species` level to our scatter plot.

```
# create plot
# create scatterplot
# customize labels
# add lines for each level of species
ggplot(data = penguins) +
  geom_point(aes(x = body_mass_g, y = bill_length_mm,
                 shape = species, color = species)) +
  xlab("body mass (g)") + ylab("bill length (mm)") +
  geom_line(aes(x = body_mass_g, y = pl_fitted, color = species))
```



Fitting a separate lines model

We now fit the separate lines regression model

$$E(\texttt{bill\_length\_mm} \mid \texttt{body\_mass\_g}, \texttt{species}) = \beta_0 + \beta_1 \texttt{body\_mass\_g} + \beta_2 D_C + \beta_3 D_G + \beta_4 \texttt{body\_mass\_g} D_C + \beta_5 \texttt{body\_mass\_g} D_G.$$

```
# fit separate lines model
# na.omit = na.exclude used to change predict behavior
lmods <- lm(bill_length_mm ~ body_mass_g + species + body_mass_g:species,
            data = penguins, na.action = na.exclude)
# extract estimated coefficients
coef(lmods)
```

```
                (Intercept)                   body_mass_g
              26.9941391367                0.0031878758
           speciesChinstrap                speciesGentoo
               5.1800537287               -0.2545906615
body_mass_g:speciesChinstrap body_mass_g:speciesGentoo
               0.0012748183                0.0009029956
```

The fitted separate lines model is

$$\begin{aligned}\hat{E}(\texttt{bill\_length\_mm} \mid \texttt{body\_mass\_g}, \texttt{species}) &= 26.99 + 0.003\texttt{body\_mass\_g} + 5.18 D_C - 0.25 D_G \\ &\quad + 0.001\texttt{body\_mass\_g} D_C + 0.0009\texttt{body\_mass\_g} D_G, (\#eq : sl - model - penguins)\end{aligned}$$

When an observation has `species` level `Adelie`, then the model simplifies to

$$\begin{aligned}\hat{E}(\texttt{bill\_length\_mm} \mid \texttt{body\_mass\_g}, \texttt{species} = \texttt{Adelie}) &= 26.99 + 0.003\texttt{body\_mass\_g} + 5.18 \cdot 0 - 0.25 \cdot 0 \\ &\quad + 0.001 \cdot \texttt{body\_mass\_g} \cdot 0 + 0.0009 \cdot \texttt{body\_mass\_g} \cdot 0 \\ &= 26.99 + 0.003\texttt{body\_mass\_g}.\end{aligned}$$

When an observation has `species` level `Chinstrap`, then the equation simplifies to

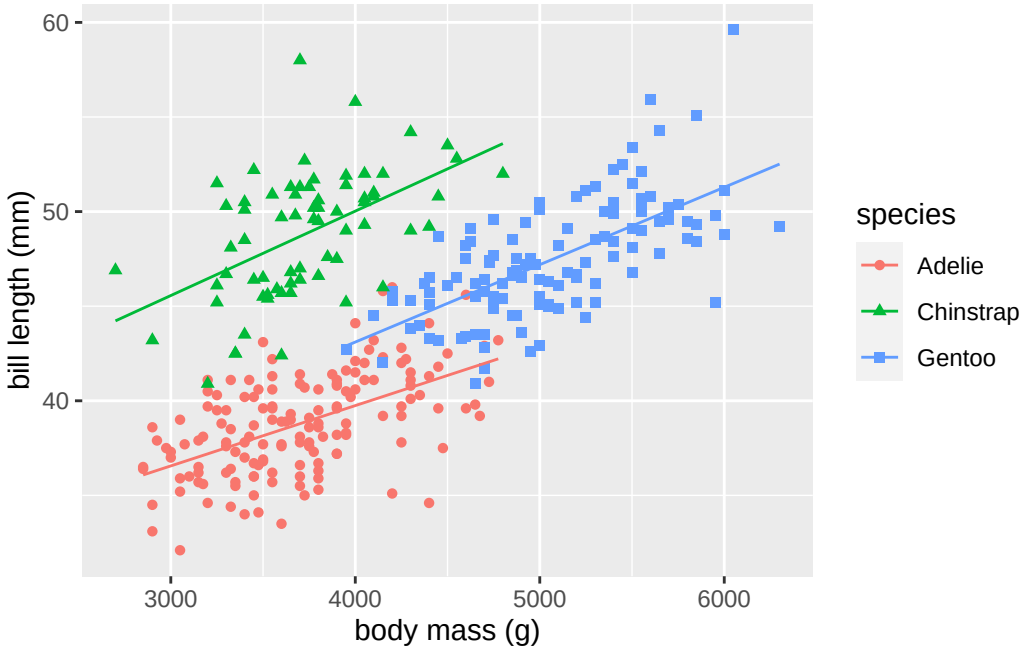
$$\begin{aligned}\hat{E}(\texttt{bill\_length\_mm} \mid \texttt{body\_mass\_g}, \texttt{species} = \texttt{Chinstrap}) &= 26.99 + 0.003\texttt{body\_mass\_g} + 5.18 \cdot 1 - 0.25 \cdot 0 \\ &\quad + 0.001 \cdot \texttt{body\_mass\_g} \cdot 1 + 0.0009 \cdot \texttt{body\_mass\_g} \cdot 0 \\ &= 31.17 + 0.004\texttt{body\_mass\_g}.\end{aligned}$$

When an observation has `species` level `Gentoo`, the model simplifies to

$$\begin{aligned}
&\hat{E}(\texttt{bill_length_mm} \mid \texttt{body_mass_g}, \texttt{species} = \texttt{Chinstrap}) \\
&= 26.99 + 0.003\texttt{body_mass_g} + 5.18 \cdot 0 - 0.25 \cdot 1 \\
&\quad + 0.001 \cdot \texttt{body_mass_g} \cdot 0 + 0.0009 \cdot \texttt{body_mass_g} \cdot 1 \\
&= 26.74 + 0.004\texttt{body_mass_g}.
\end{aligned}$$

We use the code below to display the fitted lines for the separate lines model on the `penguins` data.

```
# add separate lines fitted values to penguins data frame
penguins <-
  penguins |>
  transform(sl_fitted = predict(lmods))
# use geom_line to add fitted lines to plot
ggplot(data = penguins) +
  geom_point(aes(x = body_mass_g, y = bill_length_mm, shape = species, color = species)) +
  xlab("body mass (g)") + ylab("bill length (mm)") +
  geom_line(aes(x = body_mass_g, y = sl_fitted, col = species))
```



Question:

- Do the fitted lines match the observed data behavior reasonably well?

Evaluating model fit

The coefficient of determination

The most basic statistic measuring the fit of a regression model is the **coefficient of determination**, which is defined as

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2},$$

where $\bar{Y}$ is the sample mean of the observed response values.

Some sum-of-squares statistics

To interpret this statistic, we need to introduce some new "sum-of-squares" statistics similar to the RSS.

The **total sum of squares** (corrected for the mean) is computed as

$$TSS = \sum_{i=1}^{n}(Y_i - \bar{Y})^2.$$

- The TSS is the sum of the squared deviations of the response values from the sample mean.
- It has a more insightful interpretation.

Consider the **constant mean model**, which is the model

$$E(Y) = \beta_0.$$

Using basic calculus, we can show that the OLS estimator of β_0 for the model in Equation @ref(eq:constant-mean-model) is $\widehat{\beta}_0 = \bar{Y}$.

For the constant mean model:

- $\hat{Y}_i = \hat{\beta}_0$ for $i = 1, 2, \ldots, n$.
- The RSS of the constant mean model is $\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n}(Y_i - \bar{Y})^2$.

The TSS is the RSS for the constant mean model.

The **regression sum-of-squares** or **model sum-of-squares** is defined as

$$SS_{reg} = \sum_{i=1}^{n}(\hat{Y}_i - \bar{Y})^2.$$

- SS_{reg} is the sum of the squared deviations between the fitted values of a model and the fitted values of the constant mean model.

We have the following relationship between TSS, RSS, and SS_{reg}:

$$TSS = RSS + SS_{reg}.$$

$SS_{reg} = TSS - RSS.$

- SS_{reg} measures the reduction in RSS when comparing the fitted model to the constant mean model.

Equivalent expressiongs for R^2

Some equivalent expressions for R^2 are

$$\begin{aligned} R^2 &= 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2} \\ &= 1 - \frac{RSS}{TSS} \\ &= \frac{TSS - RSS}{TSS} \\ &= \frac{SS_{reg}}{TSS} \\ &= [\text{cor}(\mathbf{y}, \hat{\mathbf{y}})]^2. \end{aligned}$$

The last expression is the squared sample correlation between the observed and fitted values, and is a helpful way to express the coefficient of determination because it extends to regression models that are not linear.

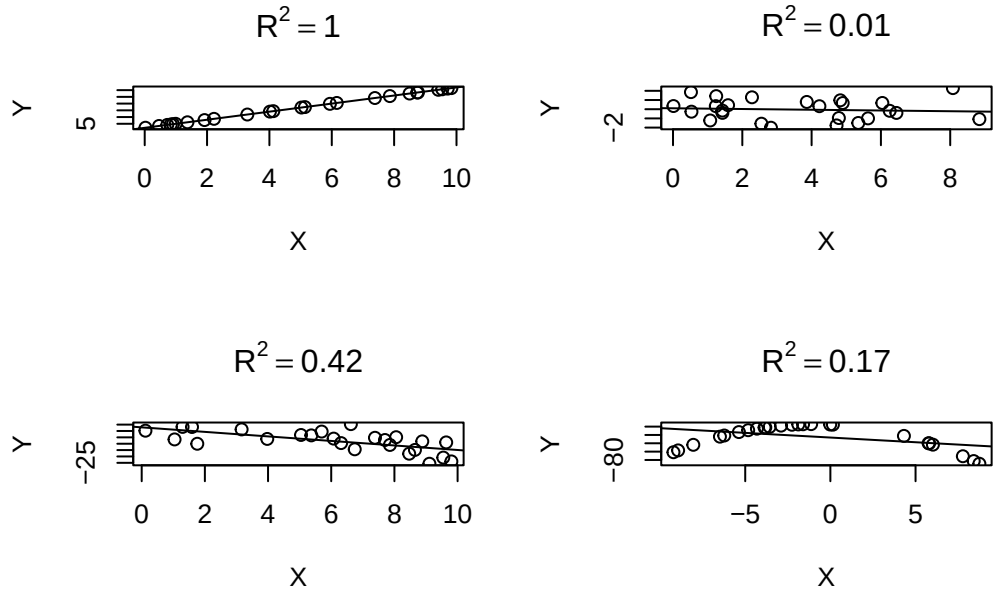
The coefficient of determination is the proportional reduction in RSS when comparing the fitted model to the constant mean model.

Comments about the coefficient of determination

- $0 \leq R^2 \leq 1$.
- $R^2 = 0$ for the constant mean model.
- $R^2 = 1$ for a fitted model that perfectly fits the data (the fitted values match the observed response values).
- Generally, larger values of R^2 suggest that the model explains a lot of the variation in the response variable.
- Smaller R^2 values suggest the fitted model does not explain a lot of the response variation.
- The `Multiple R-squared` value printed by the `summary` of an `lm` object is R^2.
- To extract R^2 from a fitted model, you can use the syntax `summary(lmod)$r.squared`, where `lmod` is your fitted model.

Examples of R^2

Consider the examples below relating R^2 to various fitted simple linear regression models.



The coefficient of determination for the parallel lines model fit to the `penguins` data is 0.81.

```
summary(lmodp)$r.squared
```

```
[1] 0.8079566
```

By adding the `body_mass_g` regressor and `species` predictor to the constant mean model of `bill_length_mm`, we reduced the RSS by 81%.

Cautions about R^2

It is not wise to use R^2 to choose between models:

- R^2 never decreases as regressors are added to an existing model.
  - We can increase R^2 by simply adding regressors to your existing model, even if they are non-sensical.
- R^2 doesn't tell you whether a model adequately describes the pattern of the observed data.
  - R^2 is a useful statistic for measuring model fit when there is approximately a linear relationship between the response values and fitted values.

Let's add some noise as a regressor to our parallel lines model.

```
set.seed(28) # for reproducibility
# create regressor of random noise
noisyx <- rnorm(344)
# add noisyx as regressor to lmodp
lmod_silly <- update(lmodp, . ~ . + noisyx)
# extract R^2 from fitted model
summary(lmod_silly)$r.squared
```

```
[1] 0.8087789
```

The R^2 value increased from 0.8080 to 0.8088!

Anscombe's Quartet

Anscombe (1973) provides a canonical data set known as "Anscombe's quartet" that illustrates how R^2 can mislead you into thinking an inappropriate model fits better than it actually does.

- The data set is comprised of 4 different data sets.
- When a simple linear regression model is fit to each data set:
  - $\hat{\beta}_0 = 3$.
  - $\hat{\beta}_1 = 0.5$.
  - $R^2 = 0.67$.

Anscombe's quartet is available as the `anscombe` data set in the **datasets** package. The data set includes 11 observations of 8 variables. The variables are:

- `x1`, `x2`, `x3` `x4`: the regressor variable for each individual data set.
- `y1`, `y2`, `y3` `y4`: the response variable for each individual data set.

```
# fit model to first data set
lmod_a1 <- lm(y1 ~ x1, data = anscombe)
# extract coefficients from fitted model
coef(lmod_a1)
```

```
(Intercept)          x1
  3.0000909   0.5000909
```

```
# extract R^2 from fitted model
summary(lmod_a1)$r.squared
```

```
[1] 0.6665425
```

```
# fit model to second data set
lmod_a2 <- lm(y2 ~ x2, data = anscombe)
coef(lmod_a2)
```

```
(Intercept)          x2
   3.000909    0.500000
```

```
summary(lmod_a2)$r.squared
```

```
[1] 0.666242
```

```r
# fit model to third data set
lmod_a3 <- lm(y3 ~ x3, data = anscombe)
coef(lmod_a3)
```

```
(Intercept)          x3
  3.0024545   0.4997273
```

```r
summary(lmod_a3)$r.squared
```

```
[1] 0.666324
```

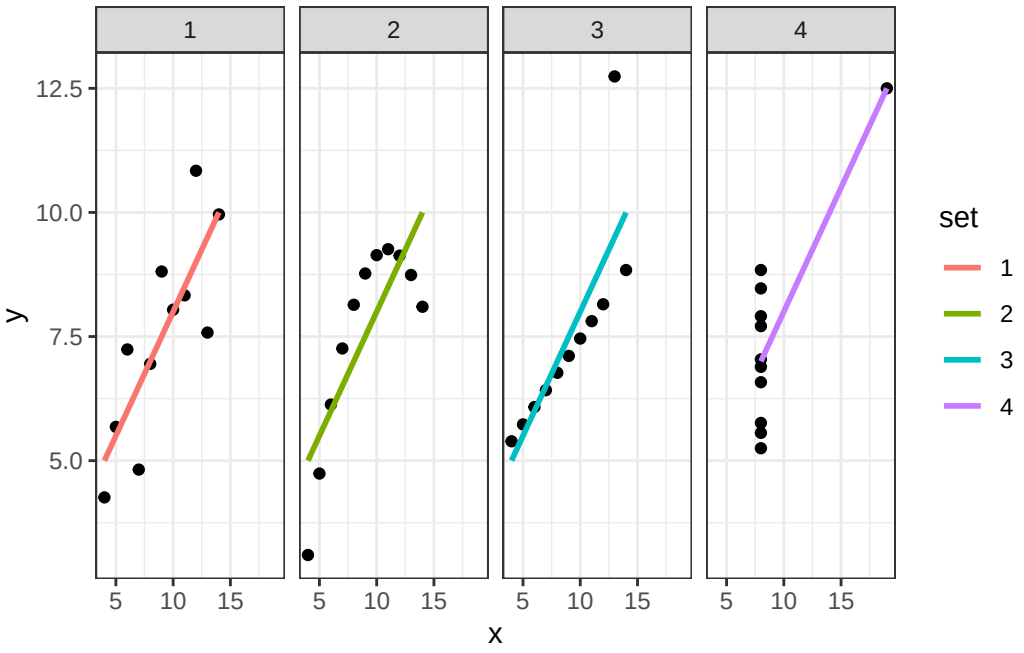
```r
# fit model to fourth data set
lmod_a4 <- lm(y4 ~ x4, data = anscombe)
coef(lmod_a4)
```

```
(Intercept)          x4
  3.0017273   0.4999091
```

```r
summary(lmod_a4)$r.squared
```

```
[1] 0.6667073
```

We overlays the fitted models on each data set.



Do all models describe the data equally well?

Adjusted R-squared

Ezekiel (1930) proposed the adjusted R-squared statistic as a better statistic for measuring model fit. The adjusted R^2 statistic is defined as

$$R_a^2 = 1 - (1 - R^2)\frac{n-1}{n-p} = 1 - \frac{RSS/(n-p)}{TSS/(n-1)}.$$

- R_a^2 will only increase when a regressors substantively improves the fit of the model to the observed data.
- We favor models with larger values of R_a^2.

What is the R_a^2 for the 4 models we previously fit to the `penguins` data? Which is the "best" model?

```
# simple linear regression model
summary(lmod)$adj.r.squared
```

```
[1] 0.3522562
```

```
# multiple linear regression model
summary(mlmod)$adj.r.squared
```

```
[1] 0.4295084
```

```
# parallel lines model
summary(lmodp)$adj.r.squared
```

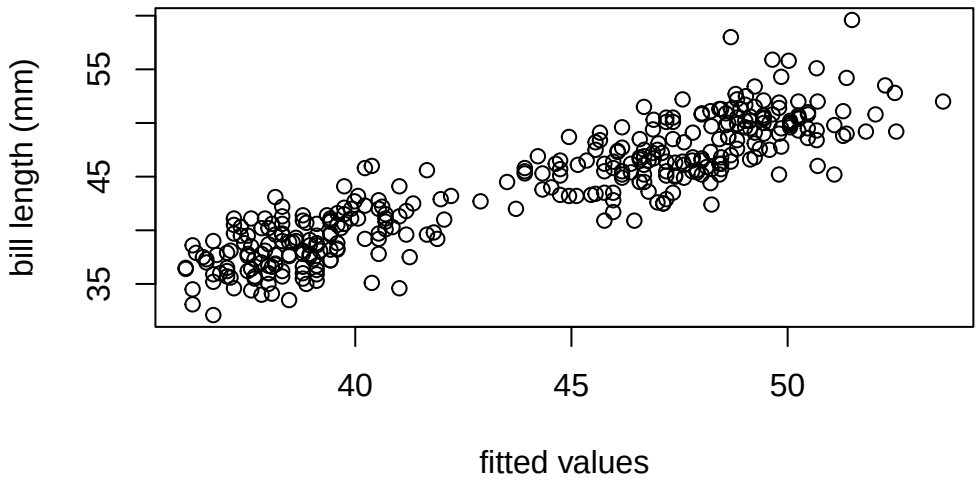
```
[1] 0.8062521
```

```
# separate lines model
summary(lmods)$adj.r.squared
```

```
[1] 0.8069556
```

We double-check that the separate lines model is a sensible model.

```
plot(penguins$bill_length_mm ~ fitted(lmods),
     xlab = "fitted values", ylab = "bill length (mm)")
```



Summary of terms

An overview of terms used to define a linear model.

Term	Description	Observable?	Random?
Y	response variable	Yes	Yes
Y_i	response value for the ith observation	Yes	Yes
$\mathbf{y}$	the $n \times 1$ column vector of response values	Yes	Yes
X	regressor variable	Yes	No
X_j	the jth regressor variable	Yes	No
$x_{i,j}$	the value of the jth regressor variable for the ith observation	Yes	No
$\mathbf{X}$	the $n \times p$ matrix of regressor values	Yes	No
$\mathbf{x}_i$	the $p \times 1$ vector of regressor values for the ith observation	Yes	No
β_j	the coefficient associated with the jth regressor variable	No	No
β	the $p \times 1$ column vector of regression coefficients	No	No
ϵ	the model error	No	Yes
ϵ_i	the error for the ith observation	No	Yes

Summary of functions

An overview of important functions discussed in this chapter.

Function	Purpose
`lm`	Fits a linear model based on a provided `formula`
`summary`	Provides summary information about the fitted model
`coef`	Extracts the vector of estimated regression coefficients from the fitted model
`residuals`	Extracts the vector of residuals from the fitted model
`fitted`	Extracts the vector of fitted values from the fitted model
`predict`	Computes the fitted values (or arbitrary predictions) based on a fitted model
`deviance`	Extracts the RSS of a fitted model
`sigma`	Extracts $\hat{\sigma}$ from the fitted model
`update`	Updates a fitted model to remove or add regressors

Going Deeper

Derivation of the OLS estimators of the simple linear regression model coefficients

Assume a simple linear regression model with n observations.

The residual sum of squares for the simple linear regression model is

$$RSS(\hat{\beta}_0, \hat{\beta}_1) = \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2.$$

OLS estimator of β_0

First, we take the partial derivative of the RSS with respect to $\hat{\beta}_0$ and simplify.

$$\begin{aligned}
\frac{\partial RSS(\hat{\beta}_0, \hat{\beta}_1)}{\partial \hat{\beta}_0} &= \frac{\partial}{\partial \hat{\beta}_0} \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 && \text{(substituting the formula for the RSS)} \\
&= \sum_{i=1}^{n} \frac{\partial}{\partial \hat{\beta}_0} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 && \text{(by the linearity property of derivatives)} \\
&= -2 \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i). && \text{(chain rule, factoring out -2)}
\end{aligned}$$

$$\begin{aligned}
0 &= \frac{\partial RSS(\hat{\beta}_0, \hat{\beta}_1)}{\partial \hat{\beta}_0} \\
0 &= -2 \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) && \text{(substitute partial deriviative)} \\
0 &= \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) && \text{(divide both sides by -2)} \\
0 &= \sum_{i=1}^{n} Y_i - \sum_{i=1}^{n} \hat{\beta}_0 - \sum_{i=1}^{n} \hat{\beta}_1 x_i && \text{(by linearity of sum)} \\
0 &= \sum_{i=1}^{n} Y_i - n\hat{\beta}_0 - \sum_{i=1}^{n} \hat{\beta}_1 x_i && (\text{summing } \hat{\beta}_0 \text{ } n \text{ times equals } n\hat{\beta}_0) \\
n\hat{\beta}_0 &= \sum_{i=1}^{n} Y_i - \sum_{i=1}^{n} \hat{\beta}_1 x_i. && \text{(algebra rearrange)} = \hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x}
\end{aligned}$$

OLS Estimator of β_1

We start by taking the partial derivative of the RSS with respect to $\hat{\beta}_1$ and simplify.

$$\begin{aligned}
\frac{\partial RSS(\hat{\beta}_0, \hat{\beta}_1)}{\partial \hat{\beta}_1} &= \frac{\partial}{\partial \hat{\beta}_1} \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 && \text{(substitute formula for RSS)} \\
&= \sum_{i=1}^{n} \frac{\partial}{\partial \hat{\beta}_1} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 && \text{(linearity property of derivatives)} \\
&= -2 \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) x_i && \text{(chain rule, factor out -2)}
\end{aligned}$$

We now set this derivative equal to 0 and rearrange the terms to solve for $\hat{\beta}_1$.

$$\begin{aligned}
0 &= \frac{\partial RSS(\hat{\beta}_0, \hat{\beta}_1)}{\partial \hat{\beta}_1} \\
0 &= -2 \sum_{i=1}^{n} (Y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) x_i && \text{(substitute partial derivative)} \\
0 &= \sum_{i=1}^{n} (Y_i - (\bar{Y} - \hat{\beta}_1 \bar{x}) - \hat{\beta}_1 x_i) x_i && \text{(substitute OLS estimator of } \hat{\beta}_0, \text{ divide both sides by -2)} \\
0 &= \sum_{i=1}^{n} x_i Y_i - \sum_{i=1}^{n} x_i \bar{Y} + \hat{\beta}_1 \bar{x} \sum_{i=1}^{n} x_i - \hat{\beta}_1 \sum_{i=1}^{n} x_i^2. && \text{(expand sum, use linearity of sum)}
\end{aligned}$$

Continuing from the previous line, we move the terms involving $\hat{\beta}_1$ to the other side of the equality.

$$\begin{aligned}
\hat{\beta}_1 \sum_{i=1}^{n} x_i^2 - \hat{\beta}_1 \bar{x} \sum_{i=1}^{n} x_i &= \sum_{i=1}^{n} x_i Y_i - \sum_{i=1}^{n} x_i \bar{Y} && \text{(move estimator to other side)} \\
\hat{\beta}_1 \sum_{i=1}^{n} x_i^2 - \hat{\beta}_1 \frac{1}{n} \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i &= \sum_{i=1}^{n} x_i Y_i - \sum_{i=1}^{n} x_i \frac{1}{n} \sum_{i=1}^{n} Y_i && \text{(rewrite using definition of sample means)} \\
\hat{\beta}_1 \sum_{i=1}^{n} x_i^2 - \hat{\beta}_1 \frac{1}{n} \left(\sum_{i=1}^{n} x_i \right)^2 &= \sum_{i=1}^{n} x_i Y_i - \frac{1}{n} \sum_{i=1}^{n} x_i \sum_{i=1}^{n} Y_i && \text{(reorder and simplify)} \\
\hat{\beta}_1 \left(\sum_{i=1}^{n} x_i^2 - \frac{1}{n} \left(\sum_{i=1}^{n} x_i \right)^2 \right) &= \sum_{i=1}^{n} x_i Y_i - \frac{1}{n} \sum_{i=1}^{n} x_i \sum_{i=1}^{n} Y_i, && \text{(factoring)}
\end{aligned}$$

which allows us to obtain

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} x_i Y_i - \frac{1}{n} \sum_{i=1}^{n} x_i \sum_{i=1}^{n} Y_i}{\sum_{i=1}^{n} x_i^2 - \frac{1}{n} \left(\sum_{i=1}^{n} x_i \right)^2}.$$

Unbiasedness of OLS estimators

We now show that the OLS estimators of the simple linear regression coefficients are unbiased.

An estimator is unbiased if the expected value is equal to the parameter it is estimating.

We want to show that

$$E(\hat{\beta}_0 \mid \mathbf{X}) = \beta_0.$$

We start by determining $E(Y_i \mid X = x_i)$.

$$\begin{aligned}
E(Y_i \mid X = x_i) &= E(\beta_0 + \beta_1 x_i + \epsilon_i \mid X = x_i) && \text{(substiute definition of } Y_i\text{)} \\
&= E(\beta_0 \mid X = x_i) + E(\beta_1 x_i \mid X = X_i) + E(\epsilon_i | X = x_i) && \text{(linearity property of expectation)} \\
&= \beta_0 + \beta_1 x_i + E(\epsilon_i | X = x_i) && \text{(the } \beta\text{s and } x_i \text{ are non-random values)} \\
&= \beta_0 + \beta_1 x_i + 0 && \text{(assumption about errors)} \\
&= \beta_0 + \beta_1 x_i.
\end{aligned}$$

Next, we note:

$$\begin{aligned}
E\left(\sum x_i Y_i \,\middle|\, \mathbf{X}\right) &= \sum E(x_i Y_i \mid \mathbf{X}) && \text{(by the linearity of the expectation operator)} \\
&= \sum x_i E(Y_i \mid \mathbf{X}) && \left(x_i \text{ is a fixed value, so it can be brought out}\right) \\
&= \sum x_i (\beta_0 + \beta_1 x_i) && \text{(substitute expected value of } Y_i\text{)} \\
&= \sum x_i \beta_0 + \sum x_i \beta_1 x_i && \text{(distribute sum)} \\
&= \beta_0 \sum x_i + \beta_1 \sum x_i^2. && \text{(factor out constants)}
\end{aligned}$$

Also,

$$\begin{aligned}
E(\bar{Y} \mid \mathbf{X}) &= E\left(\frac{1}{n} \sum Y_i \,\middle|\, \mathbf{X}\right) && \text{(definition of sample mean)} \\
&= \frac{1}{n} E\left(\sum Y_i \,\middle|\, \mathbf{X}\right) && \text{(factor out constant)} \\
&= \frac{1}{n} \sum E\left(Y_i \mid \mathbf{X}\right) && \text{(linearity of expectation)} \\
&= \frac{1}{n} \sum (\beta_0 + \beta_1 x_i) && \text{(substitute expected value of } Y_i\text{)} \\
&= \frac{1}{n} \left(\sum \beta_0 + \sum \beta_1 x_i\right) && \text{(distribute sum)} \\
&= \frac{1}{n} \left(n\beta_0 + \beta_1 \sum x_i\right) && \text{(simplify, factor out constant)} \\
&= \beta_0 + \beta_1 \bar{x}. && \text{(simplify)}
\end{aligned}$$

To simplify our derivation below, define

$$SSX = \sum x_i^2 - \frac{1}{n}\left(\sum x_i\right)^2.$$

Thus,

$$\begin{aligned}
&E(\hat{\beta}_1 \mid \mathbf{X}) \\
&= E\left(\frac{\sum x_i Y_i - \frac{1}{n}\sum x_i \sum Y_i}{\sum x_i^2 - \frac{1}{n}\left(\sum x_i\right)^2} \,\middle|\, \mathbf{X}\right) && \text{(substitute OLS estimator)} \\
&= \frac{1}{SSX} E\left(\sum x_i Y_i - \frac{1}{n}\sum x_i \sum Y_i \,\middle|\, \mathbf{X}\right) && \text{(factor out constant denominator, substitute } SSX\text{)} \\
&= \frac{1}{SSX}\left[E\left(\sum x_i Y_i \,\middle|\, \mathbf{X}\right) - E\left(\frac{1}{n}\sum x_i \sum Y_i \,\middle|\, \mathbf{X}\right)\right] && \text{(linearity of expectation)} \\
&= \frac{1}{SSX}\left[E\left(\sum x_i Y_i \,\middle|\, \mathbf{X}\right) - \left(\sum x_i\right) E\left(\bar{Y} \mid \mathbf{X}\right)\right] && \text{(factor out constant } \sum x_i\text{, use definition of } \bar{Y}\text{)} \\
&= \frac{1}{SSX}\left[\left(\beta_0 \sum x_i + \beta_1 \sum x_i^2\right) - \left(\sum x_i\right)(\beta_0 + \beta_1 \bar{x})\right] && \text{(substitute previous derivations)} \\
&= \frac{1}{SSX}\left[\beta_0 \sum x_i + \beta_1 \sum x_i^2 - \beta_0 \sum x_i - \beta_1 \bar{x} \sum x_i\right] && \text{(expand product and reorder)} \\
&= \frac{1}{SSX}\left[\beta_1 \sum x_i^2 - \beta_1 \bar{x} \sum x_i\right] && \text{(cancel terms)} \\
&= \frac{1}{SSX}\left[\beta_1 \sum x_i^2 - \beta_1 \frac{1}{n}\sum x_i \sum x_i\right] && \text{(using definition of sample mean)} \\
&= \frac{1}{SSX}\beta_1\left[\sum x_i^2 - \frac{1}{n}\left(\sum x_i\right)^2\right] && \text{(factor out } \beta_1\text{, simplify)} \\
&= \frac{1}{SSX}\beta_1[SSX] && \text{(substitute } SSX\text{)} \\
&= \beta_1. && \text{(simplify)}
\end{aligned}$$

Therefore, $\hat{\beta}_1$ is an unbiased estimator of β_1.

Next, we show that $\hat{\beta}_0$ is unbiased:

$$\begin{aligned}
E(\hat{\beta}_0 \mid \mathbf{X}) &= E(\bar{Y} - \hat{\beta}_1 \bar{x} \mid \mathbf{X}) && \text{(OLS estimator of } \beta_0\text{)} \\
&= E(\bar{Y} \mid \mathbf{X}) - E(\hat{\beta}_1 \bar{x} \mid \mathbf{X}) && \text{(linearity of expectation)} \\
&= E(\bar{Y} \mid \mathbf{X}) - \bar{x} E(\hat{\beta}_1 \mid \mathbf{X}) && \text{(factor out constant)} \\
&= \beta_0 + \beta_1 \bar{x} - \bar{x}\beta_1 && \text{(substitute previous derivations)} \\
&= \beta_0. && \text{(cancel terms)}
\end{aligned}$$

Therefore, $\hat{\beta}_0$ is an unbiased estimator of β_0.

Derivation of the OLS estimator for the multiple linear regression model coefficients

We want to determine the value of $\hat{\beta}$ that will minimize

$$\begin{aligned} RSS(\hat{\beta}) &= \sum_{i=1}^{n} \hat{\epsilon_i}^2 \\ &= \hat{\epsilon}^T \hat{\epsilon} \\ &= (\mathbf{y} - \mathbf{X}\hat{\beta})^T (\mathbf{y} - \mathbf{X}\hat{\beta}) \\ &= \mathbf{y}^T \mathbf{y} - 2\hat{\beta}^T \mathbf{X}^T \mathbf{y} + \hat{\beta}^T \mathbf{X}^T \mathbf{X} \hat{\beta}, \end{aligned}$$

where the second term in the last line comes from the fact that $\hat{\beta}^T \mathbf{X}^T \mathbf{y}$ is a 1×1 matrix, and is thus symmetric. Consequently, $\hat{\beta}^T \mathbf{X}^T \mathbf{y} = (\hat{\beta}^T \mathbf{X}^T \mathbf{y})^T = \mathbf{y}^T \mathbf{X} \hat{\beta}$.

To find the local extrema of $RSS(\hat{\beta})$, we set its derivative with respect to $\hat{\beta}$ equal to 0, and solve for $\hat{\beta}$).

We see that

$$\frac{\partial RSS(\hat{\beta})}{\partial \hat{\beta}} = -2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X} \hat{\beta}.$$

Setting $\partial RSS(\hat{\beta}) / \partial \hat{\beta} = 0$ and using some simple algebra, we derive the **normal equations**

$$\mathbf{X}^T \mathbf{X} \hat{\beta} = \mathbf{X}^T \mathbf{y}.$$

Assuming the $\mathbf{X}^T \mathbf{X}$ is invertible, which it will be when $\mathbf{X}$ is full-rank, our solution is

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}.$$

To show that the OLS estimator of β minimizes $RSS(\hat{\beta})$, we technically need to show that the Hessian matrix of $RSS(\hat{\beta})$, the matrix of second-order partial derivatives, is positive definite. In our context, the Hessian matrix is

$$\begin{aligned} \frac{\partial^2 RSS(\hat{\beta})}{\partial \hat{\beta}^2} &= \frac{\partial}{\partial \hat{\beta}} (-2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X} \hat{\beta}) \\ &= 2\mathbf{X}^T \mathbf{X}. \end{aligned}$$

The $p \times p$ matrix $2\mathbf{X}^T \mathbf{X}$ is positive definite, but it is beyond the scope of the course to prove this.

Therefore, the OLS estimator of β,

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

minimizes the RSS.

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