Applied Statistics with R

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Chapter 1

Introduction

Welcome to Applied Statistics with R!

1.1 About This Book

This book was originally (and currently) designed for use with STAT 420, Methods of Applied Statistics, at the University of Illinois at Urbana-Champaign. It may certainly be used elsewhere, but any references to "this course" in this book specifically refer to STAT 420.

This book is under active development. When possible, it would be best to always access the text online to be sure you are using the most up-to-date version. (Also, the html version provides additional features such as changing text size, font, and colors.) If you are in need of a local copy, a **pdf version** is continuously maintained.

Since this book is under active development you may encounter errors ranging from typos to broken code to poorly explained topics. If you do, please let us know! Simply send an email and we'll make the changes ASAP. (dalpiaz2 AT illinois DOT edu) Or, if you know RMarkdown and are familiar with GitHub, make a pull request and fix an issue yourself! (This process is partially automated by the edit button in the top-left corner of the html version.)

This text uses MathJax to render mathematical notation for the web. Occasionally, but rarely, a JavaScript error will prevent MathJax from rendering correctly. (In which case, will see the "code" instead of the expected mathematical equations.) From experience, this is almost always fixed by simply refreshing the page. You'll also notice that if you right-click any equation you can obtain the MathML Code (for copying into Microsoft Word) or the TeX command used to generate the equation.

$$a^2 + b^2 = c^2$$

1.2 Conventions

R code will be typeset using a monospace font which is syntax highlighted.

```
a = 3
b = 4
sqrt(a ^ 2 + b ^ 2)
```

R output lines, which would appear in the console will begin with ##. They will generally not be syntax highlighted.

[1] 5

1.3 Acknowledgements

Material in this book was heavily influenced by:

- Alex Stepanov
- David Unger
- James Balamuta

Additional corrections or suggestions provided by:

- Daniel McQuillan
- Mason Rubenstein
- Yuhang Wang
- Zhao Liu

1.4 License



 $\label{thm:commons} \begin{tabular}{ll} Figure~1.1:~This~work~is~licensed~under~a~Creative~Commons~Attribution-NonCommercial-ShareAlike~4.0~International~License. \end{tabular}$

Chapter 2

Introduction to R

"Measuring programming progress by lines of code is like measuring aircraft building progress by weight."

— Bill Gates

After reading this chapter you will be able to:

- $\bullet\,$ Interact with R using RS tudio.
- Use R as a calculator.
- Work with data as vectors and data frames.
- Make basic data visualizations.
- Write your own R functions.
- Perform hypothesis tests using R.
- Perform basic simulations in R.

2.1 R Resources

R is both a programming language and software environment for statistical computing, which is *free* and *open-source*. To get started, you will need to install two pieces of software:

- R, the actual programming language.
 - Chose your operating system, and select the most recent version, 3.3.1.
- RStudio, an excellent IDE for working with R.
 - Note, you must have R installed to use RStudio. RStudio is simply an interface used to interact
 with R.

The popularity of R is on the rise, and everyday it becomes a better tool for statistical analysis. It even generated this book! (A skill you will learn in this course.) There are many good resources for learning R. They are not necessary for this course, but you may find them useful if you would like a deeper understanding of R:

- Try R from Code School.
 - An interactive introduction to the basics of R. Could be very useful for getting up to speed on R's syntax.

- Quick-R by Robert Kabacoff.
 - A good reference for R basics.
- R Tutorial by Chi Yau.
 - A combination reference and tutorial for R basics.
- R Markdown from RStudio.
 - Reference materials for RMarkdown.
- The Art of R Programming by Norman Matloff.
 - Gentle introduction to the programming side of R. (Whereas we will focus more on the data analysis side.) A free electronic version is available through the Illinois library.
- Advanced R by Hadley Wickham.
 - From the author of several extremely popular R packages. Good follow-up to The Art of R Programming. (And more up-to-date material.)
- R for Data Science by Hadley Wickham and Garrett Grolemund.
 - Similar to Advanced R, but focuses more on data analysis, while still introducing programming concepts. At the time of writing, currently under development.
- The R Inferno by Patrick Burns.
 - Likens learning the tricks of R to descending through the levels of hell. Very advanced material, but may be important if R becomes a part of your everyday toolkit.

RStudio has a large number of useful keyboard shortcuts. A list of these can be found using a keyboard shortcut – the keyboard shortcut to rule them all:

```
On Windows: Alt + Shift + K
On Mac: Option + Shift + K
```

The RStudio team has developed a number of "cheatsheets" for working with both R and RStudio. This particular cheatseet for Base R will summarize many of the concepts in this document.

When programming, it is often a good practice to follow a style guide. (Where do spaces go? Tabs or spaces? Underscores or CamelCase when naming variables?) No style guide is "correct" but it helps to be aware of what others do. The more import thing is to be consistent within your own code.

- Hadley Wickham Style Guide from Advanced R
- Google Style Guide

For this course, our main deviation from these two guides is the use of = in place of <-. (More on that later.)

2.2 R Basics

2.2.1 Basic Calculations

To get started, we'll use R like a simple calculator. Note, in R the # symbol is used for comments. In this book, lines which begin with two such symbols, ##, indicate output.

Addition, Subtraction, Multiplication and Division

```
3 + 2
## [1] 5
3 - 2
## [1] 1
3 * 2
## [1] 6
3 / 2
## [1] 1.5
Exponents
3 ^ 2
## [1] 9
2 ^ (-3)
## [1] 0.125
100 ^ (1 / 2)
## [1] 10
sqrt(1 / 2)
## [1] 0.7071068
exp(1)
## [1] 2.718282
Mathematical Constants
рi
```

[1] 3.141593

```
exp(1)
## [1] 2.718282
Logarithms
log(10)
                  # natural log
## [1] 2.302585
log10(1000)
                  # base 10 log
## [1] 3
log2(8)
                  # base 2 log
## [1] 3
log(16, base = 4) # base 4 log
## [1] 2
Trigonometry
sin(pi / 2)
## [1] 1
cos(0)
```

2.2.2 Getting Help

[1] 1

In using R as a calculator, we have seen a number of functions: sqrt(), exp(), log() and sin(). To get documentation about a function in R, simply put a question mark in front of the function name and RStudio will display the documentation, for example:

```
?log
?sin
?paste
?lm
```

Frequently one of the most difficult things to do when learning R is asking for help. First, you need to decide to ask for help, then you need to know how to ask for help. Your very first line of defense should be to Google your error message or a short description of your issue. (The ability to solve problems using this method is quickly becoming an extremely valuable skill.) If that fails, and it eventually will, you should ask for help. There are a number of things you should include when emailing an instructor, or posting to a help website such as Stack Exchange.

- Describe what you expect the code to do.
- State the end goal you are trying to achieve. (Sometimes what you expect the code to do, is not what you want to actually do.)
- Provide the full text of any errors you have received.
- Provide enough code to recreate the error. Often for the purpose of this course, you could simply email your entire .R or .Rmd file.
- Sometimes it is also helpful to include a screenshot of your entire RStudio window when the error
 occurs.

If you follow these steps, you will get your issue resolved much quicker, and possibly learn more in the process. Do not be discouraged by running into errors and difficulties when learning R. (Or any technical skill.) It is simply part of the learning process.

2.2.3 Installing Packages

R comes with a number of built-in functions and datasets, but one of the main strengths of R as an open-source project is its package system. Packages add additional functions and data. Frequently if you want to do something in R, and it isn't available by default, there is a good chance that there is a package that will fulfill your needs.

To install a package, use the install.packages() function. Think of this as buying a recipe book from the store, bringing it home, and putting it on your shelf.

```
install.packages("ggplot2")
```

Once a package is installed, it must be loaded into your current R session before being used. Think of this as taking the book off of the shelf and opening it up to read.

```
library(ggplot2)
```

Once you close R, all the packages are closed and put back on the imaginary shelf. The next time you open R, you do not have to install the package again, but you do have to load any packages you intend to use by invoking library().

2.2.4 Data Types

R has a number of basic data types.

- Numeric
 - Also known as Double. The default type when dealing with numbers.
 - Examples: 1, 1.0, 42.5
- Integer
 - Examples: 1L, 2L, 42L

- Complex
 - Example: 4 + 2i
- Logical
 - Two possible values: TRUE and FALSE
 - You can also use T and F, but this is *not* recommended.
 - NA is also considered logical.
- Character
 - Examples: "a", "Statistics", "1 plus 2."

R also has a number of basic data *structures*. A data structure is either homogeneous (all elements are of the same data type) or heterogeneous (elements can be of more than one data type).

Dimension	Homogeneous	Heterogeneous
1	Vector	List
2	Matrix	Data Frame
3+	Array	

2.2.5 Vectors

Many operations in R make heavy use of **vectors**. Vectors in R are indexed starting at 1. That is what the [1] in the output is indicating, that the first element of the row being displayed is the first element of the vector. Larger vectors will start additional rows with [*] where * is the index of the first element of the row.

Possibly the most common way to create a vector in R is using the c() function, which is short for "combine." As the name suggests, it combines a list of numbers separated by commas.

```
c(1, 3, 5, 7, 8, 9)
```

[1] 1 3 5 7 8 9

Here R simply outputs this vector. If we would like to store this vector in a **variable** we can do so with the **assignment** operator =. In this case the variable x now holds the vector we just created, and we can access the vector by typing x.

```
x = c(1, 3, 5, 7, 8, 9)
```

[1] 1 3 5 7 8 9

As an aside, there is a long history of the assignment operator in R. For simplicity we will use =, but know that often you will see <- as the assignment operator. The pros and cons of these two are well beyond the scope of this book, but know that for our purposes you will have no issue if you simply use =.

Frequently you may wish to create a vector based on a sequence of numbers. The quickest and easiest way to do this is with the : operator, which creates a sequence of integers between two specified integers.

```
(y = 1:100)
```

```
2
##
     [1]
             1
                      3
                           4
                               5
                                    6
                                         7
                                              8
                                                   9
                                                      10
                                                           11
                                                                12
                                                                     13
                                                                         14
                                                                              15
                                                                                   16
                                                                                        17
                                                                                             18
##
    [19]
           19
                20
                     21
                          22
                              23
                                        25
                                             26
                                                 27
                                                      28
                                                           29
                                                                30
                                                                     31
                                                                         32
                                                                              33
                                                                                        35
                                                                                            36
                                   24
                                                                                   34
           37
##
                38
                     39
                          40
                                   42
                                        43
                                             44
                                                  45
                                                      46
                                                           47
                                                                48
                                                                     49
                                                                         50
                                                                                   52
                                                                                        53
                                                                                            54
                                                                                            72
##
    [55]
           55
                56
                     57
                          58
                              59
                                   60
                                        61
                                             62
                                                  63
                                                      64
                                                           65
                                                                66
                                                                     67
                                                                         68
                                                                              69
                                                                                   70
                                                                                        71
##
    [73]
           73
                74
                     75
                          76
                              77
                                   78
                                        79
                                             80
                                                 81
                                                      82
                                                           83
                                                                84
                                                                    85
                                                                         86
                                                                              87
                                                                                   88
                                                                                        89
                                                                                            90
    [91]
##
           91
                92
                     93
                          94
                              95
                                   96
                                        97
                                             98
                                                  99 100
```

Here we see R labeling the rows after the first since this is a large vector. Also, we see that by putting parentheses around the assignment, R both stores the vector in a variable called y and automatically outputs y to the console.

To subset a vector, we use square brackets, [].

```
x
```

```
## [1] 1 3 5 7 8 9
```

```
x[1]
```

```
## [1] 1
```

```
x[3]
```

[1] 5

We see that x[1] returns the first element, and x[3] returns the third element.

```
x[-2]
```

```
## [1] 1 5 7 8 9
```

We can also exclude certain indexes, in this case the second element.

```
x[1:3]
```

```
## [1] 1 3 5
```

```
x[c(1,3,4)]
```

```
## [1] 1 5 7
```

Lastly we see that we can subset based on a vector of indices.

One of the biggest strengths of R is its use of vectorized operations. (Frequently the lack of understanding of this concept leads of a belief that R is slow. R is not the fastest language, but it has a reputation for being slower than it really is.)

```
x = 1:10
    [1] 2 3 4 5 6 7 8 9 10 11
2 * x
    [1] 2 4 6 8 10 12 14 16 18 20
2 ^ x
    [1]
           2
                          16
                               32
                                    64 128 256 512 1024
##
sqrt(x)
    [1] 1.000000 1.414214 1.732051 2.000000 2.236068 2.449490 2.645751 2.828427
    [9] 3.000000 3.162278
log(x)
## [1] 0.0000000 0.6931472 1.0986123 1.3862944 1.6094379 1.7917595 1.9459101
   [8] 2.0794415 2.1972246 2.3025851
We see that when a function like log() is called on a vector x, a vector is returned which has applied the
function to each element of the vector \mathbf{x}.
vec_1 = 1:10
vec_2 = 1:1000
vec_3 = 42
```

The length of a vector can be obtained with the length() function.

```
length(vec_1)
```

[1] 10

```
length(vec_2)
```

[1] 1000

```
length(vec_3)
```

[1] 1

Note that scalars do not exists in R. They are simply vectors of length 1.

If we want to create a sequence that isn't limited to integers and increasing by 1 at a time, we can use the seq() function.

```
seq(from = 1.5, to = 4.2, by = 0.1)
```

```
## [1] 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5 2.6 2.7 2.8 2.9 3.0 3.1 3.2 3.3 ## [20] 3.4 3.5 3.6 3.7 3.8 3.9 4.0 4.1 4.2
```

We will discuss functions in detail later, but note here that the input labels from, to, and by are optional.

```
seq(1.5, 4.2, 0.1)
```

```
## [1] 1.5 1.6 1.7 1.8 1.9 2.0 2.1 2.2 2.3 2.4 2.5 2.6 2.7 2.8 2.9 3.0 3.1 3.2 3.3 ## [20] 3.4 3.5 3.6 3.7 3.8 3.9 4.0 4.1 4.2
```

Another common operation to create a vector is rep(), which can repeat a single value a number of times.

```
rep("A", times = 10)
```

Or, rep() can be used to repeat a vector a number of times.

```
rep(x, times = 3)
```

```
## [1] 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 ## [26] 6 7 8 9 10
```

We have now seen four different ways to create vectors:

- c()
- :
- seq()
- rep()

So far we have mostly used them in isolation, but they are often used together.

```
c(x, rep(seq(1, 9, 2), 3), c(1, 2, 3), 42, 2:4)
```

```
## [1] 1 2 3 4 5 6 7 8 9 10 1 3 5 7 9 1 3 5 7 9 1 3 5 7 9 
## [26] 1 2 3 42 2 3 4
```

2.2.6 Summary Statistics

R has built in functions for a large number of summary statistics.

```
у
```

```
7
                                              8
                                                   9
                                                       10
                                                                                        17
                                                                                             18
      [1]
             1
                  2
                      3
                                5
                                     6
                                                           11
                                                                12
                                                                     13
                                                                          14
                                                                               15
                                                                                    16
                     21
                              23
##
    [19]
            19
                20
                          22
                                   24
                                        25
                                             26
                                                  27
                                                       28
                                                           29
                                                                30
                                                                     31
                                                                          32
                                                                               33
                                                                                    34
                                                                                        35
                                                                                             36
    [37]
           37
                38
                     39
                          40
                               41
                                   42
                                        43
                                             44
                                                  45
                                                       46
                                                           47
                                                                48
                                                                     49
                                                                          50
                                                                               51
                                                                                    52
                                                                                        53
                                                                                             54
##
##
    [55]
            55
                56
                     57
                          58
                              59
                                   60
                                        61
                                             62
                                                  63
                                                       64
                                                           65
                                                                66
                                                                     67
                                                                          68
                                                                               69
                                                                                    70
                                                                                        71
                                                                                             72
                74
                          76
                                                                                             90
##
    [73]
            73
                     75
                              77
                                   78
                                        79
                                             80
                                                  81
                                                       82
                                                           83
                                                                84
                                                                     85
                                                                          86
                                                                               87
                                                                                    88
                                                                                        89
    [91]
                92
                     93
                          94
                               95
                                                  99 100
##
            91
                                   96
                                        97
                                             98
```

Central Tendency

```
mean(y)
## [1] 50.5
median(y)
## [1] 50.5
Spread
var(y)
## [1] 841.6667
sd(y)
## [1] 29.01149
IQR(y)
## [1] 49.5
min(y)
## [1] 1
max(y)
## [1] 100
range(y)
```

2.2.7 Matrices

1 100

[1]

R can also be used for **matrix** calculations. Matrices have rows and columns containing a single data type. In a matrix, the order of rows and columns is important. (This is not true of *data frames*, which we will see later.)

Matrices can be created using the matrix function.

```
x = 1:9
x

## [1] 1 2 3 4 5 6 7 8 9

X = matrix(x, nrow = 3, ncol = 3)
X

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

Note here that we are using two different variables: lower case x, which stores a vector and capital X, which stores a matrix. (Following the usual mathematical convention.) We can do this because R is case sensitive.

By default the matrix function reorders a vector into columns, but we can also tell R to use rows instead.

```
Y = matrix(x, nrow = 3, ncol = 3, byrow = TRUE)

## [,1] [,2] [,3]

## [1,] 1 2 3

## [2,] 4 5 6

## [3,] 7 8 9
```

We can also create a matrix of a specified dimension where every element is the same, in this case 0.

```
Z = matrix(0, 2, 4)
Z

## [,1] [,2] [,3] [,4]
## [1,] 0 0 0 0
```

Like vectors, matrices can be subsetted using square brackets, []. However, since matrices are two-dimensional, we need to specify both a row and a column when subsetting.

```
X
```

```
## [,1] [,2] [,3]
## [1,] 1 4 7
## [2,] 2 5 8
## [3,] 3 6 9
X[1, 2]
```

```
## [1] 4
```

[2,]

0

0

0

0

Here we accessed the element in the first row and the second column. We could also subset an entire row or column.

```
X[1, ]
## [1] 1 4 7

X[, 2]
## [1] 4 5 6
```

We can also use vectors to subset more than one row or column at a time. Here we subset to the first and third column of the second row.

```
X[2, c(1, 3)]
```

```
## [1] 2 8
```

##

##

[8,] 8 2 1

[9,] 9 1 1

Matrices can also be created by combining vectors as columns, using cbind, or combining vectors as rows, using rbind.

```
x = 1:9
rev(x)
## [1] 9 8 7 6 5 4 3 2 1
rep(1, 9)
## [1] 1 1 1 1 1 1 1 1 1
cbind(x, rev(x), rep(1, 9))
##
         х
##
    [1,] 1 9 1
    [2,] 2 8 1
##
##
   [3,] 3 7 1
##
    [4,] 4 6 1
    [5,] 5 5 1
##
##
    [6,] 6 4 1
##
   [7,] 7 3 1
```

```
rbind(x, rev(x), rep(1, 9))
```

```
[,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9]
##
              2
                               5
                                         7
## x
        1
                   3
                         4
                                    6
                                               8
                                                     9
##
        9
              8
                   7
                         6
                               5
                                    4
                                          3
                                               2
                                                     1
                                               1
                                                     1
##
        1
                   1
                         1
                               1
                                    1
```

R can then be used to perform matrix calculations.

```
x = 1:9
y = 9:1
X = matrix(x, 3, 3)
Y = matrix(y, 3, 3)
X
##
         [,1] [,2] [,3]
## [1,]
            1
                 4
                       7
            2
## [2,]
                 5
                       8
## [3,]
            3
                 6
                       9
Y
        [,1] [,2] [,3]
## [1,]
            9
                 6
                       3
## [2,]
            8
                 5
                       2
                       1
## [3,]
X + Y
         [,1] [,2] [,3]
##
## [1,]
           10
                10
                      10
## [2,]
                      10
           10
                10
## [3,]
           10
                10
                      10
X - Y
        [,1] [,2] [,3]
##
## [1,]
           -8
                -2
                       4
                 0
## [2,]
           -6
                       6
## [3,]
           -4
                 2
                       8
X * Y
         [,1] [,2] [,3]
##
## [1,]
            9
                24
                      21
## [2,]
           16
                25
                      16
## [3,]
           21
                24
                       9
X / Y
##
              [,1]
                         [,2]
                                   [,3]
## [1,] 0.1111111 0.6666667 2.333333
## [2,] 0.2500000 1.0000000 4.000000
## [3,] 0.4285714 1.5000000 9.000000
```

Note that X * Y is not matrix multiplication. It is element by element multiplication. (Same for X / Y). Instead, matrix multiplication uses %*%. Other matrix functions include t() which gives the transpose of a matrix and solve() which returns the inverse of a square matrix if it is invertible.

```
X %*% Y
       [,1] [,2] [,3]
##
## [1,]
       90 54 18
## [2,] 114
             69
                 24
## [3,] 138
             84
                 30
t(X)
## [,1] [,2] [,3]
## [1,] 1 2 3
       4 5 6
7 8 9
## [2,]
## [3,]
Z = matrix(c(9, 2, -3, 2, 4, -2, -3, -2, 16), 3, byrow = TRUE)
##
      [,1] [,2] [,3]
## [1,] 9 2 -3
## [2,] 2
            4 -2
## [3,] -3 -2 16
solve(Z)
             [,1] [,2] [,3]
##
## [1,] 0.12931034 -0.05603448 0.01724138
## [2,] -0.05603448 0.29094828 0.02586207
## [3,] 0.01724138 0.02586207 0.06896552
R has a number of matrix specific functions for obtaining dimension and summary information.
X = matrix(1:6, 2, 3)
X
## [,1] [,2] [,3]
## [1,] 1 3 5
## [2,] 2 4
dim(X)
## [1] 2 3
rowSums(X)
## [1] 9 12
colSums(X)
## [1] 3 7 11
```

```
rowMeans(X)
## [1] 3 4
```

```
colMeans(X)
```

```
## [1] 1.5 3.5 5.5
```

The diag() function can be used in a number of ways. We can extract the diagonal of a matrix.

```
diag(Z)
```

```
## [1] 9 4 16
```

Or create a matrix with specified elements on the diagonal. (And 0 on the off-diagonals.)

```
diag(1:5)
```

```
##
         [,1] [,2] [,3] [,4] [,5]
## [1,]
            1
                  0
                        0
                              0
                                    0
## [2,]
            0
                  2
                        0
                              0
                                    0
## [3,]
            0
                  0
                        3
                              0
                                    0
## [4,]
            0
                  0
                        0
                              4
                                    0
## [5,]
            0
                  0
                        0
                              0
                                    5
```

Or, lastly, create a square matrix of a certain dimension with 1 for every element of the diagonal and 0 for the off-diagonals.

```
diag(5)
```

```
##
         [,1] [,2] [,3] [,4] [,5]
## [1,]
                  0
                        0
                              0
                                    0
## [2,]
                        0
                              0
                                    0
            0
                  1
## [3,]
            0
                  0
                        1
                              0
                                    0
## [4,]
            0
                  0
                        0
                              1
                                    0
## [5,]
            0
                                    1
```

2.2.8 Data Frames

We have previously seen vectors and matrices for storing data as we introduced R. We will now introduce a data frame which will be the most common way that we store and interact with data in this course.

Unlike a matrix, which can be thought of as a vector rearranged into rows and columns, a data frame is not required to have the same data type for each element. A data frame is a **list** of vectors. So, each vector must contain the same data type, but the different vectors can store different data types.

example_data

```
##
                 z
           У
## 1
     1 Hello
              TRUE
## 2 3 Hello FALSE
     5 Hello TRUE
     7 Hello FALSE
## 4
## 5
     9 Hello TRUE
## 6
    1 Hello FALSE
## 7
    3 Hello TRUE
## 8 5 Hello FALSE
## 9 7 Hello TRUE
## 10 9 Hello FALSE
```

The data.frame() function above is one way to create a data frame. We can also import data from various file types in into R, as well as use data stored in packages.

The example data above can also be found here as a .csv file. To read this data into R, we would use the read.csv() function.

```
example_data_from_csv = read.csv("data/example_data.csv")
```

This particular line of code assumes that the file example_data.csv exists in a folder called data in your current working directory.

Alternatively, we could use the "Import Dataset" feature in RStudio which can be found in the environment window. (By default, the top-right pane of RStudio.)

Once completed, this process will automatically generate the code to import a file. The resulting code will be shown in the console window.

Earlier we looked at installing packages, in particular the ggplot2 package. (A package for visualization. While not necessary for this course, it is quickly growing in popularity.)

```
library(ggplot2)
```

Inside the ggplot2 package is a dataset called mpg. By loading the package using the library() function, we can now access mpg.

When using data from inside a package, there are three things we would generally like to do:

- Look at the raw data.
- Understand the data. (Where did it come from? What are the variables? Etc.)
- Visualize the data.

To look at the data, we have two useful commands: head() and str().

head(mpg, n = 10)

```
##
     manufacturer
                      model displ year cyl
                                              trans drv cty hwy fl
                                                                   class
                                                     f 18 29 p compact
## 1
            audi
                        a4
                             1.8 1999 4
                                           auto(15)
## 2
                            1.8 1999 4 manual(m5)
            audi
                        a4
                                                     f 21 29 p compact
## 3
                        a4 2.0 2008 4 manual(m6)
            audi
                                                     f 20 31 p compact
```



Figure 2.1: RStudio Import Screen

```
## 4
              audi
                                 2.0 2008
                                                 auto(av)
                                                                21
                                                                    30
                            a4
                                                             f
                                                                        p compact
## 5
                                                                16
              audi
                            а4
                                 2.8 1999
                                             6
                                                 auto(15)
                                                             f
                                                                    26
                                                                        p compact
## 6
                                                                    26 p compact
              audi
                                 2.8 1999
                                             6 manual(m5)
                                                                18
## 7
                                 3.1 2008
                                                                18
                                                                    27
              andi
                            а4
                                             6
                                                 auto(av)
                                                             f
                                                                        p compact
## 8
              audi a4 quattro
                                 1.8 1999
                                             4 manual(m5)
                                                                18
                                                                    26
                                                                        p compact
## 9
              audi a4 quattro
                                                                    25
                                                                        p compact
                                 1.8 1999
                                             4
                                                 auto(15)
                                                             4
                                                                16
## 10
              audi a4 quattro
                                 2.0 2008
                                             4 manual(m6)
                                                                20
                                                                    28 p compact
```

The function head() will display the first n observations of the data frame.

```
str(mpg)
```

```
## Classes 'tbl_df', 'tbl' and 'data.frame':
                                                234 obs. of
                                                           11 variables:
                        "audi" "audi" "audi" ...
   $ manufacturer: chr
##
                        "a4" "a4" "a4" "a4" ...
   $ model
                 : chr
##
   $ displ
                 : num 1.8 1.8 2 2 2.8 2.8 3.1 1.8 1.8 2 ...
                  : int
                        1999 1999 2008 2008 1999 1999 2008 1999 1999 2008 ...
##
   $ year
##
   $ cyl
                  : int
                        4 4 4 4 6 6 6 4 4 4 ...
                        "auto(15)" "manual(m5)" "manual(m6)" "auto(av)" ...
##
   $ trans
                 : chr
##
                 : chr
                        "f" "f" "f" "f" ...
   $ drv
##
                  : int 18 21 20 21 16 18 18 18 16 20 ...
   $ cty
                        29 29 31 30 26 26 27 26 25 28 ...
##
   $ hwy
                 : int
                        "p" "p" "p" "p" ...
##
   $ fl
                  : chr
   $ class
                  : chr
                         "compact" "compact" "compact" ...
```

The function str() will display the "structure" of the data frame. It will display the number of observations and variables, list the variables, give the type of each variable, and show some elements of each variable.

It is important to note that while matrices have rows and columns, data frames instead have observations and variables. When displayed in the console or viewer, each row is an observation and each column is a variable. However generally speaking, their order does not matter, it is simply a side-effect of how the data was entered or stored.

In this dataset an observation is for a particular model-year of a car, and the variables describe attributes of the car, for example its highway fuel efficiency.

To understand more about the data set, we use the ? operator to pull up the documentation for the data.

```
?mpg
```

R has a number of functions for quickly working with and extracting basic information from data frames. To quickly obtain a vector of the variable names, we use the names() function.

```
names(mpg)
```

```
## [1] "manufacturer" "model" "displ" "year" "cyl"
## [6] "trans" "drv" "cty" "hwy" "fl"
## [11] "class"
```

To access one of the variables as a vector, we use the \$ operator.

```
mpg$year
##
     [1] 1999 1999 2008 2008 1999 1999 2008 1999 1999 2008 2008 1999 1999 2008 2008
##
    [16] 1999 2008 2008 2008 2008 2008 1999 2008 1999 1999 2008 2008 2008 2008 2008
    [31] 1999 1999 1999 2008 1999 2008 2008 1999 1999 1999 1999 2008 2008 2008 1999
    [46] 1999 2008 2008 2008 2008 1999 1999 2008 2008 2008 1999 1999 1999 2008 2008
##
    [61] 2008 1999 2008 1999 2008 2008 2008 2008 2008 2008 1999 1999 2008 1999 1999
    [76] 1999 2008 1999 1999 1999 2008 2008 1999 1999 1999 1999 1999 2008 1999 2008
##
    [91] 1999 1999 2008 2008 1999 1999 2008 2008 2008 1999 1999 1999 1999 1999 2008
   [106] 2008 2008 2008 1999 1999 2008 2008 1999 1999 2008 1999 1999 2008 2008 2008
  [121] 2008 2008 2008 2008 1999 1999 2008 2008 2008 1999 2008 2008 1999 1999
  [136] 1999 2008 1999 2008 2008 1999 1999 1999 2008 2008 2008 2008 1999 1999 2008
  [151] 1999 1999 2008 2008 1999 1999 1999 2008 2008 1999 1999 2008 2008 2008 2008
## [166] 1999 1999 1999 1999 2008 2008 2008 2008 1999 1999 1999 1999 2008 2008 1999
## [181] 1999 2008 2008 1999 1999 2008 1999 1999 2008 2008 1999 1999 2008 1999 1999
## [196] 1999 2008 2008 1999 2008 1999 1999 2008 1999 1999 2008 2008 1999 1999 2008
## [211] 2008 1999 1999 1999 1999 2008 2008 2008 2008 1999 1999 1999 1999 1999 1999
## [226] 2008 2008 1999 1999 2008 2008 1999 1999 2008
mpg$hwy
     [1] 29 29 31 30 26 26 27 26 25 28 27 25 25 25 25 24 25 23 20 15 20 17 17 26 23
    [26] 26 25 24 19 14 15 17 27 30 26 29 26 24 24 22 22 24 24 17 22 21 23 23 19 18
##
    [51] 17 17 19 19 12 17 15 17 17 12 17 16 18 15 16 12 17 17 16 12 15 16 17 15 17
    [76] 17 18 17 19 17 19 19 17 17 17 16 16 17 15 17 26 25 26 24 21 22 23 22 20 33
## [101] 32 32 29 32 34 36 36 29 26 27 30 31 26 26 28 26 29 28 27 24 24 24 22 19 20
   [126] 17 12 19 18 14 15 18 18 15 17 16 18 17 19 19 17 29 27 31 32 27 26 26 25 25
  [151] 17 17 20 18 26 26 27 28 25 25 24 27 25 26 23 26 26 26 26 25 27 25 27 20 20
## [176] 19 17 20 17 29 27 31 31 26 26 28 27 29 31 31 26 26 27 30 33 35 37 35 15 18
## [201] 20 20 22 17 19 18 20 29 26 29 29 24 44 29 26 29 29 29 29 29 23 24 44 41 29 26
## [226] 28 29 29 29 28 29 26 26 26
We can use the dim(), nrow() and ncol() functions to obtain information about the dimension of the data
frame.
dim(mpg)
```

```
dim(mpg)
## [1] 234 11
nrow(mpg)
## [1] 234
ncol(mpg)
```

[1] 11

Here nrow() is also the number of observations, which in most cases is the sample size.

Subsetting data frames can work much like subsetting matrices using square brackets, [,]. Here, we find fuel efficient vehicles earning over 35 miles per gallon and only display manufacturer, model and year.

```
mpg[mpg$hwy > 35, c("manufacturer", "model", "year")]
```

```
##
                          model year
       manufacturer
## 106
                          civic 2008
              honda
## 107
                          civic 2008
              honda
## 197
             toyota
                        corolla 2008
## 213
         volkswagen
                          jetta 1999
## 222
         volkswagen new beetle 1999
## 223
         volkswagen new beetle 1999
```

An alternative would be to use the subset() function, which has a much more readable syntax.

```
subset(mpg, subset = hwy > 35, select = c("manufacturer", "model", "year"))
```

Lastly, we could use the filter and select functions from the dplyr package which introduces the %>% operator from the magrittr package. This is not necessary for this course, however the dplyr package is something you should be aware of as it is becoming a popular tool in the R world.

```
library(dplyr)
mpg %>% filter(hwy > 35) %>% select(manufacturer, model, year)
```

All three approaches produce the same results. Which you use will be largely based on a given situation as well as user preference.

2.2.9 Plotting

Now that we have some data to work with, and we have learned about the data at the most basic level, our next tasks is to visualize the data. Often, a proper visualization can illuminate features of the data that can inform further analysis.

We will look at three methods of visualizing data that we will use throughout the course:

- Histograms
- Boxplots
- Scatterplots

2.2.9.1 Histograms

When visualizing a single numerical variable, a **histogram** will be our go-to tool, which can be created in R using the hist() function.

```
hist(mpg$cty)
```

Histogram of mpg\$cty



The histogram function has a number of parameters which can be changed to make our plot look much nicer. Use the ? operator to read the documentation for the hist() to see a full list of these parameters.

```
hist(mpg$cty,
    xlab = "Miles Per Gallon (City)",
    main = "Histogram of MPG (City)",
    breaks = 12,
    col = "dodgerblue",
    border = "darkorange")
```

Histogram of MPG (City)



Importantly, you should always be sure to label your axes and give the plot a title. The argument breaks is specific to hist(). Entering an integer will give a suggestion to R for how many bars to use for the histogram. By default R will attempt to intelligently guess a good number of breaks, but as we can see here, it is sometimes useful to modify this yourself.

2.2.9.2 Boxplots

To visualize the relationship between a numerical and categorical variable, we will use a **boxplot**. In the mpg dataset, the drv variable takes a small, finite number of values. A car can only be front wheel drive, 4 wheel drive, or rear wheel drive.

unique(mpg\$drv)

First note that we can use a single boxplot as an alternative to a histogram for visualizing a single numerical variable. To do so in R, we use the boxplot() function.

boxplot(mpg\$hwy)



However, more often we will use boxplots to compare a numerical variable for different values of a categorical variable.

```
boxplot(hwy ~ drv, data = mpg)
```



Here used the boxplot() command to create side-by-side boxplots. However, since we are now dealing with two variables, the syntax has changed. The R syntax hwy ~ drv, data = mpg reads "Plot the hwy variable against the drv variable using the dataset mpg." We see the use of a ~ (which specifies a formula) and also a data = argument. This will be a syntax that is common to many functions we will use in this course.

```
boxplot(hwy ~ drv, data = mpg,
    xlab = "Drivetrain (f = FWD, r = RWD, 4 = 4WD)",
    ylab = "Miles Per Gallon (Highway)",
    main = "MPG (Highway) vs Drivetrain",
    pch = 20,
    cex = 2,
    col = "darkorange",
    border = "dodgerblue")
```





Again, boxplot() has a number of additional arguments which have the ability to make our plot more visually appealing.

2.2.9.3 Scatterplots

Lastly, to visualize the relationship between two numeric variables we will use a **scatterplot**. This can be done with the plot() function and the ~ syntax we just used with a boxplot. (The function plot() can also be used more generally; see the documentation for details.)

plot(hwy ~ displ, data = mpg)



MPG (Highway) vs Engine Displacement



2.2.10 Distributions

When working with different statistical distributions, we often want to make probabilistic statements based on the distribution.

We typically want to know one of four things:

- The density (pdf) at a particular value.
- The distribution (cdf) at a particular value.
- The quantile value corresponding to a particular probability.
- A random draw of values from a particular distribution.

This used to be done with statistical tables printed in the back of textbooks. Now, R has functions for obtaining density, distribution, quantile and random values.

The general naming structure of the relevant R functions is:

- dname calculates density (pdf) at input x.
- pname calculates distribution (cdf) at input x.
- qname calculates the quantile at an input probability.
- rname generates a random draw from a particular distribution.

Note that name represents the name of the given distribution.

For example, consider a random variable X which is $N(\mu = 2, \sigma^2 = 25)$. (Note, we are parameterizing using the variance σ^2 . R however uses the standard deviation.)

To calculate the value of the pdf at x = 3, that is, the height of the curve at x = 3, use:

```
dnorm(x = 3, mean = 2, sd = 5)
```

```
## [1] 0.07820854
```

To calculate the value of the cdf at x = 3, that is, $P(X \le 3)$, the probability that X is less than or equal to 3, use:

```
pnorm(q = 3, mean = 2, sd = 5)
```

```
## [1] 0.5792597
```

Or, to calculate the quantile for probability 0.975, use:

```
qnorm(p = 0.975, mean = 2, sd = 5)
```

```
## [1] 11.79982
```

Lastly, to generate a random sample of size n = 10, use:

```
rnorm(n = 10, mean = 2, sd = 5)
```

```
## [1] -9.7931600 12.7728107 -0.8234053 7.2306059 4.0522876 11.0910682
## [7] 6.5497764 0.1573191 4.6705020 -2.3744669
```

These functions exist for many other distributions, including but not limited to:

Command	Distribution
*binom	Binomial
*t	t
*pois	Poisson
*f	F
*chisq	Chi-Squared

Where * can be d, p, q, and r. Each distribution will have its own set of parameters which need to be passed to the functions as arguments. For example, dbinom() would not have arguments for mean and sd, since those are not parameters of the distribution. Instead a binomial distribution is usually parameterized by n and p, however R chooses to call them something else. To find the names that R uses we would use ?dbinom and see that R instead calls the arguments size and prob. For example:

```
dbinom(x = 6, size = 10, prob = 0.75)
```

[1] 0.145998

Also note that, when using the dname functions with discrete distributions, they are the pmf of the distribution. For example, the above command is P(Y=6) if $Y \sim b(n=10, p=0.75)$. (The probability of flipping an unfair coin 10 times and seeing 6 heads, if the probability of heads is 0.75.)

2.3 Programming Basics

2.3.1 Logical Operators

Operator	Summary	Example	Result
x < y	x less than y	3 < 42	TRUE
x > y	x greater than y	3 > 42	FALSE
x <= y	x less than or equal to y	3 <= 42	TRUE
x >= y	x greater than or equal to y	3 >= 42	FALSE
x == y	xequal to y	3 == 42	FALSE
x != y	x not equal to y	3 != 42	TRUE
!x	$\operatorname{not} \mathbf{x}$!(3 > 42)	TRUE
х у	x or y	(3 > 42) TRUE	TRUE
x & y	x and y	(3 < 4) & (42 > 13)	TRUE

In R, logical operators are vectorized. To demonstrate this, we will use the following height and weight data.

```
heights = c(110, 120, 115, 136, 205, 156, 175)
weights = c(64, 67, 62, 60, 77, 70, 66)
```

First, using the < operator, when can find which heights are less than 121. Further, we could also find which heights are less than 121 or exactly equal to 156.

```
heights < 121
```

[1] TRUE TRUE TRUE FALSE FALSE FALSE

```
heights < 121 | heights == 156
```

[1] TRUE TRUE TRUE FALSE FALSE TRUE FALSE

Often, a vector of logical values is useful for subsetting a vector. For example, we can find the heights that are larger than 150. We can then use the resulting vector to subset the heights vector, thus actually returning the heights that are above 150, instead of a vector of which values are above 150. Here we also obtain the weights corresponding to heights above 150.

```
heights > 150
```

[1] FALSE FALSE FALSE TRUE TRUE TRUE

```
heights[heights > 150]
```

```
## [1] 205 156 175
```

```
weights[heights > 150]
```

```
## [1] 77 70 66
```

When comparing vectors, be sure you are comparing vectors of the same length.

```
a = 1:10
b = 2:4
a < b
```

```
\#\# Warning in a < b: longer object length is not a multiple of shorter object \#\# length
```

```
## [1] TRUE TRUE TRUE FALSE FALSE FALSE FALSE FALSE FALSE
```

What happened here? R still performed the operation, but it also gives us a warning. (To perform the operation, R automatically made b longer by repeating b as needed.)

The one exception to this behavior is comparing to a vector of length 1. R does not warn us in this case, as comparing each value of a vector to a single value is a common operation that is usually reasonable to perform.

```
a > 5
```

```
## [1] FALSE FALSE FALSE FALSE TRUE TRUE TRUE TRUE TRUE
```

Often we will want to convert TRUE and FALSE values to 1 and 0. When performing mathematical operations on TRUE and FALSE, this is done automatically through type coercion.

```
5 + (a > 5)
```

```
## [1] 5 5 5 5 5 6 6 6 6 6
```

By calling sum() on a vector of logical values, we can essentially count the number of TRUE values.

```
sum(a > 5)
```

[1] 5

Here we count the elements of a that are larger than 5. This is an extremely useful feature.

2.3.2 Control Flow

In R, the if/else syntax is:

```
if (...) {
  some R code
} else {
  more R code
}
```

For example,

```
x = 1
y = 3
if (x > y) {
   z = x * y
   print("x is larger than y")
} else {
   z = x + 5 * y
   print("x is less than or equal to y")
}
```

[1] "x is less than or equal to y"

Z

[1] 16

R also has a special function ifelse() which is very useful. It returns one of two specified values based on a conditional statement.

```
ifelse(4 > 3, 1, 0)
```

[1] 1

The real power of ifelse() comes from its ability to be applied to vectors.

```
fib = c(1, 1, 2, 3, 5, 8, 13, 21)
ifelse(fib > 6, "Foo", "Bar")
```

```
## [1] "Bar" "Bar" "Bar" "Bar" "Foo" "Foo" "Foo"
```

Now a for loop example,

```
x = 11:15
for (i in 1:5) {
    x[i] = x[i] * 2
}
```

```
## [1] 22 24 26 28 30
```

Note that this for loop is very normal in many programming languages, but not in R. In R we would not use a loop, instead we would simply use a vectorized operation.

```
x = 11:15

x = x * 2

x = x * 2
```

[1] 22 24 26 28 30

2.3.3 Functions

So far we have been using functions, but haven't actually discussed some of their details.

```
function_name(arg1 = 10, arg2 = 20)
```

To use a function, you simply type its name, followed by an open parenthesis, then specify values of its arguments, then finish with a closing parenthesis.

An **argument** is a variable which is used in the body of the function. Specifying the values of the arguments is essentially providing the inputs to the function.

We can also write our own functions in R. For example, we often like to "standardize" variables, that is, subtracting the sample mean, and dividing by the sample standard deviation.

$$\frac{x-\bar{x}}{s}$$

In R we would write a function to do this. When writing a function, there are three thing you must do.

- Give the function a name. Preferably something that is short, but descriptive.
- Specify the arguments using function()
- Write the body of the function within curly braces, {}.

```
standardize = function(x) {
  m = mean(x)
  std = sd(x)
  result = (x - m) / std
  result
}
```

Here the name of the function is standardize, and the function has a single argument x which is used in the body of function. Note that the output of the final line of the body is what is returned by the function. In this case the function returns the vector stored in the variable results.

To test our function, we will take a random sample of size n=10 from a normal distribution with a mean of 2 and a standard deviation of 5.

```
(test_sample = rnorm(n = 10, mean = 2, sd = 5))

## [1] -9.5203429  0.7099630 -3.3555703  6.7124282 -0.6201982  4.3118075
## [7]  3.7030199 -1.2601377  3.9464309 16.9084142

standardize(x = test_sample)

## [1] -1.6756564 -0.2072147 -0.7907748  0.6543696 -0.3981439  0.3097883
## [7]  0.2224039 -0.4899998  0.2573427  2.1178851
```

This function could be written much more succinctly, simply performing all the operations on one line and immediately returning the result, without storing any of the intermediate results.

```
standardize = function(x) {
  (x - mean(x)) / sd(x)
}
```

When specifying arguments, you can provide default arguments.

```
power_of_num = function(num, power = 2) {
  num ^ power
}
```

Let's look at a number of ways that we could run this function to perform the operation 10^2 resulting in 100.

```
power_of_num(10)

## [1] 100

power_of_num(10, 2)

## [1] 100

power_of_num(num = 10, power = 2)

## [1] 100

power_of_num(power = 2, num = 10)
```

```
## [1] 100
```

Note that without using the argument names, the order matters. The following code will not evaluate to the same output as the previous example.

```
power_of_num(2, 10)
```

```
## [1] 1024
```

Also, the following line of code would produce an error since arguments without a default value must be specified.

```
power_of_num(power = 5)
```

To further illustrate a function with a default argument, we will write a function that calculates sample standard deviation two ways.

By default, is will calculate the unbiased estimate of σ , which we will call s.

$$s = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} (x - \bar{x})^2}$$

It will also have the ability to return the biased estimate (based on maximum likelihood) which we will call $\hat{\sigma}$.

$$\hat{\sigma} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (x - \bar{x})^2}$$

```
get_sd = function(x, biased = FALSE) {
  n = length(x) - 1 * !biased
  sqrt((1 / n) * sum((x - mean(x)) ^ 2))
}
```

```
get_sd(test_sample)
```

[1] 6.966777

```
get_sd(test_sample, biased = FALSE)
```

[1] 6.966777

```
sd(test_sample)
```

[1] 6.966777

We see the function is working as expected, and when returning the unbiased estimate it matches R's built in function sd(). Finally, let's examine the biased estimate of σ .

```
get_sd(test_sample, biased = TRUE)
```

[1] 6.609265

2.4 Hypothesis Tests in R

2.4.1 One Sample t-Test: Review

Suppose $x_i \sim N(\mu, \sigma^2)$ and we want to test $H_0: \mu = \mu_0$ versus $H_1: \mu \neq \mu_0$.

Assuming σ is unknown, we use the one-sample Student's t test statistic:

$$t = \frac{\bar{x} - \mu_0}{s / \sqrt{n}} \sim t_{n-1},$$

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

A $100(1-\alpha)\%$ confidence interval for μ is given by,

$$\bar{x} \pm t_{n-1}(\alpha/2) \frac{s}{\sqrt{n}}$$

where $t_{n-1}(\alpha/2)$ is the critical value such that $P(t > t_{n-1}(\alpha/2)) = \alpha/2$ for n-1 degrees of freedom.

2.4.2 One Sample t-Test: Example

Suppose a grocery store sells "16 ounce" boxes of *Captain Crisp* cereal. A random sample of 9 boxes was taken and weighed. The weight in ounces are stored in the data frame capt_crisp.

```
capt_crisp = data.frame(weight = c(15.5, 16.2, 16.1, 15.8, 15.6, 16.0, 15.8, 15.9, 16.2))
```

The company that makes *Captain Crisp* cereal claims that the average weight of a box is at least 16 ounces. We will assume the weight of cereal in a box is normally distributed and use a 0.05 level of significance to test the company's claim.

To test $H_0: \mu \geq 16$ versus $H_1: \mu < 16$, the test statistic is

$$t = \frac{\bar{x} - \mu_0}{s / \sqrt{n}}$$

The sample mean \bar{x} and the sample standard deviation s can be easily computed using R. We also create variables which store the hypothesized mean and the sample size.

```
x_bar = mean(capt_crisp$weight)
s = sd(capt_crisp$weight)
mu_0 = 16
n = 9
```

We can then easily compute the test statistic.

```
t = (x_bar - mu_0) / (s / sqrt(n))
t
```

```
## [1] -1.2
```

Under the null hypothesis, the test statistic has a t distribution with n-1 degrees of freedom, in this case 8.

To complete the test, we need to obtain the p-value of the test. Since this is a one-sided test with a less-than alternative, we need to area to the left of -1.2 for a t distribution with 8 degrees of freedom. That is,

$$P(t_8 < -1.2)$$

```
pt(t, df = n - 1)
```

```
## [1] 0.1322336
```

We now have the p-value of our test, which is greater than our significance level (0.05), so we fail to reject the null hypothesis.

Alternatively, this entire process could have been completed using one line of R code.

```
t.test(x = capt_crisp$weight, mu = 16, alternative = c("less"), conf.level = 0.95)
```

```
##
## One Sample t-test
##
## data: capt_crisp$weight
## t = -1.2, df = 8, p-value = 0.1322
## alternative hypothesis: true mean is less than 16
## 95 percent confidence interval:
## -Inf 16.05496
## sample estimates:
## mean of x
## 15.9
```

We supply R with the data, the hypothesized value of μ , the alternative, and the confidence level. R then returns a wealth of information including:

- The value of the test statistic.
- The degrees of freedom of the distribution under the null hypothesis.
- The p-value of the test.
- The confidence interval which corresponds to the test.
- An estimate of μ .

Since the test was one-sided, R returned a one-sided confidence interval. If instead we wanted a two-sided interval for the mean weight of boxes of *Captain Crisp* cereal we could modify our code.

This time we have stored the results. By doing so, we can directly access portions of the output from t.test(). To see what information is available we use the names() function.

```
names(capt_test_results)

## [1] "statistic" "parameter" "p.value" "conf.int" "estimate"

## [6] "null.value" "alternative" "method" "data.name"
```

We are interested in the confidence interval which is stored in conf.int.

capt_test_results\$conf.int

```
## [1] 15.70783 16.09217
## attr(,"conf.level")
## [1] 0.95
```

Let's check this interval "by hand." The one piece of information we are missing is the critical value, $t_{n-1}(\alpha/2) = t_8(0.025)$, which can be calculated in R using the qt() function.

```
qt(0.975, df = 8)
```

[1] 2.306004

So, the 95% CI for the mean weight of a cereal box is calculated by plugging into the formula,

$$\bar{x} \pm t_{n-1}(\alpha/2) \frac{s}{\sqrt{n}}$$

```
c(mean(capt_crisp$weight) - qt(0.975, df = 8) * sd(capt_crisp$weight) / sqrt(9),
mean(capt_crisp$weight) + qt(0.975, df = 8) * sd(capt_crisp$weight) / sqrt(9))
```

[1] 15.70783 16.09217

2.4.3 Two Sample t-Test: Review

Suppose $x_i \sim N(\mu_x, \sigma^2)$ and $y_i \sim N(\mu_y, \sigma^2)$.

Want to test $H_0: \mu_x - \mu_y = \mu_0$ versus $H_1: \mu_x - \mu_y \neq \mu_0$.

Assuming σ is unknown, use the two-sample Student's t test statistic:

$$t = \frac{(\bar{x} - \bar{y}) - \mu_0}{s_p \sqrt{\frac{1}{n} + \frac{1}{m}}} \sim t_{n+m-2},$$

where
$$\bar{x} = \frac{\sum_{i=1}^{n} x_i}{n}$$
, $\bar{y} = \frac{\sum_{i=1}^{m} y_i}{m}$, and $s_p^2 = \frac{(n-1)s_x^2 + (m-1)s_y^2}{n+m-2}$.

A $100(1-\alpha)\%$ CI for $\mu_x - \mu_y$ is given by

$$(\bar{x}-\bar{y}) \pm t_{n+m-2}(\alpha/2) \left(s_p \sqrt{\frac{1}{n}+\frac{1}{m}}\right),$$

where $t_{n+m-2}(\alpha/2)$ is the critical value such that $P(t > t_{n+m-2}(\alpha/2)) = \alpha/2$.

2.4.4 Two Sample t-Test: Example

Assume that the distributions of X and Y are $N(\mu_1, \sigma^2)$ and $N(\mu_2, \sigma^2)$, respectively. Given the n = 6 observations of X,

```
x = c(70, 82, 78, 74, 94, 82)

n = length(x)
```

and the m = 8 observations of Y,

```
y = c(64, 72, 60, 76, 72, 80, 84, 68)

m = length(y)
```

we will test $H_0: \mu_1 = \mu_2$ versus $H_1: \mu_1 > \mu_2$.

First, note that we can calculate the sample means and standard deviations.

```
x_bar = mean(x)
s_x = sd(x)
y_bar = mean(y)
s_y = sd(y)
```

We can then calculate the pooled standard deviation.

$$s_p = \sqrt{\frac{(n-1)s_x^2 + (m-1)s_y^2}{n+m-2}}$$

$$s_p = sqrt(((n-1) * s_x ^2 + (m-1) * s_y ^2) / (n + m-2))$$

Thus, the relevant t test statistic is given by

$$t = \frac{(\bar{x} - \bar{y}) - \mu_0}{s_p \sqrt{\frac{1}{n} + \frac{1}{m}}}.$$

```
t = ((x_bar - y_bar) - 0) / (s_p * sqrt(1 / n + 1 / m))
t.
```

[1] 1.823369

Note that $t \sim t_{n+m-2} = t_{12}$, so we can calculate the p-value, which is

$$P(t_{12} > 1.8233692).$$

```
1 - pt(t, df = n + m - 2)
```

[1] 0.04661961

But, then again, we could have simply performed this test in one line of R.

```
t.test(x, y, alternative = c("greater"), var.equal = TRUE)
```

Recall that a two-sample t-test can be done with or without an equal variance assumption. Here var.equal = TRUE tells R we would like to perform the test under the equal variance assumption.

Above we carried out the analysis using two vectors \mathbf{x} and \mathbf{y} . In general, we will have a preference for using data frames.

We now have the data stored in a single variables (values) and have created a second variable (group) which indicates which "sample" the value belongs to.

```
t_test_data
```

```
##
      values group
## 1
           70
                   Α
## 2
           82
           78
## 3
           74
## 4
                   Α
## 5
           94
                   Α
## 6
           82
                   Α
## 7
           64
                   В
## 8
           72
                   В
## 9
           60
                   В
## 10
           76
                   В
## 11
           72
                   В
                   В
## 12
           80
## 13
           84
                   В
## 14
                   В
           68
```

Now to perform the test, we still use the t.test() function but with the ~ syntax and a data argument.

```
##
## Two Sample t-test
##
## data: values by group
## t = 1.8234, df = 12, p-value = 0.04662
```

2.5 Simulation

One of the biggest strengths of R is its ability to carry out simulations. We'll look at two examples here, however simulation will be a topic we revisit several times throughout the course.

2.5.1 Paired Differences

Consider the model:

$$X_{11}, X_{12}, \dots, X_{1n} \sim N(\mu_1, \sigma^2)$$

 $X_{21}, X_{22}, \dots, X_{2n} \sim N(\mu_2, \sigma^2)$

Assume that $\mu_1 = 6$, $\mu_2 = 5$, $\sigma^2 = 4$ and n = 25.

Let

$$\bar{X}_{1} = \frac{1}{n} \sum_{i=1}^{n} X_{1i}$$

$$\bar{X}_{2} = \frac{1}{n} \sum_{i=1}^{n} X_{2i}$$

$$D = \bar{X}_{1} - \bar{X}_{2}.$$

Suppose we would like to calculate P(0 < D < 2). First we will need to obtain the distribution of D. Recall,

$$\bar{X}_1 \sim N\left(\mu_1, \frac{\sigma^2}{n}\right)$$

and

$$\bar{X}_2 \sim N\left(\mu_2, \frac{\sigma^2}{n}\right).$$

Then,

$$D = \bar{X}_1 - \bar{X}_2 \sim N\left(\mu_1 - \mu_2, \frac{\sigma^2}{n} + \frac{\sigma^2}{n}\right) = N\left(6 - 5, \frac{4}{25} + \frac{4}{25}\right).$$

So,

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$$D \sim N(\mu = 1, \sigma^2 = 0.32).$$

Thus,

$$P(0 < D < 2) = P(D < 2) - P(D < 0).$$

This can then be calculated using R without a need to first standardize, or use a table.

```
pnorm(2, mean = 1, sd = sqrt(0.32)) - pnorm(0, mean = 1, sd = sqrt(0.32))
```

```
## [1] 0.9229001
```

An alternative approach, would be to **simulate** a large number of observations of D then use the **empirical** distribution to calculate the probability.

Our strategy will be to repeatedly:

- Generate a sample of 25 random observations from $N(\mu_1 = 6, \sigma^2 = 4)$. Call the mean of this sample \bar{x}_{1s} .
- Generate a sample of 25 random observations from $N(\mu_1 = 5, \sigma^2 = 4)$. Call the mean of this sample \bar{x}_{2s} .
- Calculate the differences of the means, $d_s = \bar{x}_{1s} \bar{x}_{2s}$.

We will repeat the process a large number of times. Then we will use the distribution of the simulated observations of d_s as an estimate for the true distribution of D.

```
set.seed(42)
num_samples = 10000
differences = rep(0, num_samples)
```

Before starting our for loop to perform the operation, we set a seed for reproducibility, create and set a variable num_samples which will define the number of repetitions, and lastly create a variables differences which will store the simulate values, d_s .

By using set.seed() we can reproduce the random results of rnorm() each time starting from that line.

```
for (s in 1:num_samples) {
   x1 = rnorm(n = 25, mean = 6, sd = 2)
   x2 = rnorm(n = 25, mean = 5, sd = 2)
   differences[s] = mean(x1) - mean(x2)
}
```

To estimate P(0 < D < 2) we will find the proportion of values of d_s (among the 10000 values of d_s generated) that are between 0 and 2.

```
mean(0 < differences & differences < 2)</pre>
```

```
## [1] 0.9222
```

Recall that above we derived the distribution of D to be $N(\mu = 1, \sigma^2 = 0.32)$

If we look at a histogram of the differences, we find that it looks very much like a normal distribution.

```
hist(differences, breaks = 20,
    main = "Empirical Distribution of D",
    xlab = "Simulated Values of D",
    col = "dodgerblue",
    border = "darkorange")
```

Empirical Distribution of D



Also the sample mean and variance are very close to to what we would expect.

```
mean(differences)
```

[1] 1.001423

```
var(differences)
```

[1] 0.3230183

We could have also accomplished this task with a single line of more "idiomatic" R.

```
set.seed(42)
diffs = replicate(10000, mean(rnorm(25, 6, 2)) - mean(rnorm(25, 5, 2)))
```

Use ?replicate to take a look at the documentation for the replicate function and see if you can understand how this line performs the same operations that our for loop above executed.

```
mean(differences == diffs)
```

[1] 1

We see that by setting the same seed for the randomization, we actually obtain identical results!

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2.5.2 Distribution of a Sample Mean

For another example of simulation, we will simulate observations from a Poisson distribution, and examine the empirical distribution of the sample mean of these observations.

Recall, if

 $X \sim Pois(\mu)$

then

 $E[X] = \mu$

and

$$Var[X] = \mu.$$

Also, recall that for a random variable X with finite mean μ and finite variance σ^2 , the central limit theorem tells us that the mean, \bar{X} of a random sample of size n is approximately normal for large values of n. Specifically, as $n \to \infty$,

$$\bar{X} \stackrel{d}{\to} N\left(\mu, \frac{\sigma^2}{n}\right).$$

The following verifies this result for a Poisson distribution with $\mu = 10$ and a sample size of n = 50.

Histogram of Sample Means



Now we will compare sample statistics from the empirical distribution with their known values based on the parent distribution.

```
c(mean(x_bars), mu)

## [1] 10.00008 10.00000

c(var(x_bars), mu / sample_size)

## [1] 0.1989732 0.2000000

c(sd(x_bars), sqrt(mu) / sqrt(sample_size))
```

[1] 0.4460641 0.4472136

And here, we will calculate the proportion of sample means that are within 2 standard deviations of the population mean.

```
mean(x_bars > mu - 2 * sqrt(mu) / sqrt(sample_size) &
    x_bars < mu + 2 * sqrt(mu) / sqrt(sample_size))</pre>
```

[1] 0.95429

This last histogram uses a bit of a trick to approximately shade the bars that are within two standard deviations of the mean.)

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Histogram of Sample Means, Two Standard Deviations



Chapter 3

Simple Linear Regression

```
"All models are wrong, but some are useful."
```

```
— George E. P. Box
```

After reading this chapter you will be able to:

- Understand the concept of a model.
- Describe two ways in which regression coefficients are derived.
- Estimate and visualize a regression model using R.
- Interpret regression coefficients and statistics in the context of real-world problems.
- Use a regression model to make predictions.

3.1 Modeling

Let's consider a simple example of how the speed of a car affects its stopping distance, that is, how far it travels before it comes to a stop. To examine this relationship, we will use the cars dataset which, is a default R dataset. Thus, we don't need to load a package first; it is immediately available.

To get a first look at the data you can use the View() function inside RStudio.

```
View(cars)
```

We could also take a look at the variable names, the dimension of the data frame, and some sample observations with str().

```
str(cars)
```

```
## 'data.frame': 50 obs. of 2 variables:
## $ speed: num 4 4 7 7 8 9 10 10 10 11 ...
## $ dist : num 2 10 4 22 16 10 18 26 34 17 ...
```

As we have seen before with data frames, there are a number of additional functions to access some of this information directly.

```
dim(cars)
## [1] 50
nrow(cars)
## [1] 50
ncol(cars)
```

[1] 2

Other than the two variable names and the number of observations, this data is still just a bunch of numbers, so we should probably obtain some context.

```
?cars
```

Reading the documentation we learn that this is data gathered during the 1920s about the speed of cars and the resulting distance it takes for the car to come to a stop. The interesting task here is to determine how far a car travels before stopping, when traveling at a certain speed. So, we will first plot the stopping distance against the speed.

```
plot(dist ~ speed, data = cars,
     xlab = "Speed (in Miles Per Hour)",
     ylab = "Stopping Distance (in Feet)",
     main = "Stopping Distance vs Speed",
     pch = 20,
     cex = 3,
     col = "dodgerblue")
```

Stopping Distance vs Speed



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Let's now define some terminology. We have pairs of data, (x_i, y_i) , for i = 1, 2, ..., n, where n is the sample size of the dataset.

We use i as an index, simply for notation. We use x_i as the **predictor** (explanatory) variable. The predictor variable is used to help *predict* or explain the **response** (target, outcome) variable, y_i .

Other texts may use the term independent variable instead of predictor and dependent variable in place of response. However, those monikers imply mathematical characteristics that might not be true. While these other terms are not incorrect, independence is already a strictly defined concept in probability. For example, when trying to predict a person's weight given their height, would it be accurate to say that height is independent of weight? Certainly not, but that is an unintended implication of saying "independent variable." We prefer to stay away from this nomenclature.

In the cars example, we are interested in using the predictor variable speed to predict and explain the response variable dist.

Broadly speaking, we would like to model the relationship between X and Y using the form

$$Y = f(X) + \epsilon$$
.

The function f describes the functional relationship between the two variables, and the ϵ term is used to account for error. This indicates that if we plug in a given value of X as input, our output is a value of Y, within a certain range of error. You could think of this a number of ways:

- Response = Prediction + Error
- Response = Signal + Noise
- Response = Model + Unexplained
- Response = Explainable + Unexplainable

What sort of function should we use for f(X) for the cars data?

We could try to model the data with a horizontal line. That is, the model for y does not depend on the value of x. (Some function f(X) = c.) In the plot below, we see this doesn't seem to do a very good job. Many of the data points are very far from the orange line representing c. This is an example of **underfitting**. The obvious fix is to make the function f(X) actually depend on x.

Stopping Distance vs Speed



We could also try to model the data with a very "wiggly" function that tries to go through as many of the data points as possible. This also doesn't seem to work very well. The stopping distance for a speed of 5 mph shouldn't be off the chart! (Even in 1920.) This is an example of **overfitting**. (Note that in this example no function will go through every point, since there are some x values that have several possible y values in the data.)

Stopping Distance vs Speed



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Lastly, we could try to model the data with a well chosen line rather than one of the two extremes previously attempted. The line on the plot below seems to summarize the relationship between stopping distance and speed quite well. As speed increases, the distance required to come to a stop increases. There is still some variation about this line, but it seems to capture the overall trend.

Stopping Distance vs Speed



With this in mind, we would like to restrict our choice of f(X) to linear functions of X. We will write our model using β_1 for the slope, and β_0 for the intercept,

$$Y = \beta_0 + \beta_1 X + \epsilon.$$

3.1.1 Simple Linear Regression Model

We now define what we will call the simple linear regression model,

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$. That is, the ϵ_i are independent and identically distributed (iid) normal random variables with mean 0 and variance σ^2 . This model has three parameters to be estimated: β_0 , β_1 , and σ^2 , which are fixed, but unknown constants.

We have slightly modified our notation here. We are now using Y_i and x_i , since we will be fitting this model to a set of n data points, for i = 1, 2, ... n.

Recall that we use capital Y to indicate a random variable, and lower case y to denote a potential value of the random variable. Since we will have n observations, we have n random variables Y_i and their possible values y_i .

In the simple linear regression model, the x_i are assumed to be fixed, known constants, and are thus notated with a lower case variable. The response Y_i remains a random variable because of the random behavior of the error variable, ϵ_i . That is, each response Y_i is tied to an observable x_i and a random, unobservable, ϵ_i .

The random Y_i are a function of x_i , thus we can write its mean as a function of x_i ,

$$E[Y_i] = \beta_0 + \beta_1 x_i.$$

However, its variance remains constant for each x_i ,

$$Var[Y_i] = \sigma^2$$
.

This is visually displayed in the image below. We see that for any value x, the expected value of Y is $\beta_0 + \beta_1 x$. At each value of x, Y has the same variance σ^2 .



Figure 3.1: Simple Linear Regression Model UC David Stat Wiki

Often, we directly talk about the assumptions that this model makes. They can be cleverly shortened to LINE.

- Linear. The relationship between Y and x is linear, of the form $\beta_0 + \beta_1 x$.
- Independent. The errors ϵ are independent.
- Normal. The errors, ϵ are normally distributed. That is the "error" around the line follows a normal distribution.
- Equal Variance. At each value of x, the variance of Y is the same, σ^2 .

As a side note, we will often refer to simple linear regression as **SLR**. Some explanation of the name SLR:

- Simple refers to the fact that we are using a single predictor variable. Later we will use multiple predictor variables.
- Linear tells us that our model for Y is a linear combination of the predictors X. (In this case just the one.) Right now, this always results in a model that is a line, but later we will see how this is not always the case.
- Regression simply means that we are attempting to measure the relationship between a response variable and (one or more) predictor variables.

So SLR models Y as a linear function of X, but how do we actually define a good line? There are an infinite number of lines we could use, so we will attempt to find one with "small errors." That is a line with as many points as close to it as possible. The questions now becomes, how do we find such a line? There are many approaches we could take.

We could find the line that has the smallest maximum distance from any of the points to the line. That is,

$$\underset{\beta_0,\beta_1}{\operatorname{argmin}} \max |y_i - (\beta_0 + \beta_1 x_i)|.$$

We could find the line that minimizes the sum of all the distances from the points to the line. That is,

$$\underset{\beta_0,\beta_1}{\operatorname{argmin}} \sum_{i=1}^{n} |y_i - (\beta_0 + \beta_1 x_i)|.$$

We could find the line that minimizes the sum of all the squared distances from the points to the line. That is,

$$\underset{\beta_0,\beta_1}{\operatorname{argmin}} \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2.$$

This last option is called the method of **least squares**. It is essentially the de-facto method for fitting a line to data. (You may have even seen it before in a linear algebra course.) Its popularity is largely due to the fact that it is mathematically "easy." (Which was important historically, as computers are a modern contraption.) It is also very popular because many relationships are well approximated by a linear function.

3.2 Least Squares Approach

Given observations (x_i, y_i) , for i = 1, 2, ..., n, we want to find values of β_0 and β_1 which minimize

$$f(\beta_0, \beta_1) = \sum_{i=1}^n (y_i - (\beta_0 + \beta_1 x_i))^2 = \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2.$$

We will call these values $\hat{\beta}_0$ and $\hat{\beta}_1$.

First, we take a partial derivative with respect to both β_0 and β_1 .

$$\frac{\partial f}{\partial \beta_0} = -2 \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)$$
$$\frac{\partial f}{\partial \beta_1} = -2 \sum_{i=1}^n (x_i) (y_i - \beta_0 - \beta_1 x_i)$$

We then set each of the partial derivatives equal to zero and solving the resulting system of equations.

$$\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) = 0$$

$$\sum_{i=1}^{n} (x_i)(y_i - \beta_0 - \beta_1 x_i) = 0$$

While solving the system of equations, one common algebraic rearrangement results in the **normal equations**.

$$\sum_{i=1}^{n} y_i = n\beta_0 + \beta_1 \sum_{i=1}^{n} x_i$$
$$\sum_{i=1}^{n} x_i y_i = \beta_0 \sum_{i=1}^{n} x_i + \beta_1 \sum_{i=1}^{n} x_i^2$$

Finally, we finish solving the system of equations.

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n x_i y_i - \frac{(\sum_{i=1}^n x_i)(\sum_{i=1}^n y_i)}{n}}{\sum_{i=1}^n x_i^2 - \frac{(\sum_{i=1}^n x_i)^2}{n}} = \frac{S_{xy}}{S_{xx}}$$

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

Here, we have defined some notation for the expression we've obtained. Note that they have alternative forms which are much easier to work with. (We won't do it here, but you can try to prove the equalities below on your own, for "fun.") We use the capital letter S to denote "summation" which replaces the capital letter Σ when we calculate these values based on observed data, (x_i, y_i) . The subscripts such as xy denote over which variables the function $(z - \bar{z})$ is applied.

$$S_{xy} = \sum_{i=1}^{n} x_i y_i - \frac{\left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n} = \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})$$

$$S_{xx} = \sum_{i=1}^{n} x_i^2 - \frac{\left(\sum_{i=1}^{n} x_i\right)^2}{n} = \sum_{i=1}^{n} (x_i - \bar{x})^2$$

$$S_{yy} = \sum_{i=1}^{n} y_i^2 - \frac{\left(\sum_{i=1}^{n} y_i\right)^2}{n} = \sum_{i=1}^{n} (y_i - \bar{y})^2$$

Note that these summations S are not to be confused with sample standard deviation s.

By using the above alternative expressions for S_{xy} and S_{xx} , we arrive at a cleaner, more useful expression for $\hat{\beta}_1$.

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

Traditionally we would now calculate $\hat{\beta}_0$ and $\hat{\beta}_1$ by hand for the cars dataset. However because we are living in the 21st century and are intelligent (or lazy or efficient, depending on your perspective), we will utilize R to do the number crunching for us.

To keep some notation consistent with above mathematics, we will store the response variable as y and the predictor variable as x.

x = cars\$speed
y = cars\$dist

We then calculate the three sums of squares defined above.

```
Sxy = sum((x - mean(x)) * (y - mean(y)))
Sxx = sum((x - mean(x)) ^ 2)
Syy = sum((y - mean(y)) ^ 2)
c(Sxy, Sxx, Syy)
```

[1] 5387.40 1370.00 32538.98

Then finally calculate $\hat{\beta}_0$ and $\hat{\beta}_1$.

```
beta_1_hat = Sxy / Sxx
beta_0_hat = mean(y) - beta_1_hat * mean(x)
c(beta_0_hat, beta_1_hat)
```

[1] -17.579095 3.932409

What do these values tell us about our dataset?

The slope parameter β_1 tells us that for an increase in speed of one mile per hour, the **mean** stopping distance increases by β_1 . It is important to specify that we are talking about the mean. Recall that $\beta_0 + \beta_1 x$ is the estimated mean of Y, in this case stopping distance, for a particular value of x. (In this case speed.) So β_1 tells us how the mean of Y is affected by a change in x.

Similarly, the estimate $\hat{\beta}_1 = 3.932$ tells us that for an increase in speed of one mile per hour, the **estimated** mean stopping distance increases by 3.932 feet. Here we should be sure to specify we are discussing an estimated quantity. Recall that \hat{y} is the estimated mean of Y, so $\hat{\beta}_1$ tells us how the estimated mean of Y is affected by changing x.

The intercept parameter β_0 tells us the **mean** stopping distance for a car traveling zero miles per hour. (Not moving.) The estimate $\hat{\beta}_0 = -17.579$ tells us that the **estimated** mean stopping distance for a car traveling zero miles per hour is -17.579 feet. So when you apply the brakes to a car that is not moving, it moves backwards? This doesn't seem right. (Extrapolation, which we will see later, is the issue here.)

3.2.1 Making Predictions

We can now write the **fitted** or estimated line,

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x.$$

In this case,

$$\hat{y} = -17.579 + 3.932x.$$

We can now use this line to make predictions. First, let's see the possible x values in the cars dataset. Since some x values may appear more than once, we use the unique() to return each unique value only once.

```
unique(cars$speed)
```

```
## [1] 4 7 8 9 10 11 12 13 14 15 16 17 18 19 20 22 23 24 25
```

Let's make a prediction for the stopping distance of a car traveling at 8 miles per hour.

$$\hat{y} = -17.579 + 3.932 \times 8 = 13.88$$

beta_0_hat + beta_1_hat * 8

[1] 13.88018

This tells us that the estimated mean stopping distance of a car traveling at 8 miles per hour is 13.88.

Now let's make a prediction for the stopping distance of a car traveling at 21 miles per hour. This is considered **interpolation** as 21 is not an observed value of x. (But is in the data range.) We can use the special %in% operator to quickly verify this in R.

8 %in% unique(cars\$speed)

[1] TRUE

21 %in% unique(cars\$speed)

[1] FALSE

min(cars\$speed) < 21 & 21 < max(cars\$speed)</pre>

[1] TRUE

$$\hat{y} = -17.579 + 3.932 \times 21 = 65.001$$

beta_0_hat + beta_1_hat * 21

[1] 65.00149

Lastly, we can make a prediction for the stopping distance of a car traveling at 50 miles per hour. This is considered **extrapolation** as 50 is not an observed value of x and is outside data range. We should be less confident in predictions of this type.

range(cars\$speed)

[1] 4 25

range(cars\$speed)[1] < 50 & 50 < range(cars\$speed)[2]</pre>

[1] FALSE

$$\hat{y} = -17.579 + 3.932 \times 50 = 179.041$$

```
beta_0_hat + beta_1_hat * 50
```

[1] 179.0413

Cars travel 50 miles per hour rather easily today, but not in the 1920s!

This is also an issue we saw when interpreting $\hat{\beta}_0 = -17.579$, which is equivalent to making a prediction at x = 0. We should not be confident in the estimated linear relationship outside of the range of data we have observed.

3.2.2 Residuals

If we think of our model as "Response = Prediction + Error," we can then write it as

$$y = \hat{y} + e.$$

We then define a **residual** to be the observed value minus the predicted value.

$$e_i = y_i - \hat{y}_i$$

Let's calculate the residual for the prediction we made for a car traveling 8 miles per hour. First, we need to obtain the observed value of y for this x value.

```
which(cars$speed == 8)
```

[1] 5

cars[5,]

speed dist ## 5 8 16

cars[which(cars\$speed == 8),]

```
## speed dist
## 5 8 16
```

We can then calculate the residual.

$$e = 16 - 13.88 = 2.12$$

```
16 - (beta_0_hat + beta_1_hat * 8)
```

[1] 2.119825

The positive residual value indicates that the observed stopping distance is actually 2.12 feet more than what was predicted.

3.2.3 Variance Estimation

We'll now use the residuals for each of the points to create an estimate for the variance, σ^2 . Recall that,

$$E[Y_i] = \beta_0 + \beta_1 x_i.$$

So,

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

is a natural estimate for the mean of Y_i for a given value of x_i .

Also, recall that when we specified the model, we had three unknown parameters; β_0 , β_1 , and σ^2 . The method of least squares gave us estimates for β_0 and β_1 , however, we have yet to see an estimate for σ^2 . We will now define s_e^2 which will be an estimate for σ^2 .

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

This probably seems like a natural estimate, aside from the use of n-2, which we will put off explaining until the next chapter. It should actually look rather similar to something we have seen before.

$$s^{2} = \frac{1}{n-1} \sum_{i=1}^{n} (x_{i} - \bar{x})^{2}$$

Here, s^2 is the estimate of σ^2 when we have a single random variable X. In this case \bar{x} is an estimate of μ which is assumed to be the same for each x.

Now, in the regression case, with s_e^2 each y has a different mean because of the relationship with x. Thus, for each y_i , we use a different estimate of the mean, that is \hat{y}_i .

```
## [1] 236.5317
```

Just as with the univariate measure of variance, this value of 236.532 doesn't have a practical interpretation in terms of stopping distance. Taking the square root, however, computes the standard deviation of the residuals, also known as *residual standard error*.

```
s_e = sqrt(s2_e)
s_e
```

```
## [1] 15.37959
```

This tells us that our estimates of mean stopping distance are "typically" off by 15.38 feet.

3.3 Decomposition of Variation

We can re-express $y_i - \bar{y}$, which measures the deviation of an observation from the sample mean, in the following way,

$$y_i - \bar{y} = (y_i - \hat{y}_i) + (\hat{y}_i - \bar{y}).$$

This is the common mathematical trick of "adding zero." In this case we both added and subtracted \hat{y}_i .

Here, $y_i - \hat{y}_i$ measures the deviation of an observation from the fitted regression line and $\hat{y}_i - \bar{y}$ measures the deviation of the fitted regression line from the sample mean.

If we square then sum both sides of the equation above, we can obtain the following,

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

This should be somewhat alarming or amazing. How is this true? For now we will leave this questions unanswered. (Think about this, and maybe try to prove it.) We will now define three of the quantities seen in this equation.

Sum of Squares Total

$$SST = \sum_{i=1}^{n} (y_i - \bar{y})^2$$

The quantity "Sum of Squares Total," or SST, represents the **total variation** of the observed y values. This should be a familiar looking expression. Note that,

$$s^{2} = \frac{1}{n-1} \sum_{i=1}^{n} (y_{i} - \bar{y})^{2} = \frac{1}{n-1} SST.$$

Sum of Squares Regression

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

The quantity "Sum of Squares Regression," SSReg, represents the **explained variation** of the observed y values.

Sum of Squares Error

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

The quantity "Sum of Squares Error," SSE, represents the **unexplained variation** of the observed y values. You will often see SSE written as RSS, or "Residual Sum of Squares."

```
SST = sum((y - mean(y)) ^ 2)
SSReg = sum((y_hat - mean(y)) ^ 2)
SSE = sum((y - y_hat) ^ 2)
c(SST = SST, SSReg = SSReg, SSE = SSE)
```

```
## SST SSReg SSE
## 32538.98 21185.46 11353.52
```

Note that,

$$s_e^2 = \frac{SSE}{n-2}.$$

```
SSE / (n - 2)
```

[1] 236.5317

We can use R to verify that this matches our previous calculation of s_e^2 .

$$s2_e = SSE / (n - 2)$$

[1] TRUE

These three measures also do not have an important practical interpretation individually. But together, they're about to reveal a new statistic to help measure the strength of a SLR model.

3.3.1 Coefficient of Determination

The **coefficient of determination**, R^2 , is defined as

$$R^{2} = \frac{\sum_{i=1}^{n} (\hat{y}_{i} - \bar{y})^{2}}{\sum_{i=1}^{n} (y_{i} - \bar{y})^{2}} = \frac{SSReg}{SST} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - \hat{y}_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \bar{y})^{2}} = 1 - \frac{\sum_{i=1}^{n} e_{i}^{2}}{\sum_{i=1}^{n} (y_{i} - \bar{y})^{2}} = 1 - \frac{SSE}{SST}$$

The coefficient of determination is interpreted as the proportion of observed variation in y that can be explained by the simple linear regression model.

```
R2 = SSReg / SST
R2
```

[1] 0.6510794

For the cars example, we calculate $R^2 = 0.651$. We then say that 65.1% of the observed variability in stopping distance is explained by the linear relationship with speed.

The following three plots visually demonstrate the three "sums of squares" for a simulated dataset which has $R^2 = 0.901$ which is a somewhat high value. Notice in the third plot, that the orange arrows account for a larger proportion of the total arrow.

SSReg (Sum of Squares Regression)



SSE (Sum of Squares Error)



SST (Sum of Squares Total)



The next three plots again visually demonstrate the three "sums of squares," this time for a simulated dataset which has $R^2 = 0.459$. Notice in the third plot, that now the blue arrows account for a larger proportion of the total arrow.

SSReg (Sum of Squares Regression)



3.4. THE LM FUNCTION 67

SSE (Sum of Squares Error)





3.4 The lm Function

So far we have done regression by deriving the least squares estimates, then writing simple R commands to perform the necessary calculations. Since this is such a common task, this is functionality that is built

directly into R via the lm() command.

The lm() command is used to fit linear models which actually account for a broader class of models than simple linear regression, but we will use SLR as our first demonstration of lm(). The lm() function will be one of our most commonly used tools, so you may want to take a look at the documentation by using ?lm. You'll notice there is a lot of information there, but we will start with just the very basics. This is documentation you will want to return to often.

We'll continue using the cars data, and essentially use the lm() function to check the work we had previously done.

```
stop_dist_model = lm(dist ~ speed, data = cars)
```

This line of code fits our very first linear model. The syntax should look somewhat familiar. We use the dist ~ speed syntax to tell R we would like to model the response variable dist as a linear function of the predictor variable speed. In general, you should think of the syntax as response ~ predictor. The data = cars argument then tells R that that dist and speed variables are from the dataset cars. We then store this result in a variable stop_dist_model.

The variable stop_dist_model now contains a wealth of information, and we will now see how to extract and use that information. The first thing we will do is simply output whatever is stored immediately in the variable stop_dist_model.

```
stop_dist_model
```

```
##
## Call:
## lm(formula = dist ~ speed, data = cars)
##
## Coefficients:
## (Intercept) speed
## -17.579 3.932
```

We see that it first tells us the formula we input into R, that is lm(formula = dist ~ speed, data = cars). We also see the coefficients of the model. We can check that these are what we had calculated previously. (Minus some rounding that R is doing to display the results.)

```
c(beta_0_hat, beta_1_hat)
```

```
## [1] -17.579095 3.932409
```

Next, it would be nice to add the fitted line to the scatterplot. To do so we will use the abline() function.

Stopping Distance vs Speed



The abline() function is used to add lines of the form a+bx to a plot. (Hence abline.) When we give it stop_dist_model as an argument, it automatically extracts the regression coefficient estimates ($\hat{\beta}_0$ and $\hat{\beta}_1$) and uses them as the slope and intercept of the line. Here we also use lwd to modify the width of the line, as well as col to modify the color of the line.

The "thing" that is returned by the lm() function is actually an object of class lm which is a list. The exact details of this are unimportant unless you are seriously interested in the inner-workings of R, but know that we can determine the names of the elements of the list using the names() command.

names(stop_dist_model)

```
## [1] "coefficients" "residuals" "effects" "rank"

## [5] "fitted.values" "assign" "qr" "df.residual"

## [9] "xlevels" "call" "terms" "model"
```

When can then use this information to, for example, access the residuals using the \$ operator.

stop_dist_model\$residuals

```
3
##
                          2
                                                               5
                                                                            6
                                                                                         7
             1
##
     3.849460
                 11.849460
                             -5.947766
                                          12.052234
                                                        2.119825
                                                                   -7.812584
             8
                          9
                                                              12
##
                                     10
                                                  11
                                                                           13
                                                                                        14
##
     4.255007
                 12.255007
                             -8.677401
                                           2.322599
                                                     -15.609810
                                                                   -9.609810
                                                                                -5.609810
##
            15
                         16
                                     17
                                                  18
                                                              19
                                                                           20
                                                                                        21
##
    -1.609810
                 -7.542219
                              0.457781
                                           0.457781
                                                      12.457781
                                                                  -11.474628
                                                                                -1.474628
##
            22
                         23
                                     24
                                                  25
                                                              26
                                                                           27
##
    22.525372
                 42.525372
                            -21.407036
                                        -15.407036
                                                      12.592964
                                                                  -13.339445
                                                                                -5.339445
##
            29
                         30
                                     31
                                                  32
                                                              33
                                                                           34
                                                                                        35
```

```
-17.271854
               -9.271854
                            0.728146 -11.204263
                                                    2.795737
                                                               22.795737
                                   38
##
           36
                       37
                                               39
                                                           40
                                                                      41
                                                                                  42
##
   -21.136672
              -11.136672
                           10.863328 -29.069080 -13.069080
                                                               -9.069080
                                                                           -5.069080
                                               46
                                                                      48
                                                                                  49
##
           43
                       44
                                   45
                                                           47
##
     2.930920
                -2.933898 -18.866307
                                       -6.798715
                                                   15.201285
                                                               16.201285
                                                                           43.201285
##
           50
##
     4.268876
```

Another way to access stored information in stop_dist_model are the coef(), resid(), and fitted() functions. These return the coefficients, residuals, and fitted values, respectively.

```
coef(stop_dist_model)
```

```
## (Intercept) speed
## -17.579095 3.932409
```

resid(stop_dist_model)

```
##
                         2
                                     3
                                                             5
                11.849460
                                                     2.119825
##
     3.849460
                            -5.947766
                                        12.052234
                                                                -7.812584
                                                                            -3.744993
##
                         9
                                    10
                                                            12
                                                                        13
             8
                                                11
     4.255007
                            -8.677401
                                         2.322599
                                                   -15.609810
                                                                -9.609810
##
                12.255007
                                                                            -5.609810
##
           15
                        16
                                    17
                                                18
                                                            19
                                                                        20
    -1.609810
                -7.542219
                             0.457781
                                         0.457781
                                                    12.457781 -11.474628
                                                                            -1.474628
##
##
           22
                        23
                                    24
                                                25
                                                            26
                                                                        27
                           -21.407036 -15.407036
                                                    12.592964 -13.339445
##
    22.525372
                42.525372
                                                                            -5.339445
##
            29
                        30
                                    31
                                                32
                                                            33
                                                                        34
                                                                                    35
   -17.271854
                -9.271854
                             0.728146 -11.204263
                                                     2.795737
                                                                22.795737
                                                                            30.795737
##
##
           36
                        37
                                    38
                                                39
                                                            40
                                                                        41
                                                                                    42
   -21.136672 -11.136672
                            10.863328 -29.069080
                                                   -13.069080
##
                                                                -9.069080
                                                                            -5.069080
##
                        44
                                    45
                                                46
                                                            47
                                                                        48
                                                                                    49
           43
                -2.933898 -18.866307
##
     2.930920
                                        -6.798715
                                                   15.201285
                                                                16.201285
           50
##
##
     4.268876
```

fitted(stop_dist_model)

```
##
                      2
                                3
                                           4
                                                     5
                                                                6
                                                                          7
                                   9.947766 13.880175 17.812584 21.744993 21.744993
  -1.849460 -1.849460
                         9.947766
                     10
                               11
                                          12
                                                    13
                                                               14
## 21.744993 25.677401 25.677401 29.609810 29.609810 29.609810 29.609810 33.542219
          17
                     18
                               19
                                          20
                                                    21
                                                               22
                                                                         23
   33.542219 33.542219 33.542219 37.474628 37.474628 37.474628 37.474628 41.407036
##
          25
                     26
                               27
                                          28
                                                    29
                                                               30
                                                                         31
                                                                                    32
  41.407036 41.407036 45.339445 45.339445 49.271854 49.271854 49.271854 53.204263
##
          33
                     34
                               35
                                          36
                                                    37
                                                               38
## 53.204263 53.204263 53.204263 57.136672 57.136672 57.136672 61.069080 61.069080
                                          44
                                                    45
                                                               46
                                                                         47
##
## 61.069080 61.069080 61.069080 68.933898 72.866307 76.798715 76.798715 76.798715
          49
## 76.798715 80.731124
```

An R function that is useful in many situations is summary(). We see that when it is called on our model, it returns a good deal of information. By the end of the course, you will know what every value here is used for. For now, you should immediately notice the coefficient estimates, and you may recognize the R^2 value we saw earlier.

summary(stop_dist_model)

```
##
## Call:
## lm(formula = dist ~ speed, data = cars)
##
## Residuals:
##
      Min
                1Q Median
                                3Q
                                       Max
##
  -29.069
           -9.525
                   -2.272
                             9.215
                                    43.201
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -17.5791
                            6.7584
                                    -2.601
                                             0.0123 *
## speed
                 3.9324
                            0.4155
                                     9.464 1.49e-12 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 15.38 on 48 degrees of freedom
## Multiple R-squared: 0.6511, Adjusted R-squared: 0.6438
## F-statistic: 89.57 on 1 and 48 DF, p-value: 1.49e-12
```

The summary() command also returns a list, and we can again use names() to learn what about the elements of this list.

names(summary(stop_dist_model))

```
## [1] "call" "terms" "residuals" "coefficients" ## [5] "aliased" "sigma" "df" "r.squared" ## [9] "adj.r.squared" "fstatistic" "cov.unscaled"
```

So, for example, if we wanted to directly access the value of R^2 , instead of copy and pasting it out of the printed statement from summary(), we could do so.

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

```
## [1] 0.6510794
```

Another value we may want to access is s_e , which R calls sigma.

```
summary(stop_dist_model)$sigma
```

```
## [1] 15.37959
```

Note that this is the same result seen earlier as s_e. You may also notice that this value was display above as a result of the summary() command, which R labeled the "Residual Standard Error."

$$s_e = RSE = \sqrt{\frac{1}{n-2} \sum_{i=1}^{n} e_i^2}$$

Often it is useful to talk about s_e (or RSE) instead of s_e^2 because of their units. The units of s_e in the cars example is feet, while the units of s_e^2 is feet-squared.

Another useful function, which we will use almost as often as lm() is the predict() function.

```
predict(stop_dist_model, data.frame(speed = 8))
```

```
## 13.88018
```

The above code reads "predict the stopping distance of a car traveling 8 miles per hour using the stop_dist_model." Importantly, the second argument to predict() is a data frame that we make in place. We do this so that we can specify that 8 is a value of speed, so that predict knows how to use it with the model stored in stop_dist_model. We see that this result is what we had calculated "by hand" previously.

We could also predict multiple values at once.

```
predict(stop_dist_model, data.frame(speed = c(8, 21, 50)))
```

```
## 1 2 3
## 13.88018 65.00149 179.04134
```

$$\hat{y} = -17.579 + 3.932 \times 8 = 13.88$$

 $\hat{y} = -17.579 + 3.932 \times 21 = 65.001$
 $\hat{y} = -17.579 + 3.932 \times 50 = 179.041$

Or we could calculate the fitted value for each of the original data points.

```
predict(stop_dist_model, data.frame(speed = cars$speed))
```

```
7
                      2
                                3
                                                     5
                                                               6
  -1.849460 -1.849460
                                  9.947766 13.880175 17.812584 21.744993 21.744993
                        9.947766
           9
                                          12
                                                    13
  21.744993 25.677401 25.677401 29.609810 29.609810 29.609810 29.609810 33.542219
##
          17
                    18
                               19
                                          20
                                                    21
                                                              22
                                                                         23
  33.542219 33.542219 33.542219 37.474628 37.474628 37.474628 37.474628 41.407036
##
                                          28
                                                              30
##
          25
                               27
## 41.407036 41.407036 45.339445 45.339445 49.271854 49.271854 49.271854 53.204263
##
          33
                    34
                               35
                                          36
                                                    37
                                                              38
                                                                         39
## 53.204263 53.204263 53.204263 57.136672 57.136672 57.136672 61.069080 61.069080
                     42
                                         44
                                                    45
  61.069080 61.069080 61.069080 68.933898 72.866307 76.798715 76.798715 76.798715
##
          49
## 76.798715 80.731124
```

This is actually equivalent to simply calling predict() on stop_dist_model without a second argument.

predict(stop_dist_model)

```
##
                                                     5
                                                                          7
                     2
                                3
                                          4
                                                               6
                                                                                    8
   -1.849460 -1.849460
                         9.947766
                                  9.947766 13.880175 17.812584 21.744993 21.744993
           9
                    10
                               11
                                         12
                                                    13
                                                              14
                                                                         15
## 21.744993 25.677401 25.677401 29.609810 29.609810 29.609810 29.609810 33.542219
                                         20
          17
                    18
                               19
                                                    21
                                                              22
                                                                         23
   33.542219 33.542219 33.542219 37.474628 37.474628 37.474628 37.474628 41.407036
                    26
                               27
          25
                                         28
                                                    29
                                                              30
                                                                         31
## 41.407036 41.407036 45.339445 45.339445 49.271854 49.271854 49.271854 53.204263
          33
                    34
                               35
                                         36
                                                    37
                                                              38
                                                                         39
## 53.204263 53.204263 53.204263 57.136672 57.136672 57.136672 61.069080 61.069080
                               43
                                         44
                                                    45
                                                              46
                                                                         47
## 61.069080 61.069080 61.069080 68.933898 72.866307 76.798715 76.798715 76.798715
          49
## 76.798715 80.731124
```

Note that then in this case, this is the same as using fitted().

fitted(stop_dist_model)

```
2
                                3
                                                                         7
## -1.849460 -1.849460
                        9.947766
                                   9.947766 13.880175 17.812584 21.744993 21.744993
                    10
                               11
                                         12
                                                    13
                                                              14
                                                                         15
## 21.744993 25.677401 25.677401 29.609810 29.609810 29.609810 29.609810 33.542219
                    18
                               19
                                         20
                                                   21
                                                              22
                                                                        23
  33.542219 33.542219 33.542219 37.474628 37.474628 37.474628 37.474628 41.407036
                    26
                               27
                                         28
                                                   29
                                                              30
  41.407036 41.407036 45.339445 45.339445 49.271854 49.271854 49.271854 53.204263
##
          33
                    34
                               35
                                         36
                                                   37
                                                              38
                                                                         39
## 53.204263 53.204263 53.204263 57.136672 57.136672 57.136672 61.069080 61.069080
                    42
                               43
                                         44
                                                   45
                                                              46
## 61.069080 61.069080 61.069080 68.933898 72.866307 76.798715 76.798715 76.798715
          49
## 76.798715 80.731124
```

3.5 Maximum Likelihood Estimation (MLE) Approach

Recall the model,

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where $e_i \sim N(0, \sigma^2)$.

Then we can find the mean and variance of each Y_i .

$$E[Y_i] = \beta_0 + \beta_1 x_i$$

and

$$Var[Y_i] = \sigma^2$$
.

Recall that the pdf of a random variable $X \sim N(\mu, \sigma^2)$ is given by

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

Then we can write the pdf of each of the Y_i as

$$f_{Y_i}(y_i; x_i, \beta_0, \beta_1, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2} \left(\frac{y_i - (\beta_0 + \beta_1 x_i)}{\sigma}\right)^2\right].$$

Given n data points (x_i, y_i) we can write the likelihood, which is a function of the three parameters β_0 , β_1 , and σ^2 . Since the data have been observed, we use lower case y_i to denote that these values are no longer random.

$$L(\beta_0, \beta_1, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2} \left(\frac{y_i - \beta_0 - \beta_1 x_i}{\sigma}\right)^2\right]$$

Our goal is to find values of β_0 , β_1 , and σ^2 which maximize this function, which is a straightforward multivariate calculus problem.

We'll start by doing a bit of rearranging to make our task easier.

$$L(\beta_0, \beta_1, \sigma^2) = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^n \exp\left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2\right]$$

Then, as is often the case when finding MLEs, for mathematical convenience we will take the natural logarithm of the likelihood function since log is a monotonically increasing function. Then we will proceed to maximize the log-likelihood, and the resulting estimates will be the same as if we had not taken the log.

$$\log L(\beta_0, \beta_1, \sigma^2) = -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log(\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

Note that we use log to mean the natural logarithm. We now take a partial derivative with respect to each of the parameters.

$$\frac{\partial \log L(\beta_0, \beta_1, \sigma^2)}{\partial \beta_0} = \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)$$

$$\frac{\partial \log L(\beta_0, \beta_1, \sigma^2)}{\partial \beta_1} = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i)(y_i - \beta_0 - \beta_1 x_i)$$

$$\frac{\partial \log L(\beta_0, \beta_1, \sigma^2)}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

We then set each of the partial derivatives equal to zero and solve the resulting system of equations.

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$$\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) = 0$$

$$\sum_{i=1}^{n} (x_i)(y_i - \beta_0 - \beta_1 x_i) = 0$$

$$-\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 = 0$$

You may notice that the first two equations also appear in the least squares approach. Then, skipping the issue of actually checking if we have found a maximum, we then arrive at our estimates. We call these estimates the maximum likelihood estimates.

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n x_i y_i - \frac{(\sum_{i=1}^n x_i)(\sum_{i=1}^n y_i)}{n}}{\sum_{i=1}^n x_i^2 - \frac{(\sum_{i=1}^n x_i)^2}{n}} = \frac{S_{xy}}{S_{xx}}$$

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

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

Note that $\hat{\beta}_0$ and $\hat{\beta}_1$ are the same as the least squares estimates. However we now have a new estimate of σ^2 , that is $\hat{\sigma}^2$. So we now have two different estimates of σ^2 .

$$s_e^2 = \frac{1}{n-2} \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \frac{1}{n-2} \sum_{i=1}^n e_i^2 \quad \text{Least Squares}$$

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \frac{1}{n} \sum_{i=1}^n e_i^2 \quad \text{MLE}$$

In the next chapter, we will discuss in detail the difference between these two estimates, which involves biasedness.

3.6 Simulating SLR

We return again to more examples of simulation. This will be a common theme!

In practice you will almost never have a true model, and you will use data to attempt to recover information about the unknown true model. With simulation, we decide the true model and simulate data from the it. Then we apply a method to the data, in this case least squares. Now, since we know the true model, we can assess how well it did.

For this example, we will simulate n = 20 observations from the model

$$y_i = 5 + 2x_i + \epsilon_i$$
.

That is $\beta_0 = 5$, $\beta_1 = 2$, and let $\epsilon_i \sim N(\mu = 0, \sigma^2 = 1)$.

We first set the parameters of the simulation.

```
n = 20
beta_0 = 5
beta_1 = 2
sigma = 1
```

Next, we obtain simulated values of ϵ_i .

```
epsilon = rnorm(n, mean = 0, sd = sigma)
```

Now, since the x_i values in SLR are considered fixed and known, we simply generate them from a uniform distribution. Know, that this is an arbitrary, but common practice.

```
x = runif(n, 0, 10)
```

We then generate the y values according the specified functional relationship.

```
y = beta_0 + beta_1 * x + epsilon
```

Now to check how well the method of least squares works, we use lm() to fit the model to our data, then take a look at the estimated coefficients.

```
sim_fit = lm(y ~ x)
coef(sim_fit)
```

```
## (Intercept) x
## 5.098490 1.946622
```

And look at that, they aren't too far from the parameters we specified!

```
plot(y ~ x)
abline(sim_fit)
```



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We should say here, that we're being sort of lazy, and not the good kinda of lazy that could be considered efficient. Any time you simulate data, you should consider doing two things: writing a function, and storing the data in a data frame.

The function below, sim_slr() can be used for the same task as above, but is much more flexible.

Here, we use the function to repeat the analysis above.

```
sim_data = sim_slr(n = 20, beta_0 = 5, beta_1 = 2, sigma = 1)
```

This time, the simulated observations are stored in a data frame.

```
head(sim_data)
```

```
## predictor response
## 1 9.348230 23.329224
## 2 5.504941 16.195112
## 3 6.017662 17.617148
## 4 1.969945 10.339627
## 5 5.352366 14.977440
## 6 1.795557 9.893657
```

Now when we fit the model with lm() we can use a data argument, a very good practice.

```
sim_fit = lm(response ~ predictor, data = sim_data)
coef(sim_fit)
```

```
## (Intercept) predictor
## 6.162023 1.792461
```

And this time, we'll make the plot look a lot nicer.

Simulated Regression Data



3.7 History

For some brief background on the history of linear regression, see "Galton, Pearson, and the Peas: A Brief History of Linear Regression for Statistics Instructors" from the Journal of Statistics Education as well as the Wikipedia page on the history of regression analysis and lastly the article for regression to the mean which details the origins of the term "regression."

Chapter 4

Inference for Simple Linear Regression

"There are three types of lies: lies, damn lies, and statistics."

— Benjamin Disraeli

After reading this chapter you will be able to:

- Understand the distributions of regression estimates.
- Create interval estimates for regression parameters.
- Test for significance of regression.

Last chapter we defined the simple linear regression model,

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$. We then used observations (x_i, y_i) , for i = 1, 2, ..., n, to find values of β_0 and β_1 which minimized

$$f(\beta_0, \beta_1) = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2.$$

We called these values $\hat{\beta}_0$ and $\hat{\beta}_1$, which we found to be

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

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

We also estimated σ^2 using s_e^2 . In other words, we found that s_e is an estimate of σ , where;

$$s_e = RSE = \sqrt{\frac{1}{n-2} \sum_{i=1}^{n} e_i^2}$$

which we also called RSE, for "Residual Standard Error."

When applied to the cars data, we obtained the following results:

```
stop_dist_model = lm(dist ~ speed, data = cars)
summary(stop_dist_model)
```

```
##
## Call:
## lm(formula = dist ~ speed, data = cars)
##
## Residuals:
##
      Min 1Q Median
                            3Q
                                    Max
## -29.069 -9.525 -2.272 9.215 43.201
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -17.5791 6.7584 -2.601 0.0123 *
               3.9324
                          0.4155 9.464 1.49e-12 ***
## speed
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 15.38 on 48 degrees of freedom
## Multiple R-squared: 0.6511, Adjusted R-squared: 0.6438
## F-statistic: 89.57 on 1 and 48 DF, p-value: 1.49e-12
```

Last chapter, we only discussed the Estimate, Residual standard error, and Multiple R-squared values. In this chapter, we will discuss all of the information under Coefficients as well as F-statistic.

Stopping Distance vs Speed



To get started, we'll note that there is another equivalent expression for S_{xy} which we did not see last chapter,

$$S_{xy} = \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) = \sum_{i=1}^{n} (x_i - \bar{x})y_i.$$

This may be a surprising equivalence. (Maybe try to prove it.) However, it will be useful for illustrating concepts in this chapter.

Note that, $\hat{\beta}_1$ is a **statistic** when calculated with observed data as written above, as is $\hat{\beta}_0$.

However, in this chapter it will often be convenient to use both $\hat{\beta}_1$ and $\hat{\beta}_0$ as **random variables**, that is, we have not yet observed the values for each Y_i . When this is the case, we will use a slightly different notation, substituting in capital Y_i for lower case y_i .

$$\hat{\beta}_{1} = \frac{\sum_{i=1}^{n} (x_{i} - \bar{x}) Y_{i}}{\sum_{i=1}^{n} (x_{i} - \bar{x})^{2}}$$
$$\hat{\beta}_{0} = \bar{Y} - \hat{\beta}_{1} \bar{x}$$

Last chapter we argued that these estimates of unknown model parameters β_0 and β_1 were good because we obtained them by minimizing errors. We will now discuss the Gauss–Markov theorem which takes this idea further, showing that these estimates are actually the "best" estimates, from a certain point of view.

4.1 Gauss–Markov Theorem

The **Gauss–Markov theorem** tells us that when estimating the parameters of the simple linear regression model β_0 and β_1 , the $\hat{\beta}_0$ and $\hat{\beta}_1$ which we derived are the **best linear unbiased estiamtes**, or *BLUE* for short. (The actual conditions for the Gauss–Markov theorem are more relaxed than the SLR model.)

We will now discuss *linear*, *unbiased*, and *best* as is relates to these estimates.

Linear

Recall, in the SLR setup that the x_i values are considered fixed and known quantities. Then a linear estimate is one which can be written as a linear combination of the Y_i . In the case of $\hat{\beta}_1$ we see

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \bar{x}) Y_i}{\sum_{i=1}^n (x_i - \bar{x})^2} = \sum_{i=1}^n k_i Y_i = k_1 Y_1 + k_2 Y_2 + \dots + k_n Y_n$$

where
$$k_i = \frac{(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$
.

In a similar fashion, we could show that $\hat{\beta}_0$ can be written as a linear combination of the Y_i . Thus both $\hat{\beta}_0$ and $\hat{\beta}_1$ are linear estimators.

Unbiased

Now that we know our estimates are *linear*, how good are these estimates? One measure of the "goodness" of an estimate is its **bias**. Specifically, we prefer estimates that are **unbiased**, meaning their expected value is the parameter being estimated.

In the case of the regression estimates, we have,

$$E[\hat{\beta}_0] = \beta_0$$

$$E[\hat{\beta}_1] = \beta_1.$$

This tells us that, when the conditions of the SLR model are met, on average our estimates will be correct. However, as we saw last chapter when simulating from the SLR model, that does not mean that each individual estimate will be correct. Only that, if we repeated the process an infinite number of times, on average the estimate would be correct.

Best

Now, if we restrict ourselves to both *linear* and *unbiased* estimates, how do we define the *best* estimate? The estimate with the **minimum variance**.

First note that it is very easy to create an estimate for β_1 that has very low variance, but is not unbiased. For example, define:

$$\hat{\theta}_{BAD} = 5.$$

Then, since $\hat{\theta}_{BAD}$ is a constant value,

$$Var[\hat{\theta}_{BAD}] = 0.$$

However since,

$$E[\hat{\theta}_{BAD}] = 5$$

we say that $\hat{\theta}_{BAD}$ is a biased estimator unless $\beta_1 = 5$, which we would not know ahead of time. For this reason, it is a terrible estimate (unless by chance $\beta_1 = 5$) even though it has the smallest possible variance.

This is part of the reason we restrict ourselves to *unbiased* estimates. What good is an estimate, if it estimates the wrong quantity?

So now, the natural question is, what are the variances of $\hat{\beta}_0$ and $\hat{\beta}_1$? They are,

$$Var[\hat{\beta}_0] = \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}} \right)$$
$$Var[\hat{\beta}_1] = \frac{\sigma^2}{S_{xx}}.$$

These quantify the variability of the estimates due to random chance during sampling. Are these "the best"? Are these variances as small as we can possibility get? You'll just have to take our word for it that they are because showing that this is true is beyond the score of this course.

4.2 Sampling Distributions

Now that we have "redefined" the estimates for $\hat{\beta}_0$ and $\hat{\beta}_1$ as random variables, we can discuss their **sampling distribution**, which is the distribution when a statistic is considered a random variable.

Since both $\hat{\beta}_0$ and $\hat{\beta}_1$ are a linear combination of the Y_i and each Y_i is normally distributed, then both $\hat{\beta}_0$ and $\hat{\beta}_1$ also follow a normal distribution.

Then, putting all of the above together, we arrive at the distributions of $\hat{\beta}_0$ and $\hat{\beta}_1$.

For $\hat{\beta}_1$ we say,

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = \frac{\sum_{i=1}^n (x_i - \bar{x})Y_i}{\sum_{i=1}^n (x_i - \bar{x})^2} \sim N\left(\beta_1, \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}\right).$$

Or more succinctly,

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma^2}{S_{xx}}\right).$$

And for $\hat{\beta}_0$,

$$\hat{\beta}_0 = \bar{Y} - \hat{\beta}_1 \bar{x} \sim N\left(\beta_0, \frac{\sigma^2 \sum_{i=1}^n x_i^2}{n \sum_{i=1}^n (x_i - \bar{x})^2}\right).$$

Or more succinctly,

$$\hat{\beta}_0 \sim N\left(\beta_0, \sigma^2\left(\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}\right)\right)$$

At this point we have neglected to prove a number of these results. Instead of working through the tedious derivations of these sampling distributions, we will instead justify these results to ourselves using simulation.

A note to current readers: These derivations and proofs may be added to an appendix at a later time. You can also find these results in nearly any standard linear regression textbook. At UIUC, these results will likely be presented in both STAT 424 and STAT 425. However, since you will not be asked to perform derivations of this type in this course, they are for now omitted.

4.2.1 Simulating Sampling Distributions

To verify the above results, we will simulate samples of size n = 100 from the model

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$. In this case, the parameters are known to be:

- $\beta_0 = 3$ $\beta_1 = 6$ $\sigma^2 = 4$

Then, based on the above, we should find that

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma^2}{S_{xx}}\right)$$

and

$$\hat{\beta}_0 \sim N\left(\beta_0, \sigma^2\left(\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}\right)\right).$$

First we need to decide ahead of time what our x values will be for this simulation, since the x values in SLR are also considered known quantities. The choice of x values is arbitrary. Here we also set a seed for randomization, and calculate S_{xx} which we will need going forward.

```
set.seed(42)
sample_size = 100 # this is n
x = seq(-1, 1, length = sample_size)
Sxx = sum((x - mean(x)) ^ 2)
```

We also fix our parameter values.

```
beta_0 = 3
beta_1 = 6
sigma = 2
```

With this information, we know the sampling distributions should be:

```
(var_beta_1_hat = sigma ^ 2 / Sxx)
## [1] 0.1176238
(var_beta_0_hat = sigma ^ 2 * (1 / sample_size + mean(x) ^ 2 / Sxx))
```

```
## [1] 0.04
```

 $\hat{\beta}_1 \sim N(6, 0.1176238)$

and

 $\hat{\beta}_0 \sim N(3, 0.04).$

That is,

$$E[\hat{\beta}_1] = 6$$
 $Var[\hat{\beta}_1] = 0.1176238$

and

$$E[\hat{\beta}_0] = 3$$

$$Var[\hat{\beta}_0] = 0.04.$$

We now simulate this model 10,000 times. Note this may not be the most R way of doing the simulation. We perform the simulation in this manner in an attempt at clarity.

```
num_samples = 10000
beta_0_hats = rep(0, num_samples)
beta_1_hats = rep(0, num_samples)

for(i in 1:num_samples) {
   eps = rnorm(sample_size, mean = 0, sd = sigma)
   y = beta_0 + beta_1 * x + eps

   sim_model = lm(y ~ x)

   beta_0_hats[i] = coef(sim_model)[1]
   beta_1_hats[i] = coef(sim_model)[2]
}
```

The variables beta_0_hats and beta_1_hats now store 10,000 simulated values of $\hat{\beta}_0$ and $\hat{\beta}_1$ respectively. We first verify the distribution of $\hat{\beta}_1$.

```
mean(beta_1_hats) # empirical mean

## [1] 6.001998

beta_1  # true mean

## [1] 6

var(beta_1_hats) # empirical variance
```

[1] 0.11899

```
var_beta_1_hat # true variance
```

[1] 0.1176238

We see that the empirical and true means and variances are *very* similar. We also verify that the empirical distribution is normal. We plot a histogram of the beta_1_hats, and add the curve for the true distribution of β_1 . We use prob = TRUE to put the histogram on the same scale as the normal curve.



We then repeat the process for $\hat{\beta}_0$.

```
mean(beta_0_hats) # empirical mean
```

[1] 3.001147

```
beta_0 # true mean
```

[1] 3

```
var(beta_0_hats) # empirical variance
```

[1] 0.04017924

```
var_beta_0_hat # true variance
```

[1] 0.04



In this simulation study, we have only simulated a finite number of samples. To truly verify the distributional results, we would need to observe an infinite number of samples. However, the following plot should make it clear that if we continued simulating, the empirical results would get closer and closer to what we should expect.





4.3 Standard Errors

So now we believe the two distributional results,

$$\hat{\beta}_0 \sim N\left(\beta_0, \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}\right)\right)$$

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma^2}{S_{xx}}\right).$$

Then by standardizing these results we find that

$$\frac{\hat{\beta}_0 - \beta_0}{SD[\hat{\beta}_0]} \sim N(0, 1)$$

and

$$\frac{\hat{\beta}_1 - \beta_1}{SD[\hat{\beta}_1]} \sim N(0, 1)$$

where

$$SD[\hat{\beta}_0] = \sigma \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}}$$

and

$$SD[\hat{\beta}_1] = \frac{\sigma}{\sqrt{S_{xx}}}.$$

Since we don't know σ in practice, we will have to estimate it using s_e , which we plug into our existing expression for the standard deviations of our estimates. We choose s_e instead of $\hat{\sigma}$ because, as you've seen recently, we prize unbiased estimators over biased ones.

These two new expressions are called **standard errors** which are the *estimated* standard deviations of the sampling distributions.

$$SE[\hat{\beta}_0] = s_e \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}}$$
$$SE[\hat{\beta}_1] = \frac{s_e}{\sqrt{S_{xx}}}$$

Now if we divide by the standard error, instead of the standard deviation, we obtain the following results which will allow us to make confidence intervals and perform hypothesis testing.

$$\frac{\hat{\beta}_0 - \beta_0}{SE[\hat{\beta}_0]} \sim t_{n-2}$$

$$\frac{\hat{\beta}_1 - \beta_1}{SE[\hat{\beta}_1]} \sim t_{n-2}$$

To see this, first note that,

$$\frac{RSS}{\sigma^2} = \frac{(n-2)s_e^2}{\sigma^2} \sim \chi_{n-2}^2.$$

Then we use the classic trick of "multiply by 1" and some rearranging to arrive at

$$\begin{split} \frac{\hat{\beta}_1 - \beta_1}{SE[\hat{\beta}_1]} &= \frac{\hat{\beta}_1 - \beta_1}{s_e/\sqrt{S_{xx}}} \\ &= \frac{\hat{\beta}_1 - \beta_1}{s_e/\sqrt{S_{xx}}} \cdot \frac{\sigma/\sqrt{S_{xx}}}{\sigma/\sqrt{S_{xx}}} \\ &= \frac{\hat{\beta}_1 - \beta_1}{\sigma/\sqrt{S_{xx}}} \cdot \frac{\sigma/\sqrt{S_{xx}}}{s_e/\sqrt{S_{xx}}} \\ &= \frac{\hat{\beta}_1 - \beta_1}{\sigma/\sqrt{S_{xx}}} \bigg/ \sqrt{\frac{s_e^2}{\sigma^2}} \sim \frac{Z}{\sqrt{\frac{\chi_{n-2}^2}{n-2}}} \sim t_{n-2} \end{split}$$

where $Z \sim N(0, 1)$.

Recall that a random variable T defined as,

$$T = \frac{Z}{\sqrt{\frac{\chi_d^2}{d}}}$$

follows a t distribution with d degrees of freedom, where χ_d^2 is a χ^2 random variable with d degrees of freedom.

That is,

$$T \sim t_d$$
.

4.4 Confidence Intervals for Slope and Intercept

Recall that confidence intervals for means often take the form:

$$EST \pm CRIT \cdot SE$$

or

$$EST \pm MARGIN$$

where EST is an estimate for the parameter of interest, SE is the standard error of the estimate and $MARGIN = CRIT \cdot SE$.

Then, for β_0 and β_1 we can create confidence intervals using

$$\hat{\beta}_0 \pm t_{\alpha/2, n-2} \cdot SE[\hat{\beta}_0]$$
 $\hat{\beta}_0 \pm t_{\alpha/2, n-2} \cdot s_e \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}}$

and

$$\hat{\beta}_1 \pm t_{\alpha/2, n-2} \cdot SE[\hat{\beta}_1] \qquad \quad \hat{\beta}_1 \pm t_{\alpha/2, n-2} \cdot \frac{s_e}{\sqrt{S_{xx}}}$$

where $t_{\alpha/2,n-2}$ is the critical value such that $P(t_{n-2} > t_{\alpha/2,n-2}) = \alpha/2$.

4.5 Hypothesis Tests

"We may speak of this hypothesis as the 'null hypothesis', and it should be noted that the null hypothesis is never proved or established, but is possibly disproved, in the course of experimentation."

— Ronald Aylmer Fisher

Recall that a test statistic (TS) for testing means often take the form:

$$TS = \frac{EST - HYP}{SE}$$

where EST is an estimate for the parameter of interest, HYP is a hypothesized value of the parameter, and SE is the standard error of the estimate.

So, to test

$$H_0: \beta_0 = \beta_{00}$$
 vs $H_1: \beta_0 \neq \beta_{00}$

we use the test statistic

$$t = \frac{\hat{\beta}_0 - \beta_{00}}{SE[\hat{\beta}_0]} = \frac{\hat{\beta}_0 - \beta_{00}}{s_e \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}}}$$

which, under the null hypothesis, follows a t distribution with n-2 degrees of freedom. We use β_{00} to denote the hypothesized value of β_0 .

Similarly, to test

$$H_0: \beta_1 = \beta_{10}$$
 vs $H_1: \beta_1 \neq \beta_{10}$

we use the test statistic

$$t = \frac{\hat{\beta}_1 - \beta_{10}}{SE[\hat{\beta}_1]} = \frac{\hat{\beta}_1 - \beta_{10}}{s_e/\sqrt{S_{xx}}}$$

which again, under the null hypothesis, follows a t distribution with n-2 degrees of freedom. We now use β_{10} to denote the hypothesized value of β_1 .

4.6 cars Example

We now return to the cars example from last chapter to illustrate these concepts. We first fit the model using lm() then use summary() to view the results in greater detail.

```
stop_dist_model = lm(dist ~ speed, data = cars)
summary(stop_dist_model)
```

```
##
## Call:
## lm(formula = dist ~ speed, data = cars)
##
## Residuals:
##
      Min
                1Q Median
                                3Q
                                      Max
  -29.069 -9.525
                   -2.272
                             9.215
                                   43.201
##
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) -17.5791
                            6.7584 -2.601
                                             0.0123 *
                                     9.464 1.49e-12 ***
## speed
                 3.9324
                            0.4155
##
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 15.38 on 48 degrees of freedom
## Multiple R-squared: 0.6511, Adjusted R-squared: 0.6438
## F-statistic: 89.57 on 1 and 48 DF, p-value: 1.49e-12
```

4.6.1 Tests in R

We will now discuss the results displayed called Coefficients. First recall that we can extract this information directly.

4.6. CARS EXAMPLE 93

names(summary(stop_dist_model))

```
## [1] "call" "terms" "residuals" "coefficients" ## [5] "aliased" "sigma" "df" "r.squared" ## [9] "adj.r.squared" "fstatistic" "cov.unscaled"
```

summary(stop_dist_model)\$coefficients

```
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) -17.579095 6.7584402 -2.601058 1.231882e-02
## speed 3.932409 0.4155128 9.463990 1.489836e-12
```

The names() function tells us what information is available, and then we use the \$ operator and coefficients to extract the information we are interested in. Two values here should be immediately familiar.

$$\hat{\beta}_0 = -17.5790949$$

and

$$\hat{\beta}_1 = 3.9324088$$

which are our estimates for the model parameters β_0 and β_1 .

Let's now focus on the second row of output, which is relevant to β_1 .

summary(stop_dist_model)\$coefficients[2,]

```
## Estimate Std. Error t value Pr(>|t|)
## 3.932409e+00 4.155128e-01 9.463990e+00 1.489836e-12
```

Again, the first value, Estimate is

$$\hat{\beta}_1 = 3.9324088.$$

The second value, Std. Error, is the standard error of $\hat{\beta}_1$,

$$SE[\hat{\beta}_1] = \frac{s_e}{\sqrt{S_{xx}}} = 0.4155128.$$

The third value, t value, is the value of the test statistics for testing $H_0: \beta_1 = 0$ vs $H_1: \beta_1 \neq 0$,

$$t = \frac{\hat{\beta}_1 - 0}{SE[\hat{\beta}_1]} = \frac{\hat{\beta}_1 - 0}{s_e/\sqrt{S_{xx}}} = 9.46399.$$

Lastly, Pr(>|t|), gives us the p-value of that test.

p-value =
$$1.4898365 \times 10^{-12}$$

Note here, we are specifically testing whether or not $\beta_1 = 0$.

The first row of output reports the same values, but for β_0 .

```
summary(stop_dist_model)$coefficients[1,]
```

```
## Estimate Std. Error t value Pr(>|t|)
## -17.57909489 6.75844017 -2.60105800 0.01231882
```

In summary, the following code stores the information of summary(stop_dist_model)\$coefficients in a new variable stop_dist_model_test_info, then extracts each element into a new variable which describes the information it contains.

We can then verify some equivalent expressions: the t test statistic for $\hat{\beta}_1$ and the two-sided p-value associated with that test statistic.

```
(beta_1_hat - 0) / beta_1_hat_se

## [1] 9.46399

beta_1_hat_t

## [1] 9.46399

2 * pt(abs(beta_1_hat_t), df = length(resid(stop_dist_model)) - 2, lower.tail = FALSE)

## [1] 1.489836e-12

beta_1_hat_pval
```

[1] 1.489836e-12

4.6.2 Significance of Regression, t-Test

We pause to discuss the **significance of regression** test. First, note that based on the above distributional results, we could test β_0 and β_1 against any particular value, and perform both one and two-sided tests.

However, one very specific test,

$$H_0: \beta_1 = 0 \text{ vs } H_1: \beta_1 \neq 0$$

4.6. CARS EXAMPLE 95

is used most often. Let's think about this test in terms of the simple linear regression model,

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i.$$

If we assume the null hypothesis is true, then $\beta_1 = 0$ and we have the model,

$$Y_i = \beta_0 + \epsilon_i.$$

In this model, the response does **not** depend on the predictor. So then we could think of this test in the following way,

- Under H_0 there is not a significant linear relationship between x and y.
- Under H_1 there is a significance linear relationship between x and y.

For the cars example,

- \bullet Under H_0 there is not a significant linear relationship between speed and stopping distance.
- Under H_1 there is a significant linear relationship between speed and stopping distance.

Again, that test is seen in the output from summary(),

p-value =
$$1.4898365 \times 10^{-12}$$
.

With this extremely low p-value, we would reject the null hypothesis at any reasonable α level, say for example $\alpha = 0.01$. So we say there is a significant **linear** relationship between speed and stopping distance. Notice that we emphasize **linear**.



In this plot of simulated data, we see a clear relationship between x and y, however it is not a linear relationship. If we fit a line to this data, it is very flat. The resulting test for $H_0: \beta_1 = 0$ vs $H_1: \beta_1 \neq 0$ gives a large p-value, in this case 0.7564548, so we would fail to reject and say that there is no significant linear relationship between x and y. We will see later how to fit a curve to this data using a "linear" model, but for now, realize that testing $H_0: \beta_1 = 0$ vs $H_1: \beta_1 \neq 0$ can only detect straight line relationships.

4.6.3 Confidence Intervals in R

Using R we can very easily obtain the confidence intervals for β_0 and β_1 .

This automatically calculates 99% confidence intervals for both β_0 and β_1 , the first row for β_0 , the second row for β_1 .

For the cars example when interpreting these intervals, we say, we are 99% confident that for an increase in speed of 1 mile per hour, the average increase in stopping distance is between 2.8179187 and 5.0468988 feet, which is the interval for β_1 .

Note that this 99% confidence interval does **not** contain the hypothesized value of 0. Since it does not contain 0, it is equivalent to rejecting the test of $H_0: \beta_1 = 0$ vs $H_1: \beta_1 \neq 0$ at $\alpha = 0.01$, which we had seen previously.

You should be somewhat suspicious of the confidence interval for β_0 , as it covers negative values, which correspond to negative stopping distances. Technically the interpretation would be that we are 99% confident that the average stopping distance of a car traveling 0 miles per hour is between -35.7066103 and 0.5484205 feet, but we don't really believe that, since we are actually certain that it would be non-negative.

Note, we can extract specific values from this output a number of ways. This code is not run, and instead, you should check how it relates to the output of the code above.

```
confint(stop_dist_model, level = 0.99)[1,]
confint(stop_dist_model, level = 0.99)[1,1]
confint(stop_dist_model, level = 0.99)[1,2]
confint(stop_dist_model, parm = "(Intercept)", level = 0.99)
confint(stop_dist_model, level = 0.99)[2,]
confint(stop_dist_model, level = 0.99)[2,1]
confint(stop_dist_model, level = 0.99)[2,2]
confint(stop_dist_model, parm = "speed", level = 0.99)
```

4.7 Confidence Interval for Mean Response

In addition to confidence intervals for β_0 and β_1 there two other common interval estimates used with regression. The first is called a **confidence interval for the mean response**. Often, we would like an interval estimate for the mean, E[Y] for a particular value of x.

In this situation we use \hat{y} as our estimate of E[Y].

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$$

Recall that,

$$E[Y] = \beta_0 + \beta_1 x$$

Thus, \hat{y} is a good estimate since it is unbiased:

$$E[\hat{y}] = \beta_0 + \beta_1 x.$$

We could then derive,

$$Var[\hat{y}] = \sigma^2 \left(\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}} \right).$$

Like the other estimates we have seen, \hat{y} also follows a normal distribution,

$$\hat{y} \sim N\left(\beta_0 + \beta_1 x, \sigma^2 \left(\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}\right)\right).$$

And lastly, since we need to estimate this variance, we arrive at the standard error of our estimate,

$$SE[\hat{y}] = s_e \sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}.$$

We can then use this to find the confidence interval for the mean response,

$$\hat{y} \pm t_{\alpha/2, n-2} \cdot s_e \sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}$$

To find confidence intervals for the mean response using R, we use the predict() function. We give the function our fitted model as well as new data, stored as a data frame. (This is important, so that R knows the name of the predictor variable.) Here, we are finding the confidence interval for the mean stopping distance when a car is travelling 5 miles per hour and when a car is travelling 21 miles per hour.

```
## fit lwr upr
## 1 2.082949 -10.89309 15.05898
## 2 65.001489 56.45836 73.54462
```

4.8 Prediction Interval for New Observations

Sometimes we would like an interval estimate for a new observation, Y for a particular value of x. This is very similar to an interval for the mean response, E[Y], but different in one very important way.

Our best guess for a new observation is still \hat{y} . The estimated mean is still the best prediction we can make. The difference is in the amount of variability, since we know that observations will vary about the true regression line according to a $N(0, \sigma^2)$ distribution. Because of this we add an extra factor of σ^2 to our estimates variability.

$$Var[\hat{y}] = \sigma^2 \left(1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}} \right)$$

$$\hat{y} \sim N\left(\beta_0 + \beta_1 x, \sigma^2 \left(1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}\right)\right)$$

$$SE[\hat{y}] = s_e \sqrt{1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}$$

We can then find a **prediction interval** using,

$$\hat{y} \pm t_{\alpha/2, n-2} \cdot s_e \sqrt{1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}.$$

To calculate this for a set of points in R notice there is only a minor change in syntax from finding a confidence interval for the mean response.

Also notice that these two intervals are wider than the corresponding confidence intervals for the mean response.

4.9 Confidence and Prediction Bands

Often we will like to plot both confidence intervals for the mean response and prediction intervals for all possible values of x. We calls these confidence and prediction bands.

```
speed_grid = seq(min(cars$speed), max(cars$speed), by = 0.01)
dist_ci_band = predict(stop_dist_model,
                           newdata = data.frame(speed = speed_grid),
                           interval = "confidence", level = 0.99)
dist pi band = predict(stop dist model,
                           newdata = data.frame(speed = speed grid),
                           interval = "prediction", level = 0.99)
plot(dist ~ speed, data = cars,
     xlab = "Speed (in Miles Per Hour)",
     ylab = "Stopping Distance (in Feet)",
     main = "Stopping Distance vs Speed",
     pch = 20,
     cex = 2,
     col = "dodgerblue",
     ylim = c(-50, 140))
abline(stop_dist_model, lwd = 5, col = "darkorange")
lines(speed_grid, dist_ci_band[,"lwr"], col = "red", lwd = 3, lty = 2)
lines(speed_grid, dist_ci_band[,"upr"], col = "red", lwd = 3, lty = 2)
lines(speed_grid, dist_pi_band[,"lwr"], col = "green", lwd = 3, lty = 3)
lines(speed_grid, dist_pi_band[,"upr"], col = "green", lwd = 3, lty = 3)
points(mean(cars$speed), mean(cars$dist), pch = "+", cex = 3)
```

Stopping Distance vs Speed



Some things to notice:

- We use the ylim argument to stretch the y-axis of the plot, since the bands extend further than the points.
- We add a point at the point (\bar{x}, \bar{y}) .
 - This is a point that the regression line will **always** pass through. (Think about why.)
 - This is the point where both the confidence and prediction bands are the narrowest. Look at the standard errors of both to understand why.
- The prediction bands (green) are less curved than the confidence bands (red). This is a result of the extra factor of σ^2 added to the variance at any value of x.

4.10 Significance of Regression, F-Test

In the case of simple linear regression, the t test for the significance of the regression is equivalent to another test, the F test for the significance of the regression. This equivalence will only be true for simple linear regression, and in the next chapter we will only use the F test for the significance of the regression.

Recall from last chapter the decomposition of variance we saw before calculating R^2 ,

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

or, in short,

$$SST = SSReq + SSE.$$

To develop the F test, we will arrange this information in an **ANOVA** table,

Source	Sum of Squares	Degrees of Freedom	Mean Square	F
Regression	$\sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2$	1	SSReg/1	$\overline{MSReg/MSE}$
Error Total	$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ \sum_{i=1}^{n} (y_i - \bar{y})^2$	n-2 $n-1$	SSE/(n-2)	

ANOVA, or Analysis of Variance will be a concept we return to often in this course. For now, we will focus on the results of the table, which is the F statistic,

$$F = \frac{\sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2 / 1}{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 / (n-2)} \sim F_{1,n-2}$$

which follows an F distribution with degrees of freedom 1 and n-2 under the null hypothesis. An F distribution is a continuous distribution which takes only positive values and has two parameters, which are the two degrees of freedom.

Recall, in the significance of the regression test, Y does **not** depend on x in the null hypothesis.

$$H_0: \beta_1 = 0 \qquad Y_i = \beta_0 + \epsilon_i$$

While in the alternative hypothesis Y may depend on x.

$$H_1: \beta_1 \neq 0$$
 $Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$

We can use the F statistic to perform this test.

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

In particular, we will reject the null when the F statistic is large, that is, when there is a low probability that the observations could have come from the null model by chance. We will let R calculate the p-value for us.

To perform the F test in R you can look at the last row of the output from summary() called F-statistic which gives the value of the test statistic, the relevant degrees of freedom, as well as the p-value of the test.

summary(stop_dist_model)

```
##
## Call:
  lm(formula = dist ~ speed, data = cars)
## Residuals:
##
       Min
                10 Median
                                 3Q
                                         Max
                              9.215
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -17.5791
                                     -2.601
                             6.7584
                                       9.464 1.49e-12 ***
## speed
                  3.9324
                             0.4155
```

```
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 15.38 on 48 degrees of freedom
## Multiple R-squared: 0.6511, Adjusted R-squared: 0.6438
## F-statistic: 89.57 on 1 and 48 DF, p-value: 1.49e-12
```

Additionally, you can use the anova() function to display the information in an ANOVA table.

```
anova(stop_dist_model)
```

This also gives a p-value for the test. You should notice that the p-value from the t test was the same. You might also notice that the value of the test statistic for the t test, 9.46399, can be squared to obtain the value of the F statistic, 89.5671065.

Note that there is another equivalent way to do this in R, which we will return to often to compare two models.

```
anova(lm(dist ~ 1, data = cars), lm(dist ~ speed, data = cars))
```

```
## Analysis of Variance Table
##
## Model 1: dist ~ 1
## Model 2: dist ~ speed
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 49 32539
## 2 48 11354 1 21186 89.567 1.49e-12 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

The model statement $lm(dist \sim 1, data = cars)$ applies the model $Y_i = \beta_0 + \epsilon_i$ to the cars data. Note that $\hat{y} = \bar{y}$ when $Y_i = \beta_0 + \epsilon_i$.

The model statement lm(dist ~ speed, data = cars) applies the model $Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$.

We can then think of this usage of anova() as directly comparing the two models. (Notice we get the same p-value again.)

Chapter 5

Multiple Linear Regression

"Life is really simple, but we insist on making it complicated."

— Confucius

After reading this chapter you will be able to:

- Construct and interpret linear regression models with more than one predictor.
- Understand how regression models are derived using matrices.
- Create interval estimates and perform hypothesis tests for multiple regression parameters.
- Formulate and interpret interval estimates for the mean response under various conditions.
- Compare nested models using an ANOVA F-Test.

The last two chapters we saw how to fit a model that assumed a linear relationship between a response variable and a single predictor variable. Specifically, we defined the simple linear regression model,

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$.

However, it is rarely the case that a dataset will have a single predictor variable. It is also rarely the case that a response variable will only depend on a single variable. So in this chapter, we will extend our current linear model to allow a response to depend on *multiple* predictors.

```
# read the data from the web
autompg = read.table(
   "http://archive.ics.uci.edu/ml/machine-learning-databases/auto-mpg/auto-mpg.data",
   quote = "\"",
   comment.char = "",
   stringsAsFactors = FALSE)
# give the dataframe headers
colnames(autompg) = c("mpg", "cyl", "disp", "hp", "wt", "acc", "year", "origin", "name")
# remove missing data, which is stored as "?"
autompg = subset(autompg, autompg$hp != "?")
# remove the plymouth reliant, as it causes some issues
autompg = subset(autompg, autompg$name != "plymouth reliant")
# give the dataset row names, based on the engine, year and name
rownames(autompg) = paste(autompg$cyl, "cylinder", autompg$year, autompg$name)
```

```
# remove the variable for name, as will as origin
autompg = subset(autompg, select = c("mpg", "cyl", "disp", "hp", "wt", "acc", "year"))
# change horsepower from character to numeric
autompg$hp = as.numeric(autompg$hp)
str(autompg)
```

```
## 'data.frame': 390 obs. of 7 variables:
## $ mpg : num   18 15 18 16 17 15 14 14 14 15 ...
## $ cyl : int   8 8 8 8 8 8 8 8 ...
## $ disp: num   307 350 318 304 302 429 454 440 455 390 ...
## $ hp : num   130 165 150 150 140 198 220 215 225 190 ...
## $ wt : num   3504 3693 3436 3433 3449 ...
## $ acc : num   12 11.5 11 12 10.5 10 9 8.5 10 8.5 ...
## $ year: int   70 70 70 70 70 70 70 70 70 ...
```

We will once again discuss a dataset with information about cars. This dataset, which can be found at the UCI Machine Learning Repository contains a response variable mpg which stores the city fuel efficiency of cars, as well as several predictor variables for the attributes of the vehicles. We load the data, and perform some basic tidying before moving on to analysis.

For now we will focus on using two variables, wt and year, as predictor variables. That is, we would like to model the fuel efficiency (mpg) of a car as a function of its weight (wt) and model year (year). To do so, we will define the following linear model,

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i, \qquad i = 1, 2, \dots, n$$

where $\epsilon_i \sim N(0, \sigma^2)$. In this notation we will define:

- x_{i1} as the weight (wt) of the *i*th car.
- x_{i2} as the model year (year) of the *i*th car.

The picture below will visualize what we would like to accomplish. The data points (x_{i1}, x_{i2}, y_i) now exist in 3-dimensional space, so instead of fitting a line to the data, we will fit a plane. (We'll soon move to higher dimensions, so this will be the last example that is easy to visualize and think about this way.)



How do we find such a plane? Well, we would like a plane that is as close as possible to the data points. That is, we would like it to minimize the errors it is making. How will we define these errors? Squared distance of course! So, we would like to minimize

$$f(\beta_0, \beta_1, \beta_2) = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2}))^2$$

with respect to β_0 , β_1 , and β_2 . How do we do so? It is another straightforward multivariate calculus problem. All we have done is add an extra variable since we did this last time. So again, we take a derivative with respect to each of β_0 , β_1 , and β_2 and set them equal to zero, then solve the resulting system of equations. That is,

$$\frac{\partial f}{\partial \beta_0} = 0$$
$$\frac{\partial f}{\partial \beta_1} = 0$$
$$\frac{\partial f}{\partial \beta_2} = 0$$

After doing so, we will once again obtain the **normal equations**.

$$n\beta_0 + \beta_1 \sum_{i=1}^n x_{i1} + \beta_2 \sum_{i=1}^n x_{i2} = \sum_{i=1}^n y_i$$

$$\beta_0 \sum_{i=1}^n x_{i1} + \beta_1 \sum_{i=1}^n x_{i1}^2 + \beta_2 \sum_{i=1}^n x_{i1} x_{i2} = \sum_{i=1}^n x_{i1} y_i$$

$$\beta_0 \sum_{i=1}^n x_{i2} + \beta_1 \sum_{i=1}^n x_{i1} x_{i2} + \beta_2 \sum_{i=1}^n x_{i2}^2 = \sum_{i=1}^n x_{i2} y_i$$

We now have three equations and three variables, which we could solve, or we could simply let R solve for us

```
mpg_model = lm(mpg ~ wt + year, data = autompg)
coef(mpg_model)
```

```
## (Intercept) wt year
## -14.637641945 -0.006634876 0.761401955
```

$$\hat{y} = -14.6376419 + -0.0066349x_1 + 0.761402x_2$$

Here we have once again fit our model using lm(), however we have introduced a new syntactical element. The formula mpg ~ wt + year now reads: "model the response variable mpg as a linear function of wt and year". That is, it will estimate an intercept, as well as slope coefficients for wt and year. We then extract these as we have done before using coef().

In the multiple linear regression setting, some of the interpretations of the coefficients change slightly.

Here, $\hat{\beta}_0 = -14.6376419$ is our estimate for β_0 , the mean miles per gallon for a car that weighs 0 pounds and was built in 1900. We see our estimate here is negative, which is a physical impossibility. However, this isn't unexpected, as we shouldn't expect our model to be accurate for cars from 1900 which weigh 0 pounds. (Because they never existed!) This isn't much of a change from SLR. That is, β_0 is still simply the mean when all of the predictors are 0.

The interpretation of the coefficients in front of our predictors are slightly different than before. For example $\hat{\beta}_1 = -0.0066349$ is our estimate for β_1 , the average change in miles per gallon for an increase in weight (x_1) of one-pound for a car of a certain model year, that is, for a fixed value of x_2 . Note that this coefficient is actually the same for any given value of x_2 . Later, we will look at models that allow for a different change in mean response for different values of x_2 . Also note that this estimate is negative, which we would expect since, in general, fuel efficiency decreases for larger vehicles. Recall that in the multiple linear regression setting, this interpretation is dependent on a fixed value for x_2 , that is, "for a car of a certain model year." It is possible that the indirect relationship between fuel efficiency and weight does not hold when an additional factor, say year, is included, and thus we could have the sign of our coefficient flipped.

Lastly, $\hat{\beta}_2 = 0.761402$ is our estimate for β_2 , the average change in miles per gallon for a one-year increase in model year (x_2) for a car of a certain weight, that is, for a fixed value of x_1 . It is not surprising that the estimate is positive. We expect that as time passes and the years march on, technology would improve so that a car of a specific weight would get better mileage now as compared to their predecessors. And yet, the coefficient could have been negative because we are also including weight as variable, and not strictly as a fixed value.

5.1 Matrix Approach to Regression

In our above example we used two predictor variables, but it will only take a little more work to allow for an arbitrary number of predictor variables and derive their coefficient estimates. We can consider the model,

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_{p-1} x_{i(p-1)} + \epsilon_i, \qquad i = 1, 2, \dots, n$$

where $\epsilon_i \sim N(0, \sigma^2)$. In this model, there are p-1 predictor variables, x_1, x_2, \dots, x_{p-1} . There are a total of p β -parameters and a single parameter σ^2 for the variance of the errors. (It should be noted that almost as often, authors will use p as the number of predictors, making the total number of β parameters p+1. This is always something you should be aware of when reading about multiple regression. There is not a standard that is used most often.)

If we were to stack together the n linear equations that represent each Y_i into a column vector, we get the following.

$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1(p-1)} \\ 1 & x_{21} & x_{22} & \cdots & x_{2(p-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{n(p-1)} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{p-1} \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$Y = X\beta + \epsilon$$

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1(p-1)} \\ 1 & x_{21} & x_{22} & \cdots & x_{2(p-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{n(p-1)} \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{p-1} \end{bmatrix}, \quad \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

So now with data,

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Just as before, we can estimate β by minimizing,

$$f(\beta_0, \beta_1, \beta_2, \cdots, \beta_{p-1}) = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_{p-1} x_{i(p-1)}))^2,$$

which would require taking p derivatives, which result in following **normal equations**.

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_{i1} & \sum_{i=1}^{n} x_{i2} & \cdots & \sum_{i=1}^{n} x_{i(p-1)} \\ \sum_{i=1}^{n} x_{i1} & \sum_{i=1}^{n} x_{i1}^{2} & \sum_{i=1}^{n} x_{i1} x_{i2} & \cdots & \sum_{i=1}^{n} x_{i(p-1)} \end{bmatrix} \begin{bmatrix} \beta_{0} \\ \beta_{1} \\ \vdots \\ \sum_{i=1}^{n} x_{i(p-1)} & \sum_{i=1}^{n} x_{i(p-1)} x_{i1} & \sum_{i=1}^{n} x_{i(p-1)} x_{i2} & \cdots & \sum_{i=1}^{n} x_{i(p-1)}^{2} \end{bmatrix} \begin{bmatrix} \beta_{0} \\ \beta_{1} \\ \vdots \\ \beta_{p-1} \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_{i} \\ \sum_{i=1}^{n} x_{i1} y_{i} \\ \vdots \\ \sum_{i=1}^{n} x_{i(p-1)} y_{i} \end{bmatrix}$$

The normal equations can be written much more succinctly in matrix notation,

$$X^{\top}X\beta = X^{\top}y.$$

We can then solve this expression by multiplying both sides by the inverse of $X^{\top}X$, which exists, provided the columns of X are linearly independent. Then as always, we denote our solution with a hat.

$$\hat{\beta} = \left(X^{\top} X \right)^{-1} X^{\top} y$$

To verify that this is what R has done for us in the case of two predictors, we create an X matrix. Note that the first column is all 1s, and the remaining columns contain the data.

```
n = nrow(autompg)
p = length(coef(mpg_model))
X = cbind(rep(1, n), autompg$wt, autompg$year)
y = autompg$mpg
(beta_hat = solve(t(X) %*% X) %*% t(X) %*% y)
```

```
## [,1]
## [1,] -14.637641945
## [2,] -0.006634876
## [3,] 0.761401955
```

```
coef(mpg_model)
```

```
## (Intercept) wt year
## -14.637641945 -0.006634876 0.761401955
```

$$\hat{\beta} = \begin{bmatrix} -14.6376419 \\ -0.0066349 \\ 0.761402 \end{bmatrix}$$

In our new notation, the fitted values can be written

$$\hat{y} = X\hat{\beta}.$$

$$\hat{y} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix}$$

Then, we can create a vector for the residual values,

$$e = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix}.$$

And lastly, we can update our estimate for σ^2 .

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

Recall, we like this estimate because it is unbiased, that is,

$$E[s_e^2] = \sigma^2$$

Note that the change from the SLR estimate to now is in the denominator. Specifically we now divide by n-p instead of n-2. Or actually, we should note that in the case of SLR, there are two β parameters and thus p=2.

Also note that if we fit the model $Y_i = \beta + \epsilon_i$ that $\hat{y} = \bar{y}$ and p = 1 and s_e^2 would become

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

which is likely the very first sample standard deviation you saw in a mathematical statistics class. The same reason for n-1 in this case, that we estimated one parameter, so we lose one degree of freedom. Now, in general, we are estimating p parameters, the β parameters, so we lose p degrees of freedom.

Also, recall that most often we will be interested in s_e , the residual standard error as R calls it,

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

In R, we could directly access s_e for a fitted model, as we have seen before.

```
summary(mpg_model)$sigma
```

```
## [1] 3.431367
```

And we can now verify that our math above is indeed calculating the same quantities.

```
y_hat = X %*% solve(t(X) %*% X) %*% t(X) %*% y
e = y - y_hat
sqrt(t(e) %*% e / (n - p))
```

```
## [,1]
## [1,] 3.431367
```

```
sqrt(sum((y - y_hat) ^ 2) / (n - p))
```

[1] 3.431367

5.2 Sampling Distribution

As we can see in the output below, the results of calling summary() are similar to SLR, but there are some differences, most obviously a new row for the added predictor variable.

summary(mpg_model)

```
##
## Call:
## lm(formula = mpg ~ wt + year, data = autompg)
##
##
  Residuals:
##
     Min
              1Q Median
                                  Max
  -8.852 -2.292 -0.100 2.039 14.325
##
##
## Coefficients:
##
                  Estimate
                            Std. Error t value Pr(>|t|)
  (Intercept) -14.6376419
                             4.0233914 -3.638 0.000312 ***
                -0.0066349
                             0.0002149 -30.881 < 2e-16 ***
## wt
                 0.7614020
                             0.0497266 15.312 < 2e-16 ***
## year
## Signif. codes:
                  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.431 on 387 degrees of freedom
## Multiple R-squared: 0.8082, Adjusted R-squared: 0.8072
## F-statistic: 815.6 on 2 and 387 DF, p-value: < 2.2e-16
```

To understand these differences in detail, we will need to first obtain the sampling distribution of $\hat{\beta}$.

The derivation of the sampling distribution of $\hat{\beta}$ involves the multivariate normal distribution. These brief notes from semesters past give a basic overview. These are simply for your information, as we will not present the derivation in full here.

Our goal now is to obtain the distribution of the $\hat{\beta}$ vector,

$$\hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_{p-1} \end{bmatrix}$$

Recall from last time that when discussing sampling distributions, we now consider $\hat{\beta}$ to be a random vector, thus we use Y instead of the data vector y.

$$\hat{\beta} = \left(X^{\top}X\right)^{-1}X^{\top}Y$$

Then it is a consequence of the multivariate normal distribution that,

$$\hat{\beta} \sim N\left(\beta, \sigma^2 \left(X^{\top} X\right)^{-1}\right).$$

We then have

$$E[\hat{\beta}] = \beta$$

and for any $\hat{\beta}_j$ we have

$$E[\hat{\beta}_j] = \beta_j.$$

We also have

$$Var[\hat{\beta}] = \sigma^2 \left(X^{\top} X \right)^{-1}$$

and for any $\hat{\beta}_j$ we have

$$Var[\hat{\beta}_j] = \sigma^2 C_{jj}$$

where

$$C = \left(X^{\top}X\right)^{-1}$$

and the elements of C are denoted

$$C = \begin{bmatrix} C_{00} & C_{01} & C_{02} & \cdots & C_{0(p-1)} \\ C_{10} & C_{11} & C_{12} & \cdots & C_{1(p-1)} \\ C_{20} & C_{21} & C_{22} & \cdots & C_{2(p-1)} \\ \vdots & \vdots & \vdots & & \vdots \\ C_{(p-1)0} & C_{(p-1)1} & C_{(p-1)2} & \cdots & C_{(p-1)(p-1)} \end{bmatrix}.$$

Essentially, the diagonal elements correspond to the β vector.

Then the standard error for the $\hat{\beta}$ vector is given by

$$SE[\hat{\beta}] = s_e \sqrt{(X^{\top}X)^{-1}}$$

and for a particular $\hat{\beta}_j$

$$SE[\hat{\beta}_j] = s_e \sqrt{C_{jj}}.$$

Lastly, each of the $\hat{\beta}_j$ follows a normal distribution,

$$\hat{\beta}_j \sim N\left(\beta_j, \sigma^2 C_{jj}\right).$$

thus

$$\frac{\hat{\beta}_j - \beta_j}{s_e \sqrt{C_{jj}}} \sim t_{n-p}.$$

Now that we have the necessary distributional results, we can move on to perform tests and make interval estimates.

5.2.1 Single Parameter Tests

The first test we will see is a test for a single β_i .

$$H_0: \beta_j = 0$$
 vs $H_1: \beta_j \neq 0$

Again, the test statistic takes the form

$$TS = \frac{EST - HYP}{SE}.$$

In particular,

$$t = \frac{\hat{\beta}_j - \beta_j}{SE[\hat{\beta}_j]} = \frac{\hat{\beta}_j - 0}{s_e \sqrt{C_{jj}}},$$

which, under the null hypothesis, follows a t distribution with n-p degrees of freedom.

Recall our model for mpg,

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i, \qquad i = 1, 2, \dots, n$$

where $\epsilon_i \sim N(0, \sigma^2)$.

- x_{i1} as the weight (wt) of the *i*th car.
- x_{i2} as the model year (year) of the *i*th car.

Then the test

$$H_0: \beta_1 = 0$$
 vs $H_1: \beta_1 \neq 0$

can be found in the summary() output, in particular:

summary(mpg_model)\$coef

```
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) -14.637641945 4.0233913563 -3.638135 3.118311e-04
## wt -0.006634876 0.0002148504 -30.881372 1.850466e-106
## year 0.761401955 0.0497265950 15.311765 1.036597e-41
```

The estimate (Estimate), standard error (Std. Error), test statistic (t value), and p-value (Pr(>|t|)) for this test are displayed in the second row, labeled wt. Remember that the p-value given here is specifically for a two-sided test, where the hypothesized value is 0.

Also note in this case, by hypothesizing that $\beta_1 = 0$ the null and alternative essentially specify two different models:

```
• H_0: Y = \beta_0 + \beta_2 x_2 + \epsilon
• H_1: Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon
```

This is important. We are not simply testing whether or not there is a relationship between weight and fuel efficiency. We are testing if there is a relationship between weight and fuel efficiency, given that a term for year is in the model. (Note, we dropped some indexing here, for readability.)

5.2.2 Confidence Intervals

Since $\hat{\beta}_j$ is our estimate for β_j and we have

$$E[\hat{\beta}_j] = \beta_j$$

as well as the standard error,

$$SE[\hat{\beta}_i] = s_e \sqrt{C_{ii}}$$

and the sampling distribution of $\hat{\beta}_j$ is Normal, then we can easily construct confidence intervals for each of the $\hat{\beta}_j$.

$$\hat{\beta}_j \pm t_{\alpha/2, n-p} \cdot s_e \sqrt{C_{jj}}$$

We can find these in R using the same method as before. Now there will simply be additional rows for the additional β .

```
confint(mpg_model, level = 0.99)
```

```
## 0.5 % 99.5 %

## (Intercept) -25.052563681 -4.222720208

## wt -0.007191036 -0.006078716

## year 0.632680051 0.890123859
```

5.2.3 Confidence Intervals for Mean Response

As we saw in SLR, we can create confidence intervals for mean response, that is, an interval estimate for E[Y]. In SLR, the mean of Y was only dependent on a single value x. Now, in multiple regression, E[Y] is dependent on the value of each of the predictors, so we define the vector x_0 to be,

$$x_0 = \begin{bmatrix} 1 \\ x_{01} \\ x_{02} \\ \vdots \\ x_{0(p-1)} \end{bmatrix}.$$

Then our estimate of E[Y] for a set of values x_0 is given by

$$\hat{y} = x_0^{\top} \hat{\beta}$$

= $\hat{\beta}_0 + \hat{\beta}_1 x_{01} + \hat{\beta}_2 x_{02} + \dots + \hat{\beta}_{p-1} x_{0(p-1)}$.

As with SLR, this is an unbiased estimate.

$$E[\hat{y}] = x_0^{\top} \beta$$

= $\beta_0 + \beta_1 x_{01} + \beta_2 x_{02} + \dots + \beta_{p-1} x_{0(p-1)}$

To make an interval estimate, we will also need its standard error.

$$SE[\hat{y}] = s_e \sqrt{x_0^\top \left(X^\top X\right)^{-1} x_0}$$

Putting it all together, we obtain a confidence interval for the mean response.

$$\hat{y} \pm t_{\alpha/2, n-p} \cdot s_e \sqrt{x_0^\top \left(X^\top X\right)^{-1} x_0}$$

The math has changed a bit, but the process in R remains almost identical. Here, we create a data frame for two additional cars. One car that weighs 3500 pounds produced in 1976, as well as a second car that weighs 5000 pounds which was produced in 1981.

```
new_cars = data.frame(wt = c(3500, 5000), year = c(76, 81))
new_cars
```

```
## wt year
## 1 3500 76
## 2 5000 81
```

We can then use the predict() function with interval = "confidence" to obtain intervals for the mean fuel efficiency for both new car. Again, it is important to make the data passed to newdata a data frame, so that R knows which values are for which variables.

```
predict(mpg_model, newdata = new_cars, interval = "confidence", level = 0.99)
```

```
## fit lwr upr
## 1 20.00684 19.4712 20.54248
## 2 13.86154 12.3341 15.38898
```

R then reports the estimate \hat{y} (fit) for each, as well as the lower (lwr) and upper (upr) bounds for the interval at a desired level (99%).

A word of caution here: one of these estimates is good while one is suspect.

```
new_cars$wt
```

[1] 3500 5000

```
range(autompg$wt)
```

```
## [1] 1613 5140
```

Note that both of the weights of the new cars are within the range of observed values.

```
new_cars$year
```

```
## [1] 76 81
```

range(autompg\$year)

[1] 70 82

As are the years of each of the new cars.

```
plot(year ~ wt, data = autompg, pch = 20, col = "dodgerblue", cex = 1.5)
points(new_cars, col = "darkorange", cex = 3, pch = "X")
```



However, we have to consider weight and year together now. And based on the above plot, one of the new cars is within the "blob" of observed values, while the other, the car from 1981 weighing 5000 pounds, is noticeably outside of the observed values. This is a hidden extrapolation which you should be aware of when using multiple regression.

Shifting gears back to the new data pair that can be reasonably estimated, we do a quick verification of some of the mathematics in R.

```
x0 = c(1, 3500, 76)
x0 %*% beta_hat
```

$$x_0 = \begin{bmatrix} 1\\3500\\76 \end{bmatrix}$$

$$\hat{\beta} = \begin{bmatrix} -14.6376419 \\ -0.0066349 \\ 0.761402 \end{bmatrix}$$

$$\hat{y} = x_0^{\top} \hat{\beta} = \begin{bmatrix} 1 & 3500 & 76 \end{bmatrix} \begin{bmatrix} -14.6376419 \\ -0.0066349 \\ 0.761402 \end{bmatrix} = 20.0068411$$

Also note that, using a particular value for x_0 , we can essentially extract certain $\hat{\beta}_i$ values.

```
x0 = c(0, 0, 1)

x0 %*% beta_hat
```

```
## [,1]
## [1,] 0.761402
```

beta_hat

```
## [,1]
## [1,] -14.637641945
## [2,] -0.006634876
## [3,] 0.761401955
```

With this in mind, confidence intervals for the individual $\hat{\beta}_j$ are actually a special case of a confidence interval for mean response.

5.2.4 Prediction Intervals

As with SLR, creating prediction intervals involves one slight change to the standard error to account for the fact that we are now considering an observation, instead of a mean.

Here we use \hat{y}_{Pred} to estimate Y_0 , the value of Y for the predictor vector x_0

$$\hat{y}_{Pred} = x_0^{\top} \hat{\beta}$$

$$= \hat{\beta}_0 + \hat{\beta}_1 x_{01} + \hat{\beta}_2 x_{02} + \dots + \hat{\beta}_{p-1}$$

$$E[\hat{y}_{Pred}] = Y_0$$

$$= x_0^{\top} \beta$$

$$= \beta_0 + \beta_1 x_{01} + \beta_2 x_{02} + \dots + \beta_{p-1} x_{0(p-1)}$$

$$SE[\hat{y}_{Pred}] = s_e \sqrt{1 + x_0^{\top} (X^{\top} X)^{-1} x_0}$$

$$\hat{y}_{Pred} \pm t_{\alpha/2, n-p} \cdot s_e \sqrt{1 + x_0^{\top} (X^{\top} X)^{-1} x_0}$$

new_cars

```
## wt year
## 1 3500 76
## 2 5000 81
```

predict(mpg_model, newdata = new_cars, interval = "prediction", level = 0.99)

```
## fit lwr upr
## 1 20.00684 11.108294 28.90539
## 2 13.86154 4.848751 22.87432
```

5.3 Signifiance of Regression

The decomposition of variation that we had seen in SLR still remains true,

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

Which means that, we can still calculate R^2 in the same manner as before, which R continues to do automatically.

summary(mpg_model)\$r.squared

[1] 0.8082355

The interpretation changes slightly as compared to SLR. In this MLR case, we say that 80.82% for the observed variation in miles per gallon is explained by the linear relationship with the two predictor variables, weight and year.

We can also create the ANOVA table as before and perform the significance of regression test. In multiple regression, the significance of regression test is

$$H_0: \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0.$$

Here, we see that the null hypothesis sets all of the β_j equal to 0, except the intercept, β_0 . We could then say that the null model, or "model under the null hypothesis" is

$$Y_i = \beta_0 + \epsilon_i$$
.

This is a model where the regression is insignificant. None of the predictors have a significant linear relationship with the response. Notationally, we will denote the fitted values of this model as \hat{y}_{0i} , which in this case happens to be:

$$\hat{y}_{0i} = \bar{y}$$
.

The alternative hypothesis here is that at least one of the β_j from the null hypothesis is not 0.

$$H_1$$
: At least one of $\beta_i \neq 0, j = 1, 2, \cdots, (p-1)$

We could then say that the full model, or "model under the alternative hypothesis" is

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_n x_{i(n-1)} + \epsilon_i$$

This is a model where the regression is significant. At least one of the predictors has a significant linear relationship with the response. We will denote the fitted values of this model as \hat{y}_{1i} . The ANOVA table is then nearly identical to the ANOVA table from SLR, with two exceptions in the degrees of freedom column.

Source	Sum of Squares	Degrees of Freedom	Mean Square	F
Regression	$\sum_{i=1}^{n} (\hat{y}_{1i} - \bar{y})^2$	p-1	SSReg/(p-1)	$\overline{MSReg/MSE}$
Error Total	$\sum_{i=1}^{n} (y_i - \hat{y}_{1i})^2 $ $\sum_{i=1}^{n} (y_i - \bar{y})^2$	n-p $n-1$	SSE/(n-p)	

In summary, the F statistic is

$$F = \frac{\sum_{i=1}^{n} (\hat{y}_{1i} - \bar{y})^{2} / (p-1)}{\sum_{i=1}^{n} (y_{i} - \hat{y}_{1i})^{2} / (n-p)},$$

and the p-value is calculated as

$$P(F_{p-1,n-p} > F)$$

since we reject for large values of F. Here $F_{p-1,n-p}$ represents a random variable which follows an F distribution with p-1 and n-p degrees of freedom.

To perform this test in R, we first explicitly specify the two models in R and save the results in different variables. We then use anova() to compare the two models, giving anova() the null model first and the alternative (full) model second.

In this case,

• H_0 : $Y_i = \beta_0 + \epsilon_i$ • H_1 : $Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i$

That is, in the null model, we use neither of the predictors, whereas in the full (alternative) model, at least one of the predictors is useful.

```
null_mpg_model = lm(mpg ~ 1, data = autompg)
full_mpg_model = lm(mpg ~ wt + year, data = autompg)
anova(null_mpg_model, full_mpg_model)
```

```
## Analysis of Variance Table
##
## Model 1: mpg ~ 1
## Model 2: mpg ~ wt + year
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 389 23761.7
## 2 387 4556.6 2 19205 815.55 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1</pre>
```

First, notice that R does not display the results in the same manner as the table above. More important than the layout of the table are its contents. We see that the value of the F statistic is 815.55, and the p-value is extremely low, so we reject the null hypothesis at any reasonable α and say that the regression is significant. At least one of wt or year has a useful linear relationship with mpg.

```
summary(mpg_model)
##
## Call:
## lm(formula = mpg ~ wt + year, data = autompg)
##
## Residuals:
    Min
           1Q Median
                       3Q
## -8.852 -2.292 -0.100 2.039 14.325
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) -14.6376419   4.0233914   -3.638   0.000312 ***
             ## year
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 3.431 on 387 degrees of freedom
## Multiple R-squared: 0.8082, Adjusted R-squared: 0.8072
## F-statistic: 815.6 on 2 and 387 DF, p-value: < 2.2e-16
```

Notice that the value reported in the row for F-statistic is indeed the F test statistic for the significance of the regression test, and additionally it reports the two relevant degrees of freedom.

Also, note that none of the individual t-tests are equivalent to the F-test as they were in SLR. This equivalence only holds for SLR because the individual test for β_1 is the same as testing for all non-intercept parameters, since there is only one.

We can also verify the sums of squares and degrees of freedom directly in R. You should match these to the table from R and use this to match R's output to the written table above.

```
# SSReg
sum((fitted(full_mpg_model) - fitted(null_mpg_model)) ^ 2)

## [1] 19205.03

# SSE
sum(resid(full_mpg_model) ^ 2)

## [1] 4556.646

# SST
sum(resid(null_mpg_model) ^ 2)

## [1] 23761.67

# Degrees of Freedom: Regression
length(coef(full_mpg_model)) - length(coef(null_mpg_model))
```

```
# Degrees of Freedom: Error
length(resid(full_mpg_model)) - length(coef(full_mpg_model))
```

[1] 387

```
# Degrees of Freedom: Total
length(resid(null_mpg_model)) - length(coef(null_mpg_model))
```

[1] 389

5.4 Nested Models

The significance of the regression test is actually a special case of testing what we will call **nested models**. More generally we can compare two models, where one model is "nested" inside the other, meaning one model contains a subset of the predictors from only the larger model.

Consider the following full model,

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_p x_{i(p-1)} + \epsilon_i$$

This model has p-1 predictors, for a total of p β -parameters. We will denote the fitted values of this model as \hat{y}_{1i} .

Let the null model be

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_{(q-1)} x_{i(q-1)} + \epsilon_i$$

where q < p. This model has q - 1 predictors, for a total of q β -parameters. We will denote the fitted values of this model as \hat{y}_{0i} .

The difference between these two models can be codified by the null hypothesis of a test.

$$H_0: \beta_q = \beta_{q+1} = \dots = \beta_{p-1} = 0.$$

Specifically, the β -parameters from the full model that are not in the null model are zero. The resulting model, which is nested, is the null model.

We can then perform this test using an F-test, which is the result of the following ANOVA table.

Source	Sum of Squares	Degrees of Freedom	Mean Square	F
Diff	$\sum_{i=1}^{n} (\hat{y}_{1i} - \hat{y}_{0i})^2$	p-q	SSD/(p-q)	MSD/MSE
Full	$\sum_{i=1}^{n} (y_i - \hat{y}_{1i})^2$	n-p	SSE/(n-p)	
Null	$\sum_{i=1}^{n} (\hat{y}_{1i} - \hat{y}_{0i})^{2}$ $\sum_{i=1}^{n} (y_{i} - \hat{y}_{1i})^{2}$ $\sum_{i=1}^{n} (y_{i} - \hat{y}_{0i})^{2}$	n-q		

$$F = \frac{\sum_{i=1}^{n} (\hat{y}_{1i} - \hat{y}_{0i})^2 / (p-1)}{\sum_{i=1}^{n} (y_i - \hat{y}_{1i})^2 / (n-p)}.$$

Notice that the row for "Diff" compares the sum of the squared differences of the fitted values. The degrees

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of freedom is then the difference of the number of β -parameters estimated between the two models.

For example, the autompg dataset has a number of additional variables that we have yet to use.

```
names(autompg)
```

```
## [1] "mpg" "cyl" "disp" "hp" "wt" "acc" "year"
```

We'll continue to use mpg as the response, but now we will consider two different models.

```
Full: mpg ~ wt + year + cyl + disp + hp + acc
Null: mpg ~ wt + year
```

Note that these are nested models, as the null model contains a subset of the predictors from the full model, and no additional predictors. Both models have an intercept β_0 as well as a coefficient in front of each of the predictors. We could then write the null hypothesis for comping these two models as,

$$H_0: \beta_{cyl} = \beta_{disp} = \beta_{hp} = \beta_{acc} = 0$$

The alternative is simply that at least one of the β_i from the null is not 0.

To perform this test in R we first define both models, then give them to the anova() commands.

```
null_mpg_model = lm(mpg ~ wt + year, data = autompg)
#full_mpg_model = lm(mpg ~ wt + year + cyl + disp + hp + acc, data = autompg)
full_mpg_model = lm(mpg ~ ., data = autompg)
anova(null_mpg_model, full_mpg_model)
```

```
## Analysis of Variance Table
##
## Model 1: mpg ~ wt + year
## Model 2: mpg ~ cyl + disp + hp + wt + acc + year
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 387 4556.6
## 2 383 4530.5 4 26.18 0.5533 0.6967
```

Here we have used the formula $mpg \sim .$ to define to full model. This is the same as the commented out line. Specifically, this a common shortcut in R which reads, "model mpg as the response with each of the remaining variables in the data frame as predictors."

Here we see that the value of the F statistic is 0.553, and the p-value is very large, so we fail to reject the null hypothesis at any reasonable α and say that none of cyl, disp, hp, and acc are significant with wt and year already in the model.

Again, we verify the sums of squares and degrees of freedom directly in R. You should match these to the table from R, and use this to match R's output to the written table above.

```
# SSDiff
sum((fitted(full_mpg_model) - fitted(null_mpg_model)) ^ 2)
```

```
## [1] 26.17981
```

```
# SSE (For Full)
sum(resid(full_mpg_model) ^ 2)

## [1] 4530.466

# SST (For Null)
sum(resid(null_mpg_model) ^ 2)

## [1] 4556.646

# Degrees of Freedom: Diff
length(coef(full_mpg_model)) - length(coef(null_mpg_model))

## [1] 4

# Degrees of Freedom: Full
length(resid(full_mpg_model)) - length(coef(full_mpg_model))

## [1] 383

# Degrees of Freedom: Null
length(resid(null_mpg_model)) - length(coef(null_mpg_model))

## [1] 387
```

5.5 Simulation

Since we ignored the derivation of certain results, we will again use simulation to convince ourselves of some of the above results. In particular, we will simulate samples of size $\tt n = 100$ from the model

$$Y_i = 5 + -2x_{i1} + 6x_{i2} + \epsilon_i, \qquad i = 1, 2, \dots, n$$

where $\epsilon_i \sim N(0, \sigma^2 = 16)$. Here we have two predictors, so p = 3.

```
set.seed(1337)
n = 100 # sample size
p = 3

beta_0 = 5
beta_1 = -2
beta_2 = 6
sigma = 4
```

As is the norm with regression, the x values are considered fixed and known quantities, so we will simulate those first, and they remain the same for the rest of the simulation study. Also note we create an x0 which is all 1, which we need to create our X matrix. If you look at the matrix formulation of regression, this unit vector of all 1s is a "predictor" that puts the intercept into the model. We also calculate the C matrix for later use.

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```
x0 = rep(1, n)
x1 = sample(seq(1, 10, length = n))
x2 = sample(seq(1, 10, length = n))
X = cbind(x0, x1, x2)
C = solve(t(X) %*% X)
```

We then simulate the response according the model above. Lastly, we place the two predictors and response into a data frame. Note that we do **not** place x0 in the data frame. This is a result of R adding an intercept by default.

```
eps = rnorm(n, mean = 0, sd = sigma)
y = beta_0 + beta_1 * x1 + beta_2 * x2 + eps
sim_data = data.frame(x1, x2, y)
```

Plotting this data and fitting the regression produces the following plot.



We then calculate

$$\hat{\beta} = \left(X^{\top} X \right)^{-1} X^{\top} y.$$

```
(beta_hat = C %*% t(X) %*% y)
```

```
##  [,1]
## x0  5.293609
## x1 -1.798593
## x2  5.775081
```

Notice that these values are the same as the coefficients found using lm() in R.

```
coef(lm(y \sim x1 + x2, data = sim_data))
```

```
## (Intercept) x1 x2
## 5.293609 -1.798593 5.775081
```

Also, these values are close to what we would expect.

```
c(beta_0, beta_1, beta_2)
```

```
## [1] 5 -2 6
```

We then calculated the fitted values in order to calculate s_e , which we see is the same as the sigma which is returned by summary().

```
y_hat = X %*% beta_hat
(s_e = sqrt(sum((y - y_hat) ^ 2) / (n - p)))
```

[1] 3.976044

```
summary(lm(y ~ x1 + x2, data = sim_data))$sigma
```

```
## [1] 3.976044
```

So far so good. Everything checks out. Now we will finally simulate from this model repeatedly in order to obtain an empirical distribution of $\hat{\beta}_2$.

We expect $\hat{\beta}_2$ to follow a normal distribution,

$$\hat{\beta}_2 \sim N\left(\beta_2, \sigma^2 C_{22}\right).$$

In this case,

$$\hat{\beta}_2 \sim N \left(\mu = 6, \sigma^2 = 16 \times 0.0014777 = 0.0236438 \right).$$

$$\hat{\beta}_2 \sim N \left(\mu = 6, \sigma^2 = 0.0236438 \right).$$

Note that C_{22} corresponds to the element in the **third** row and **third** column since R is indexed starting at 1, but we index the C matrix starting at 0 to match the diagonal elements to the corresponding β_j .

Note that C_{22} corresponds to the element in the **third** row and **third** column since β_2 is the **third** parameter in the model and because R is indexed starting at 1. However, we index the C matrix starting at 0 to match the diagonal elements to the corresponding β_i .

```
C[3, 3]
```

```
## [1] 0.00147774
```

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```
C[2 + 1, 2 + 1]
```

[1] 0.00147774

```
sigma ^ 2 * C[2 + 1, 2 + 1]
```

[1] 0.02364383

We now perform the simulation a large number of times. Each time, we update the y variable in the data frame, leaving the x variables the same. We then fit a model, and store $\hat{\beta}_2$.

We then see that the mean of the simulated values is close to the true value of β_2 .

```
mean(beta_hat_2)
```

[1] 5.99871

beta_2

[1] 6

We also see that the variance of the simulated values is close to the true variance of $\hat{\beta}_2$.

$$Var[\hat{\beta}_2] = \sigma^2 C_{22} = 16 \times 0.0014777 = 0.0236438$$

```
var(beta_hat_2)
```

[1] 0.02360853

```
sigma ^ 2 * C[2 + 1, 2 + 1]
```

[1] 0.02364383

The standard deviations found from the simulated data and the parent population are also very close.

```
sd(beta_hat_2)
```

```
## [1] 0.1536507
```

```
sqrt(sigma ^ 2 * C[2 + 1, 2 + 1])
```

[1] 0.1537655

Lastly, we plot a histogram of the simulated values, and overlay the true distribution.



This looks good! The simulation-based histogram appears to be Normal with mean 6 and spread of about 0.15 as you measure from center to inflection point. That matches really well with the sampling distribution of $\hat{\beta}_2 \sim N$ ($\mu = 6, \sigma^2 = 0.0236438$).

One last check, we verify the 68 - 95 - 99.7 rule.

```
sd_bh2 = sqrt(sigma ^ 2 * C[2 + 1, 2 + 1])
# We expect these to be: 0.68, 0.95, 0.997
mean(beta_2 - 1 * sd_bh2 < beta_hat_2 & beta_hat_2 < beta_2 + 1 * sd_bh2)

## [1] 0.6811

mean(beta_2 - 2 * sd_bh2 < beta_hat_2 & beta_hat_2 < beta_2 + 2 * sd_bh2)

## [1] 0.955

mean(beta_2 - 3 * sd_bh2 < beta_hat_2 & beta_hat_2 < beta_2 + 3 * sd_bh2)</pre>
```

```
## [1] 0.9972
```

Chapter 6

Categorical Predictors and Interactions

"The greatest value of a picture is when it forces us to notice what we never expected to see."

— John Tukey

After reading this chapter you will be able to:

- Include and interpret categorical variables in a linear regression model by way of dummy variables.
- Understand the implications of using a model with a categorical variable in two ways: levels serving as unique predictors versus levels serving as a comparison to a baseline.
- Construct and interpret linear regression models with interaction terms.
- Identify categorical variables in a data set and convert them into factor variables, if necessary, using R.

So far in each of our analyses, we have only used numeric variables as predictors. We have also only used additive models, meaning the effect any predictor had on the response was not dependent on the other predictors. In this chapter, we will remove both of these restrictions. We will fit models with categorical predictors, and use models that allow predictors to interact. The mathematics of multiple regression will remain largely unchanging, however, we will pay close attention to interpretation, as well as some difference in R usage.

6.1 Dummy Variables

For this chapter, we will briefly use the built in dataset mtcars before returning to our autompg dataset that we created in the last chapter. The mtcars dataset is somewhat smaller, so we'll quickly take a look at the entire dataset.

mtcars

```
##
                        mpg cyl disp hp drat
                                                  wt qsec vs am gear carb
## Mazda RX4
                              6 160.0 110 3.90 2.620 16.46
                              6 160.0 110 3.90 2.875 17.02
                                                                          4
## Mazda RX4 Wag
                       21.0
## Datsun 710
                       22.8
                              4 108.0 93 3.85 2.320 18.61
                                                                          1
                       21.4
## Hornet 4 Drive
                              6 258.0 110 3.08 3.215 19.44
                                                                          1
```

```
## Hornet Sportabout
                      18.7
                             8 360.0 175 3.15 3.440 17.02
                             6 225.0 105 2.76 3.460 20.22
                                                                  3
                                                                       1
## Valiant
                      18.1
                                                          1
                                                             0
## Duster 360
                      14.3
                             8 360.0 245 3.21 3.570 15.84
                                                                       4
                                                                       2
## Merc 240D
                      24.4
                             4 146.7 62 3.69 3.190 20.00
                                                                  4
## Merc 230
                      22.8
                             4 140.8 95 3.92 3.150 22.90
                                                                  4
                                                                       2
## Merc 280
                      19.2
                             6 167.6 123 3.92 3.440 18.30
                                                                  4
                                                                       4
                                                             0
## Merc 280C
                             6 167.6 123 3.92 3.440 18.90
                      17.8
                             8 275.8 180 3.07 4.070 17.40
                                                                  3
## Merc 450SE
                      16.4
                                                          0
                                                             0
                                                                       3
## Merc 450SL
                      17.3
                             8 275.8 180 3.07 3.730 17.60
                                                          0
                                                             0
                                                                  3
                                                                       3
                                                                  3
## Merc 450SLC
                      15.2
                             8 275.8 180 3.07 3.780 18.00
                                                             Ω
                                                                       3
## Cadillac Fleetwood 10.4
                             8 472.0 205 2.93 5.250 17.98
                                                                  3
                                                                       4
## Lincoln Continental 10.4
                             8 460.0 215 3.00 5.424 17.82
                                                                  3
                                                                       4
                                                          0
                                                             0
## Chrysler Imperial 14.7
                             8 440.0 230 3.23 5.345 17.42
                                                          0
                                                             0
                                                                  3
                                                                       4
## Fiat 128
                      32.4
                                                                  4
                             4 78.7
                                      66 4.08 2.200 19.47
                                                                       1
## Honda Civic
                      30.4
                             4 75.7
                                      52 4.93 1.615 18.52
                                                                  4
                                                                       2
                                                          1
                                                             1
## Toyota Corolla
                      33.9
                             4 71.1
                                      65 4.22 1.835 19.90
                                                           1
                                                                  4
                                                                       1
                             4 120.1 97 3.70 2.465 20.01
                                                                  3
## Toyota Corona
                      21.5
                                                          1
                                                             Ω
                                                                       1
## Dodge Challenger
                      15.5
                             8 318.0 150 2.76 3.520 16.87
                                                                  3
                                                                       2
## AMC Javelin
                             8 304.0 150 3.15 3.435 17.30
                                                                  3
                                                                       2
                      15.2
                                                          0
                                                             0
                                                                  3
## Camaro Z28
                      13.3
                             8 350.0 245 3.73 3.840 15.41
                                                                       4
## Pontiac Firebird 19.2
                             8 400.0 175 3.08 3.845 17.05
                                                          0
                                                             0
                                                                  3
                                                                       2
## Fiat X1-9
                    27.3
                             4 79.0 66 4.08 1.935 18.90
                                                                       1
                    26.0
## Porsche 914-2
                             4 120.3 91 4.43 2.140 16.70
                                                                  5
                                                                       2
                                                          0 1
## Lotus Europa
                      30.4
                            4 95.1 113 3.77 1.513 16.90
                                                                  5
                                                                       2
                                                                  5
                                                                       4
## Ford Pantera L
                      15.8 8 351.0 264 4.22 3.170 14.50
                                                          0 1
## Ferrari Dino
                      19.7
                             6 145.0 175 3.62 2.770 15.50
                                                          0 1
                                                                  5
                                                                       6
## Maserati Bora
                      15.0 8 301.0 335 3.54 3.570 14.60
                                                                  5
                                                                       8
                                                          0 1
                      21.4 4 121.0 109 4.11 2.780 18.60 1 1
                                                                       2
## Volvo 142E
```

We will be interested in three of the variables: mpg, hp, and am.

- mpg: fuel efficiency, in miles per gallon.
- hp: horsepower, in foot-pounds per second.
- am: transmission. Automatic or manual.

As we often do, we will start by plotting the data. We are interested in mpg as the response variable, and hp as a predictor.

```
plot(mpg ~ hp, data = mtcars, col = am + 1, pch = am + 1, cex = 2)
```



We used a common R "trick" when plotting this data. The am variable takes two possible values; 0 for automatic transmission, and 1 for manual transmissions. R can use numbers to represent colors, however the color for 0 is white. So we take the am vector and add 1 to it. Then observations with automatic transmissions are now represented by 1, which is black in R, and manual transmission are represented by 2, which is red in R. (Note, we are only adding 1 inside the call to plot(), we are not actually modifying the values stored in am.)

We now fit the SLR model

$$Y = \beta_0 + \beta_1 x_1 + \epsilon,$$

where Y is mpg and x_1 is hp. For notational brevity, we drop the index i for observations.

```
mpg_hp_slr = lm(mpg ~ hp, data = mtcars)
```

We then re-plot the data and add the fitted line to the plot.

```
plot(mpg ~ hp, data = mtcars, col = am + 1, pch = am + 1, cex = 2)
abline(mpg_hp_slr, lwd = 2, col = "green")
```



We should notice a pattern here. The red, manual observations largely fall above the line, while the black, automatic observations are mostly below the line. This means our model underestimates the fuel efficiency of manual transmissions, and overestimates the fuel efficiency of automatic transmissions. To correct for this, we will add a predictor to our model, namely, am as x_2 .

Our new model is

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon,$$

where x_1 and Y remain the same, but now

$$x_2 = \begin{cases} 1 & \text{manual transmission} \\ 0 & \text{automatic transmission} \end{cases}.$$

In this case, we call x_2 a **dummy variable**. A dummy variable is somewhat unfortunately named, as it is in no way "dumb". In fact, it is actually somewhat clever. A dummy variable is a numerical variable that is used in a regression analysis to "code" for a binary categorical variable. Let's see how this works.

First, note that am is already a dummy variable, since it uses the values 0 and 1 to represent automatic and manual transmissions. Often, a variable like am would store the character values auto and man and we would either have to convert these to 0 and 1, or, as we will see later, R will take care of creating dummy variables for us.

So, to fit the above model, we do so like any other multiple regression model we have seen before.

Briefly checking the output, we see that R has estimated the three β parameters.

mpg_hp_add

```
##
## Call:
## lm(formula = mpg ~ hp + am, data = mtcars)
##
## Coefficients:
## (Intercept) hp am
## 26.58491 -0.05889 5.27709
```

Since x_2 can only take values 0 and 1, we can effectively write two different models, one for manual and one for automatic transmissions.

For automatic transmissions, that is $x_2 = 0$, we have,

$$Y = \beta_0 + \beta_1 x_1 + \epsilon.$$

Then for manual transmissions, that is $x_2 = 1$, we have,

$$Y = (\beta_0 + \beta_2) + \beta_1 x_1 + \epsilon.$$

Notice that these models share the same slope, β_1 , but have different intercepts, differing by β_2 . So the change in mpg is the same for both models, but on average mpg differs by β_2 between the two transmission types.

We'll now calculate the estimated slope and intercept of these two models so that we can add them to a plot. Note that:

```
• \hat{\beta}_0 = \text{coef(mpg_hp_add)}[1] = 26.5849137
• \hat{\beta}_1 = \text{coef(mpg_hp_add)}[2] = -0.0588878
• \hat{\beta}_2 = \text{coef(mpg_hp_add)}[3] = 5.2770853
```

We can then combine these to calculate the estimated slope and intercepts.

```
int_auto = coef(mpg_hp_add)[1]
int_manu = coef(mpg_hp_add)[1] + coef(mpg_hp_add)[3]

slope_auto = coef(mpg_hp_add)[2]
slope_manu = coef(mpg_hp_add)[2]
```

Re-plotting the data, we use these slopes and intercepts to add the "two" fitted models to the plot.

```
plot(mpg ~ hp, data = mtcars, col = am + 1, pch = am + 1, cex = 2)
abline(int_auto, slope_auto, col = 1, lty = 1, lwd = 2) # add line for auto
abline(int_manu, slope_manu, col = 2, lty = 2, lwd = 2) # add line for manual
```



We notice right away that the points are no longer systematically incorrect. The red, manual observations vary about the red line in no particular pattern without underestimating the observations as before. The black, automatic points vary about the black line, also without an obvious pattern.

They say a picture is worth a thousand words, but as a statistician, sometimes a picture is worth an entire analysis. The above picture makes it plainly obvious that β_2 is significant, but let's verify mathematically. Essentially we would like to test:

$$H_0: \beta_2 = 0$$
 vs $H_1: \beta_2 \neq 0$.

This is nothing new. Again, the math is the same as the multiple regression analyses we have seen before. We could perform either a t or F test here. The only difference is a slight change in interpretation. We could think of this as testing a model with a single line (H_0) against a model that allows two lines (H_1) .

To obtain the test statistic and p-value for the t-test, we would use

```
summary(mpg_hp_add)$coef[3,]
```

```
## Estimate Std. Error t value Pr(>|t|)
## 5.27708530818 1.07954057578 4.88826953480 0.00003460318
```

To do the same for the F test, we would use

```
anova(mpg_hp_slr, mpg_hp_add)
```

```
## Analysis of Variance Table
##
## Model 1: mpg ~ hp
## Model 2: mpg ~ hp + am
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 30 447.67
```

6.2. INTERACTIONS

```
## 2 29 245.44 1 202.24 23.895 0.0000346 ***

## ---

## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' ' 1
```

Notice that these are indeed testing the same thing, as the p-values are exactly equal. (And the F test statistic is the t test statistic squared.)

Recapping some interpretations:

- $\hat{\beta}_0 = 26.5849137$ is the estimated average mpg for a car with an automatic transmission and **0** hp.
- $\hat{\beta}_0 + \hat{\beta}_2 = 31.8619991$ is the estimated average mpg for a car with a manual transmission and **0** hp.
- $\hat{\beta}_2 = 5.2770853$ is the estimated **difference** in average mpg for cars with manual transmissions as compared to those with automatic transmission, for **any** hp.
- $\hat{\beta}_1 = -0.0588878$ is the estimated change in average mpg for an increase in one hp, for either transmission types.

We should take special notice of those last two. In the model,

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon,$$

we see β_1 is the average change in Y for an increase in x_1 , no matter the value of x_2 . Also, β_2 is always the difference in the average of Y for any value of x_1 . These are two restrictions we won't always want, so we need a way to specify a more flexible model.

Here we restricted ourselves to a single numerical predictor x_1 and one dummy variable x_2 . However, the concept of a dummy variable can be used with larger multiple regression models. We only use a single numerical predictor here for ease of visualization since we can think of the "two lines" interpretation. But in general, we can think of a dummy variable as creating "two models," one for each category of a binary categorical variable.

6.2 Interactions

To remove the "same slope" restriction, we will now discuss **interaction**. To illustrate this concept, we will return to the **autompg** dataset we created in the last chapter, with a few more modifications.

```
# read data frame from the web
autompg = read.table(
   "http://archive.ics.uci.edu/ml/machine-learning-databases/auto-mpg/auto-mpg.data",
   quote = "\"",
   comment.char = "",
   stringsAsFactors = FALSE)
# give the dataframe headers
colnames(autompg) = c("mpg", "cyl", "disp", "hp", "wt", "acc", "year", "origin", "name")
# remove missing data, which is stored as "?"
autompg = subset(autompg, autompg$hp != "?")
# remove the plymouth reliant, as it causes some issues
autompg = subset(autompg, autompg$name != "plymouth reliant")
# give the dataset row names, based on the engine, year and name
rownames(autompg) = paste(autompg$cyl, "cylinder", autompg$year, autompg$name)
# remove the variable for name, as will as origin
```

```
autompg = subset(autompg, select = c("mpg", "cyl", "disp", "hp", "wt", "acc", "year", "origin"))
# change horsepower from character to numeric
autompg$hp = as.numeric(autompg$hp)
# create a dummary variable for foreign vs domestic cars. domestic = 1.
autompg$domestic = as.numeric(autompg$origin == 1)
# remove 3 and 5 cylinder cars (which are very rare.)
autompg = autompg[autompg$cyl != 5,]
autompg = autompg[autompg$cyl != 3,]
# the following line would verify the remaining cylinder possibilities are 4, 6, 8
#unique(autompg$cyl)
# change cyl to a factor variable
autompg$cyl = as.factor(autompg$cyl)
```

str(autompg)

```
## 'data.frame':
                   383 obs. of 9 variables:
## $ mpg
          : num 18 15 18 16 17 15 14 14 14 15 ...
             : Factor w/ 3 levels "4", "6", "8": 3 3 3 3 3 3 3 3 3 3 ...
## $ cyl
## $ disp
             : num 307 350 318 304 302 429 454 440 455 390 ...
## $ hp
             : num 130 165 150 150 140 198 220 215 225 190 ...
## $ wt
             : num 3504 3693 3436 3433 3449 ...
## $ acc
             : num 12 11.5 11 12 10.5 10 9 8.5 10 8.5 ...
             : int 70 70 70 70 70 70 70 70 70 70 ...
## $ year
## $ origin : int 1 1 1 1 1 1 1 1 1 ...
## $ domestic: num 1 1 1 1 1 1 1 1 1 ...
```

We've removed cars with 3 and 5 cylinders, as well as created a new variable domestic which indicates whether or not a car was built in the United States. Removing the 3 and 5 cylinders is simply for ease of demonstration later in the chapter and would not be done in practice. The new variable domestic takes the value 1 if the car was built in the United States, and 0 otherwise, which we will refer to as "foreign." (We are arbitrarily using the United States as the reference point here.) We have also made cyl and origin into factor variables, which we will discuss later.

We'll now be concerned with three variables: mpg, disp, and domestic. We will use mpg as the response. We can fit a model,

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon,$$

where

- Y is mpg, the fuel efficiency in miles per gallon,
- x_1 is disp, the displacement in cubic inches,
- x_2 is domestic as described above, which is a dummy variable.

We will fit this model, extract the slope and intercept for the "two lines," plot the data and add the lines.

```
mpg_disp_add = lm(mpg ~ disp + domestic, data = autompg)
int_for = coef(mpg_disp_add)[1]
int_dom = coef(mpg_disp_add)[1] + coef(mpg_disp_add)[3]
slope_for = coef(mpg_disp_add)[2]
```

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```
slope_dom = coef(mpg_disp_add)[2]

plot(mpg ~ disp, data = autompg, col = domestic + 1, pch = domestic + 1)
abline(int_for, slope_for, col = 1, lty = 1, lwd = 2) # add line for foreign cars
abline(int_dom, slope_dom, col = 2, lty = 2, lwd = 2) # add line for domestic cars
```



This is a model that allows for two *parallel* lines, meaning the mpg can be different on average between foreign and domestic cars of the same engine displacement, but the change in average mpg for an increase in displacement is the same for both. We can see this model isn't doing very well here. The red line fits the red points fairly well, but the black line isn't doing very well for the black points, it should clearly have a more negative slope. Essentially, we would like a model that allows for two different slopes.

Consider the following model,

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon,$$

where x_1 , x_2 , and Y are the same as before, but we have added a new **interaction** term x_1x_2 which multiplies x_1 and x_2 , so we also have an additional β parameter β_3 .

This model essentially creates two slopes and two intercepts, β_2 being the difference in intercepts and β_3 being the difference in slopes. To see this, we will break down the model into the two "sub-models" for foreign and domestic cars.

For foreign cars, that is $x_2 = 0$, we have

$$Y = \beta_0 + \beta_1 x_1 + \epsilon.$$

For domestic cars, that is $x_2 = 1$, we have

$$Y = (\beta_0 + \beta_2) + (\beta_1 + \beta_3)x_1 + \epsilon.$$

These two models have both different slopes and intercepts.

- β_0 is the average mpg for a foreign car with **0** disp.
- β_1 is the change in average mpg for an increase of one disp, for foreign cars.
- $\beta_0 + \beta_2$ is the average mpg for a domestic car with **0** disp.
- $\beta_1 + \beta_3$ is the change in average mpg for an increase of one disp, for domestic cars.

How do we fit this model in R? There are a number of ways.

One method would be to simply create a new variable, then fit a model like any other.

```
autompg$x3 = autompg$disp * autompg$domestic # THIS CODE NOT RUN!
do_not_do_this = lm(mpg ~ disp + domestic + x3, data = autompg) # THIS CODE NOT RUN!
```

You should only do this as a last resort. We greatly prefer not to have to modify our data simply to fit a model. Instead, we can tell R we would like to use the existing data with an interaction term, which it will create automatically when we use the : operator.

```
mpg_disp_int = lm(mpg ~ disp + domestic + disp:domestic, data = autompg)
```

An alternative method, which will fit the exact same model as above would be to use the * operator. This method automatically creates the interaction term, as well as any "lower order terms," which in this case are the first order terms for disp and domestic

```
mpg\_disp\_int2 = lm(mpg \sim disp * domestic, data = autompg)
```

We can quickly verify that these are the doing the same thing.

```
coef(mpg_disp_int)
##
     (Intercept)
                           disp
                                      domestic disp:domestic
##
      46.0548423
                     -0.1569239
                                   -12.5754714
                                                    0.1025184
coef(mpg_disp_int2)
##
     (Intercept)
                           disp
                                      domestic disp:domestic
      46.0548423
                     -0.1569239
                                   -12.5754714
                                                    0.1025184
##
```

We see that both the variables, and their coefficient estimates are indeed the same for both models.

```
summary(mpg_disp_int)
```

```
##
## Call:
## lm(formula = mpg ~ disp + domestic + disp:domestic, data = autompg)
##
## Residuals:
##
        Min
                  1Q
                       Median
                                     3Q
                                             Max
## -10.8332 -2.8956 -0.8332
                                 2.2828
                                         18.7749
##
## Coefficients:
                  Estimate Std. Error t value Pr(>|t|)
##
```

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```
## (Intercept)
                 46.05484
                            1.80582 25.504 < 2e-16 ***
## disp
                 -0.15692
                            0.01668 -9.407 < 2e-16 ***
## domestic
                -12.57547
                             1.95644 -6.428 3.90e-10 ***
                  0.10252
                             0.01692
                                      6.060 3.29e-09 ***
## disp:domestic
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 4.308 on 379 degrees of freedom
## Multiple R-squared: 0.7011, Adjusted R-squared: 0.6987
## F-statistic: 296.3 on 3 and 379 DF, p-value: < 2.2e-16
```

We see that using summary() gives the usual output for a multiple regression model. We pay close attention to the row for disp:domestic which tests,

$$H_0: \beta_3 = 0.$$

In this case, testing for $\beta_3 = 0$ is testing for two lines with parallel slopes versus two lines with possibly different slopes. The disp:domestic line in the summary() output uses a t-test to perform the test.

We could also use an ANOVA F-test. The additive model, without interaction is our null model, and the interaction model is the alternative.

```
anova(mpg_disp_add, mpg_disp_int)
```

```
## Analysis of Variance Table
##
## Model 1: mpg ~ disp + domestic
## Model 2: mpg ~ disp + domestic + disp:domestic
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 380 7714.0
## 2 379 7032.6 1 681.36 36.719 3.294e-09 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

Again we see this test has the same p-value as the t-test. Also the p-value is extremely low, so between the two, we choose the interaction model.

```
int_for = coef(mpg_disp_int)[1]
int_dom = coef(mpg_disp_int)[1] + coef(mpg_disp_int)[3]

slope_for = coef(mpg_disp_int)[2]
slope_dom = coef(mpg_disp_int)[2] + coef(mpg_disp_int)[4]
```

Here we again calculate the slope and intercepts for the two lines for use in plotting.

```
plot(mpg ~ disp, data = autompg, col = domestic + 1, pch = domestic + 1)
abline(int_for, slope_for, col = 1, lty = 1, lwd = 2) # add line for foreign cars
abline(int_dom, slope_dom, col = 2, lty = 2, lwd = 2) # add line for domestic cars
```



We see that these lines fit the data much better, which matches the result of our tests.

So far we have only seen interaction between a categorical variable (domestic) and a numerical variable (disp). While this is easy to visualize, since it allows for different slopes for two lines, it is not the only type of interaction we can use in a model. We can also consider interactions between two numerical variables.

Consider the model,

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon,$$

where

- Y is mpg, the fuel efficiency in miles per gallon,
- x_1 is disp, the displacement in cubic inches,
- x_2 is hp, the horsepower, in foot-pounds per second.

How does mpg change based on disp in this model? We can rearrange some terms to see how.

$$Y = \beta_0 + (\beta_1 + \beta_3 x_2) x_1 + \beta_2 x_2 + \epsilon$$

So, for a one unit increase in x_1 (disp), the mean of Y (mpg) increases $\beta_1 + \beta_3 x_2$, which is a different value depending on the value of x_2 (hp)!

Since we're now working in three dimensions, this model can't be easily justified via visualizations like the previous example. Instead, we will have to rely on a test.

```
mpg_disp_add_hp = lm(mpg ~ disp + hp, data = autompg)
mpg_disp_int_hp = lm(mpg ~ disp * hp, data = autompg)
summary(mpg_disp_int_hp)
```

##

Call:

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```
## lm(formula = mpg ~ disp * hp, data = autompg)
##
## Residuals:
##
       \mathtt{Min}
                 1Q
                     Median
                                    ЗQ
                                           Max
## -10.7849 -2.3104 -0.5699
                               2.1453
##
## Coefficients:
##
                 Estimate Std. Error t value Pr(>|t|)
## (Intercept) 52.40819978 1.52272673
                                        34.42
                                                 <2e-16 ***
              -0.10017377 0.00663825
                                      -15.09
                                                 <2e-16 ***
## hp
              -0.21981997 0.01986944 -11.06
                                                 <2e-16 ***
               0.00056583 0.00005165
## disp:hp
                                       10.96
                                                 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.896 on 379 degrees of freedom
## Multiple R-squared: 0.7554, Adjusted R-squared: 0.7535
## F-statistic: 390.2 on 3 and 379 DF, p-value: < 2.2e-16
```

Using summary() we focus on the row for disp:hp which tests,

$$H_0: \beta_3 = 0.$$

Again, we see a very low p-value so we reject the null (additive model) in favor of the interaction model. Again, there is an equivalent F-test.

```
anova(mpg_disp_add_hp, mpg_disp_int_hp)
```

```
## Analysis of Variance Table
##
## Model 1: mpg ~ disp + hp
## Model 2: mpg ~ disp * hp
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 380 7576.6
## 2 379 5754.2 1 1822.3 120.03 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1</pre>
```

We can take a closer look at the coefficients of our fitted interaction model.

```
coef(mpg_disp_int_hp)
```

```
## (Intercept) disp hp disp:hp
## 52.4081997848 -0.1001737655 -0.2198199720 0.0005658269
```

- $\hat{\beta}_0 = 52.4081998$ is the estimated average mpg for a car with 0 disp and 0 hp.
- $\hat{\beta}_1 = -0.1001738$ is the estimated change in average mpg for an increase in 1 disp, for a car with 0 hp.
- $\hat{\beta}_2 = -0.21982$ is the estimated change in average mpg for an increase in 1 hp, for a car with 0 disp.
- $\hat{\beta}_3 = 0.0005658$ is an estimate of the modification to the change in average mpg for an increase in disp, for a car of a certain hp (or vice versa).

That last coefficient needs further explanation. Recall the rearrangement we made earlier

$$Y = \beta_0 + (\beta_1 + \beta_3 x_2) x_1 + \beta_2 x_2 + \epsilon.$$

So, our estimate for $\beta_1 + \beta_3 x_2$, is $\hat{\beta}_1 + \hat{\beta}_3 x_2$, which in this case is

$$-0.1001738 + 0.0005658x_2$$
.

This says that, for an increase of one disp we see an estimated change in average mpg of $-0.1001738 + 0.0005658x_2$. So how disp and mpg are related, depends on the hp of the car.

So for a car with 50 hp, the estimated change in average mpg for an increase of one disp is

$$-0.1001738 + 0.000565850 = -0.0718824$$

And for a car with 350 hp, the estimated change in average mpg for an increase of one disp is

$$-0.1001738 + 0.0005658350 = 0.0978657$$

Notice the sign changed!

6.3 Factor Variables

So far in this chapter, we have limited our use of categorical variables to binary categorical variables. Specifically, we have limited ourselves to dummy variables which take a value of 0 or 1 and represent a categorical variable numerically.

We will now discuss **factor** variables, which is a special way that R deals with categorical variables. With factor variables, a human user can simply think about the categories of a variable, and R will take care of the necessary dummy variables without any 0/1 assignment being done by the user.

```
is.factor(autompg$domestic)
```

```
## [1] FALSE
```

Earlier when we used the domestic variable, it was **not** a factor variable. It was simply a numerical variable that only took two possible values, 1 for domestic, and 0 for foreign. Let's create a new variable origin that stores the same information, but in a different way.

```
autompg$origin[autompg$domestic == 1] = "domestic"
autompg$origin[autompg$domestic == 0] = "foreign"
head(autompg$origin)
```

```
## [1] "domestic" "domestic" "domestic" "domestic" "domestic"
```

Now the origin variable stores "domestic" for domestic cars and "foreign" for foreign cars.

```
is.factor(autompg$origin)
```

[1] FALSE

However, this is simply a vector of character values. A vector of car models is a character variable in R. A vector of Vehicle Identification Numbers (VINs) is a character variable as well. But those don't represent a short list of levels that might influence a response variable. We will want to **coerce** this origin variable to be something more: a factor variable.

```
autompg$origin = as.factor(autompg$origin)
```

Now when we check the structure of the autompg dataset, we see that origin is a factor variable.

str(autompg)

```
'data.frame':
                   383 obs. of 9 variables:
             : num 18 15 18 16 17 15 14 14 14 15 ...
   $ mpg
             : Factor w/ 3 levels "4", "6", "8": 3 3 3 3 3 3 3 3 3 ...
   $ cyl
   $ disp
             : num 307 350 318 304 302 429 454 440 455 390 ...
             : num 130 165 150 150 140 198 220 215 225 190 ...
##
   $ hp
##
             : num 3504 3693 3436 3433 3449 ...
   $ wt
             : num 12 11.5 11 12 10.5 10 9 8.5 10 8.5 ...
##
  $ acc
             : int 70 70 70 70 70 70 70 70 70 70 ...
  $ year
   $ origin : Factor w/ 2 levels "domestic", "foreign": 1 1 1 1 1 1 1 1 1 1 ...
   $ domestic: num 1 1 1 1 1 1 1 1 1 ...
```

Factor variables have **levels** which are the possible values (categories) that the variable may take, in this case foreign or domestic.

```
levels(autompg$origin)
```

```
## [1] "domestic" "foreign"
```

Recall that previously we have fit the model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon,$$

where

- Y is mpg, the fuel efficiency in miles per gallon,
- x_1 is disp, the displacement in cubic inches,
- x_2 is domestic a dummy variable where 1 indicates a domestic car.

```
(mod_dummy = lm(mpg ~ disp * domestic, data = autompg))
```

```
##
## Call:
## lm(formula = mpg ~ disp * domestic, data = autompg)
##
## Coefficients:
## (Intercept) disp domestic disp:domestic
## 46.0548 -0.1569 -12.5755 0.1025
```

So here we see that

$$\hat{\beta}_0 + \hat{\beta}_2 = 46.0548423 + -12.5754714 = 33.4793709$$

is the estimated average mpg for a domestic car with 0 disp.

Now let's try to do the same, but using our new factor variable.

```
(mod_factor = lm(mpg ~ disp * origin, data = autompg))
```

```
##
## Call:
## lm(formula = mpg ~ disp * origin, data = autompg)
##
## Coefficients:
## (Intercept) disp originforeign disp:originforeign
## 33.47937 -0.05441 12.57547 -0.10252
```

It seems that it doesn't produce the same results. Right away we notice that the intercept is different, as is the the coefficient in front of disp. We also notice that the remaining two coefficients are of the same magnitude as their respective counterparts using the domestic variable, but with a different sign. Why is this happening?

It turns out, that by using a factor variable, R is automatically creating a dummy variable for us. However, it is not the dummy variable that we had originally used ourselves.

R is fitting the model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon,$$

where

- Y is mpg, the fuel efficiency in miles per gallon,
- x_1 is disp, the displacement in cubic inches,
- x_2 is a dummy variable create by R. It uses 1 to represent a foreign car.

So now,

$$\hat{\beta}_0 = 33.4793709$$

is the estimated average mpg for a domestic car with 0 disp, which is indeed the same as before.

When R created x_2 , the dummy variable, it used domestic cars as the **reference** level, that is the default value of the factor variable. So when the dummy variable is 0, the model represents this reference level, which is domestic. (R makes this choice because domestic comes before foreign alphabetically.)

So the two models have different estimated coefficients, but due to the different model representations, they are actually the same model.

6.3.1 Factors with More Than Two Levels

Let's now consider a factor variable with more than two levels. In this dataset, cyl is an example.

```
is.factor(autompg$cyl)
```

[1] TRUE

```
levels(autompg$cyl)
```

```
## [1] "4" "6" "8"
```

Here the cyl variable has three possible levels: 4, 6, and 8. You may wonder, why not simply use cyl as a numerical variable? You certainly could.

However, that would force the difference in average mpg between 4 and 6 cylinders to be the same as the difference in average mpg between 6 and 8 cylinders. That usually make senses for a continuous variable, but not for a discrete variable with so few possible values. In the case of this variable, there is no such thing as a 7-cylinder engine or a 6.23-cylinder engine in personal vehicles. For these reasons, we will simply consider cyl to be categorical. This is a decision that will commonly need to be made with ordinal variables. Often, with a large number of categories, the decision to treat them as numerical variables is appropriate because a large number of dummy variables are then needed to represent these variables.

Let's define three dummy variables related to the cyl factor variable.

$$v_1 = \begin{cases} 1 & 4 \text{ cylinder} \\ 0 & \text{not 4 cylinder} \end{cases}$$

$$v_2 = \begin{cases} 1 & 6 \text{ cylinder} \\ 0 & \text{not 6 cylinder} \end{cases}$$

$$v_3 = \begin{cases} 1 & 8 \text{ cylinder} \\ 0 & \text{not 8 cylinder} \end{cases}$$

Now, let's fit an additive model in R, using mpg as the response, and disp and cyl as predictors. This should be a model that uses "three regression lines" to model mpg, one for each of the possible cyl levels. They will all have the same slope (since it is an additive model), but each will have its own intercept.

```
(mpg_disp_add_cyl = lm(mpg ~ disp + cyl, data = autompg))
```

```
##
## Call:
## lm(formula = mpg ~ disp + cyl, data = autompg)
##
## Coefficients:
## (Intercept) disp cyl6 cyl8
## 34.99929 -0.05217 -3.63325 -2.03603
```

The question is, what is the model that R has fit here? It has chosen to use the model

$$Y = \beta_0 + \beta_1 x + \beta_2 v_2 + \beta_3 v_3 + \epsilon,$$

where

- Y is mpg, the fuel efficiency in miles per gallon,
- x is disp, the displacement in cubic inches,
- v_2 and v_3 are the dummy variables define above.

Why doesn't R use v_1 ? Essentially because it doesn't need to. To create three lines, it only needs two dummy variables since it is using a reference level, which in this case is a 4 cylinder car. The three "sub models" are then:

```
    4 Cylinder: Y = β<sub>0</sub> + β<sub>1</sub>x + ε
    6 Cylinder: Y = (β<sub>0</sub> + β<sub>2</sub>) + β<sub>1</sub>x + ε
    8 Cylinder: Y = (β<sub>0</sub> + β<sub>3</sub>) + β<sub>1</sub>x + ε
```

Notice that they all have the same slope. However, using the two dummy variables, we achieve the three intercepts.

- β_0 is the average mpg for a 4 cylinder car with 0 disp.
- $\beta_0 + \beta_2$ is the average mpg for a 6 cylinder car with 0 disp.
- $\beta_0 + \beta_3$ is the average mpg for a 8 cylinder car with 0 disp.

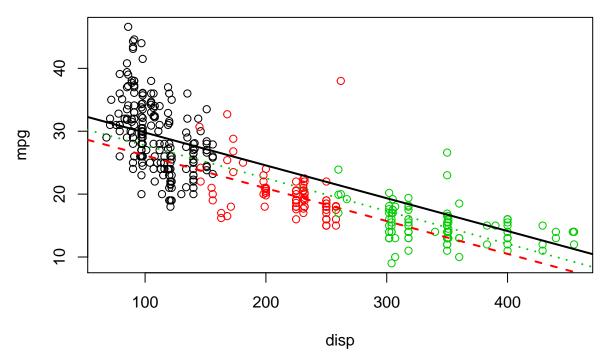
So because 4 cylinder is the reference level, β_0 is specific to 4 cylinders, but β_2 and β_3 are used to represent quantities relative to 4 cylinders.

As we have done before, we can extract these intercepts and slopes for the three lines, and plot them accordingly.

```
int_4cyl = coef(mpg_disp_add_cyl)[1]
int_6cyl = coef(mpg_disp_add_cyl)[1] + coef(mpg_disp_add_cyl)[3]
int_8cyl = coef(mpg_disp_add_cyl)[1] + coef(mpg_disp_add_cyl)[4]

slope_all_cyl = coef(mpg_disp_add_cyl)[2]

plot(mpg ~ disp, data = autompg, col = cyl)
abline(int_4cyl, slope_all_cyl, col = 1, lty = 1, lwd = 2)
abline(int_6cyl, slope_all_cyl, col = 2, lty = 2, lwd = 2)
abline(int_8cyl, slope_all_cyl, col = 3, lty = 3, lwd = 2)
```



On this plot, we have

- 4 Cylinder: black dots, solid black line.
- 6 Cylinder: red dots, dashed red line.
- 8 Cylinder: green dots, dotted green line.

The odd result here is that we're estimating that 8 cylinder cars have better fuel efficiency than 6 cylinder cars at **any** displacement! The dotted green line is always above the dashed red line. That doesn't seem right. Maybe for very large displacement engines that could be true, but that seems wrong for medium to low displacement.

To attempt to fix this, we will try using an interaction model, that is, instead of simply three intercepts and one slope, we will allow for three slopes. Again, we'll let R take the wheel, (no pun intended) then figure out what model it has applied.

```
(mpg_disp_int_cyl = lm(mpg ~ disp * cyl, data = autompg))
```

```
##
## Call:
## lm(formula = mpg ~ disp * cyl, data = autompg)
##
## Coefficients:
##
   (Intercept)
                        disp
                                       cyl6
                                                    cyl8
                                                             disp:cyl6
                                                                           disp:cyl8
##
      43.59052
                    -0.13069
                                 -13.20026
                                               -20.85706
                                                               0.08299
                                                                             0.10817
```

```
\# could also use mpg \sim disp + cyl + disp:cyl
```

R has again chosen to use 4 cylinder cars as the reference level, but this also now has an effect on the interaction terms. R has fit the model.

$$Y = \beta_0 + \beta_1 x + \beta_2 v_2 + \beta_3 v_3 + \gamma_2 x v_2 + \gamma_3 x v_3 + \epsilon$$

We're using γ like a β parameter for simplicity, so that, for example β_2 and γ_2 are both associated with v_2 . Now, the three "sub models" are:

```
4 Cylinder: Y = β<sub>0</sub> + β<sub>1</sub>x + ε.
6 Cylinder: Y = (β<sub>0</sub> + β<sub>2</sub>) + (β<sub>1</sub> + γ<sub>2</sub>)x + ε.
8 Cylinder: Y = (β<sub>0</sub> + β<sub>3</sub>) + (β<sub>1</sub> + γ<sub>3</sub>)x + ε.
```

Interpreting some parameters and coefficients then:

- $(\beta_0 + \beta_2)$ is the average mpg of a 6 cylinder car with 0 disp
- $(\hat{\beta}_1 + \hat{\gamma}_3) = -0.1306935 + 0.1081714 = -0.0225221$ is the estimated change in average mpg for an increase of one disp, for an 8 cylinder car.

So, as we have seen before β_2 and β_3 change the intercepts for 6 and 8 cylinder cars relative to the reference level of β_0 for 4 cylinder cars.

Now, similarly γ_2 and γ_3 change the slopes for 6 and 8 cylinder cars relative to the reference level of β_1 for 4 cylinder cars.

Once again, we extract the coefficients and plot the results.

```
int_4cyl = coef(mpg_disp_int_cyl)[1]
int_6cyl = coef(mpg_disp_int_cyl)[1] + coef(mpg_disp_int_cyl)[3]
int_8cyl = coef(mpg_disp_int_cyl)[1] + coef(mpg_disp_int_cyl)[4]

slope_4cyl = coef(mpg_disp_int_cyl)[2]
slope_6cyl = coef(mpg_disp_int_cyl)[2] + coef(mpg_disp_int_cyl)[5]
slope_8cyl = coef(mpg_disp_int_cyl)[2] + coef(mpg_disp_int_cyl)[6]

plot(mpg ~ disp, data = autompg, col = cyl)
abline(int_4cyl, slope_4cyl, col = 1, lty = 1, lwd = 2)
abline(int_6cyl, slope_6cyl, col = 2, lty = 2, lwd = 2)
abline(int_8cyl, slope_8cyl, col = 3, lty = 3, lwd = 2)
```



This looks much better! We can see that for medium displacement cars, 6 cylinder cars now perform better than 8 cylinder cars, which seems much more reasonable than before.

To completely justify the interaction model (i.e., a unique slope for each cyl level) compared to the additive model (single slope), we can perform an F-test. Notice first, that there is no t-test that will be able to do this since the difference between the two models is not a single parameter.

We will test,

$$H_0: \gamma_2 = \gamma_3 = 0$$

which represents the parallel regression lines we saw before,

$$Y = \beta_0 + \beta_1 x + \beta_2 v_2 + \beta_3 v_3 + \epsilon.$$

Again, this is a difference of two parameters, thus no t-test will be useful.

```
anova(mpg_disp_add_cyl, mpg_disp_int_cyl)
```

```
## Analysis of Variance Table
##
## Model 1: mpg ~ disp + cyl
## Model 2: mpg ~ disp * cyl
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 379 7299.5
## 2 377 6551.7 2 747.79 21.515 1.419e-09 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

As expected, we see a very low p-value, and thus reject the null. We prefer the interaction model over the additive model.

Recapping a bit:

- Null Model: $Y = \beta_0 + \beta_1 x + \beta_2 v_2 + \beta_3 v_3 + \epsilon$
 - Number of parameters: q = 4
- Full Model: $Y = \beta_0 + \beta_1 x + \beta_2 v_2 + \beta_3 v_3 + \gamma_2 x v_2 + \gamma_3 x v_3 + \epsilon$
 - Number of parameters: p = 6

```
length(coef(mpg_disp_int_cyl)) - length(coef(mpg_disp_add_cyl))
```

```
## [1] 2
```

We see there is a difference of two parameters, which is also displayed in the resulting ANOVA table from R. Notice that the following two values also appear on the ANOVA table.

```
nrow(autompg) - length(coef(mpg_disp_int_cyl))
```

```
## [1] 377
```

```
nrow(autompg) - length(coef(mpg_disp_add_cyl))
## [1] 379
```

6.4 Parameterization

So far we have been simply letting R decide how to create the dummy variables, and thus R has been deciding the parameterization of the models. To illustrate the ability to use alternative parameterizations, we will recreate the data, but directly creating the dummy variables ourselves.

```
new_param_data = data.frame(
    y = autompg$mpg,
    x = autompg$disp,
    v1 = 1 * as.numeric(autompg$cyl == 4),
    v2 = 1 * as.numeric(autompg$cyl == 6),
    v3 = 1 * as.numeric(autompg$cyl == 8))
head(new_param_data, 20)
```

```
x v1 v2 v3
## 1
     18 307
              0
## 2
     15 350
              0
                 0
     18 318
## 4
     16 304
              0
                0
## 5
     17 302
                   1
## 6
     15 429
     14 454
              0
     14 440
## 8
              0
                 0
## 9
     14 455
              0
                0
## 10 15 390
              0 0
## 11 15 383
              0
                0 1
## 12 14 340
## 13 15 400
              0
                0
## 14 14 455
## 15 24 113
              1
                0
                   0
## 16 22 198
## 17 18 199
              0 1 0
## 18 21 200
              1 0 0
## 19 27
         97
## 20 26 97
```

Now,

- y is mpg
- x is disp, the displacement in cubic inches,
- v1, v2, and v3 are dummy variables as defined above.

First let's try to fit an additive model using x as well as the three dummy variables.

```
lm(y \sim x + v1 + v2 + v3, data = new_param_data)
```

```
##
## Call:
## lm(formula = y ~ x + v1 + v2 + v3, data = new_param_data)
##
## Coefficients:
## (Intercept) x v1 v2 v3
## 32.96326 -0.05217 2.03603 -1.59722 NA
```

What is happening here? Notice that R is essentially ignoring v3, but why? Well, because R uses an intercept, it cannot also use v3. This is because

$$1 = v_1 + v_2 + v_3$$

which means that $\mathbf{1}$, v_1 , v_2 , and v_3 are linearly dependent. This would make the $X^{\top}X$ matrix singular, but we need to be able to invert it to solve the normal equations and obtain $\hat{\beta}$. With the intercept, $\mathtt{v1}$, and $\mathtt{v2}$, R can make the necessary "three intercepts". So, in this case $\mathtt{v3}$ is the reference level.

If we remove the intercept, then we can directly obtain all "three intercepts" without a reference level.

```
lm(y \sim 0 + x + v1 + v2 + v3, data = new_param_data)
```

Here, we are fitting the model

$$Y = \mu_1 v_1 + \mu_2 v_2 + \mu_3 v_3 + \beta x + \epsilon.$$

Thus we have:

• 4 Cylinder: $Y = \mu_1 + \beta x + \epsilon$ • 6 Cylinder: $Y = \mu_2 + \beta x + \epsilon$ • 8 Cylinder: $Y = \mu_3 + \beta x + \epsilon$

We could also do something similar with the interaction model, and give each line an intercept and slope, without the need for a reference level.

```
lm(y \sim 0 + v1 + v2 + v3 + x:v1 + x:v2 + x:v3, data = new_param_data)
```

```
##
## Call:
## lm(formula = y ~ 0 + v1 + v2 + v3 + x:v1 + x:v2 + x:v3, data = new_param_data)
##
## Coefficients:
## v1 v2 v3 v1:x v2:x v3:x
## 43.59052 30.39026 22.73346 -0.13069 -0.04770 -0.02252
```

```
Y = \mu_1 v_1 + \mu_2 v_2 + \mu_3 v_3 + \beta_1 x v_1 + \beta_2 x v_2 + \beta_3 x v_3 + \epsilon
```

```
    4 Cylinder: Y = μ<sub>1</sub> + β<sub>1</sub>x + ε
    6 Cylinder: Y = μ<sub>2</sub> + β<sub>2</sub>x + ε
    8 Cylinder: Y = μ<sub>3</sub> + β<sub>3</sub>x + ε
```

Using the original data, we have (at least) three equivalent ways to specify the interaction model with R.

```
lm(mpg ~ disp * cyl, data = autompg)
##
## Call:
## lm(formula = mpg ~ disp * cyl, data = autompg)
## Coefficients:
## (Intercept)
                       disp
                                     cyl6
                                                   cyl8
                                                           disp:cyl6
                                                                        disp:cyl8
##
      43.59052
                   -0.13069
                                -13.20026
                                             -20.85706
                                                             0.08299
                                                                           0.10817
lm(mpg \sim 0 + cyl + disp : cyl, data = autompg)
##
## Call:
## lm(formula = mpg ~ 0 + cyl + disp:cyl, data = autompg)
##
## Coefficients:
##
        cyl4
                   cyl6
                               cyl8
                                     cyl4:disp cyl6:disp
                                                            cyl8:disp
    43.59052
                           22.73346
               30.39026
                                      -0.13069
                                                 -0.04770
                                                             -0.02252
lm(mpg ~ 0 + disp + cyl + disp : cyl, data = autompg)
##
## lm(formula = mpg ~ 0 + disp + cyl + disp:cyl, data = autompg)
##
## Coefficients:
##
        disp
                   cyl4
                               cyl6
                                          cyl8 disp:cyl6 disp:cyl8
    -0.13069
               43.59052
                           30.39026
                                      22.73346
                                                   0.08299
                                                              0.10817
```

They all fit the same model, importantly each using six parameters, but the coefficients mean slightly different things in each. However, once they are interpreted as slopes and intercepts for the "three lines" they will have the same result.

Use ?all.equal to learn about the all.equal() function, and think about how the following code verifies that the residuals of the two models are the same.

```
## [1] TRUE
```

6.5 Building Larger Models

Now that we have seen how to incorporate categorical predictors as well as interaction terms, we can start to build much larger, much more flexible models which can potentially fit data better.

Let's define a "big" model,

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + \beta_6 x_2 x_3 + \beta_7 x_1 x_2 x_3 + \epsilon.$$

Here.

- Y is mpg.
- x₁ is disp.
- x_2 is hp.
- x_3 is domestic, which is a dummy variable we defined, where 1 is a domestic vehicle.

First thing to note here, we have included a new term $x_1x_2x_3$ which is a three-way interaction. Interaction terms can be larger and larger, up to the number of predictors in the model.

Since we are using the three-way interaction term, we also use all possible two-way interactions, as well as each of the first order (**main effect**) terms. This is the concept of a **hierarchy**. Any time a "higher-order" term is in a model, the related "lower-order" terms should also be included. Mathematically their inclusion or exclusion is sometimes irrelevant, but from an interpretation standpoint, it is best to follow the hierarchy rules.

Let's do some rearrangement to obtain a "coefficient" in front of x_1 .

$$Y = \beta_0 + \beta_2 x_2 + \beta_3 x_3 + \beta_6 x_2 x_3 + (\beta_1 + \beta_4 x_2 + \beta_5 x_3 + \beta_7 x_2 x_3) x_1 + \epsilon.$$

Specifically, the "coefficient" in front of x_1 is

$$(\beta_1 + \beta_4 x_2 + \beta_5 x_3 + \beta_7 x_2 x_3).$$

Let's discuss this "coefficient" to help us understand the idea of the *flexibility* of a model. Recall that,

- β_1 is the coefficient for a first order term,
- β_4 and β_5 are coefficients for two-way interactions,
- β_7 is the coefficient for the three-way interaction.

If the two and three way interactions were not in the model, the whole "coefficient" would simply be

$$\beta_1$$
.

Thus, no matter the values of x_2 and x_3 , β_1 would determine the relationship between x_1 (disp) and Y (mpg).

With the addition of the two-way interactions, now the "coefficient" would be

$$(\beta_1 + \beta_4 x_2 + \beta_5 x_3).$$

Now, changing x_1 (disp) has a different effect on Y (mpg), depending on the values of x_2 and x_3 .

Lastly, adding the three-way interaction gives the whole "coefficient"

$$(\beta_1 + \beta_4 x_2 + \beta_5 x_3 + \beta_7 x_2 x_3)$$

which is even more flexible. Now changing x_1 (disp) has a different effect on Y (mpg), depending on the values of x_2 and x_3 , but in a more flexible way which we can see with some more rearrangement. Now the "coefficient" in front of x_3 in this "coefficient" is dependent on x_2 .

$$(\beta_1 + \beta_4 x_2 + (\beta_5 + \beta_7 x_2)x_3)$$

It is so flexible, it is becoming hard to interpret!

Let's fit this three-way interaction model in R.

```
big_model = lm(mpg ~ disp * hp * domestic, data = autompg)
summary(big_model)
```

```
##
## Call:
## lm(formula = mpg ~ disp * hp * domestic, data = autompg)
##
## Residuals:
##
        Min
                  1Q
                       Median
                                    3Q
                                            Max
  -11.9410 -2.2147
                      -0.4008
                                1.9430
                                        18.4094
##
## Coefficients:
##
                       Estimate
                                 Std. Error t value Pr(>|t|)
## (Intercept)
                     60.6457838
                                  6.6000851
                                              9.189
                                                       < 2e-16 ***
                                             -2.232
                                                        0.0262 *
## disp
                     -0.1415870
                                  0.0634395
                                             -4.364 0.0000165 ***
## hp
                     -0.3544717
                                  0.0812261
                    -12.5718884
                                             -1.780
                                                       0.0759 .
## domestic
                                  7.0643505
## disp:hp
                      0.0013690
                                  0.0006727
                                              2.035
                                                        0.0426 *
## disp:domestic
                      0.0493298
                                  0.0640046
                                              0.771
                                                        0.4414
## hp:domestic
                                  0.0870881
                                              2.126
                                                        0.0342 *
                      0.1851530
## disp:hp:domestic -0.0009163
                                  0.0006768
                                            -1.354
                                                        0.1766
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.88 on 375 degrees of freedom
## Multiple R-squared: 0.76, Adjusted R-squared: 0.7556
## F-statistic: 169.7 on 7 and 375 DF, p-value: < 2.2e-16
```

Do we actually need this large of a model? Let's first test for the necessity of the three-way interaction term. That is,

$$H_0: \beta_7 = 0.$$

So,

- Full Model: $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + \beta_6 x_2 x_3 + \beta_7 x_1 x_2 x_3 + \epsilon$
- Null Model: $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + \beta_6 x_2 x_3 + \epsilon$

We fit the null model in R as two_way_int_mod, then use anova() to perform an F-test as usual.

```
two_way_int_mod = lm(mpg ~ disp * hp + disp * domestic + hp * domestic, data = autompg)
anova(two_way_int_mod, big_model)
```

```
## Analysis of Variance Table
##
## Model 1: mpg ~ disp * hp + disp * domestic + hp * domestic
## Model 2: mpg ~ disp * hp * domestic
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 376 5673.2
## 2 375 5645.6 1 27.599 1.8332 0.1766
```

We see the p-value is somewhat large, so we would fail to reject. We prefer the smaller, less flexible, null model, without the three-way interaction.

A quick note here: the full model does still "fit better." Notice that it has a smaller RMSE than the null model, which means the full model makes smaller (squared) errors on average.

```
mean(resid(big_model) ^ 2)
```

```
## [1] 14.74053
```

```
mean(resid(two_way_int_mod) ^ 2)
```

```
## [1] 14.81259
```

However, it is not much smaller. We could even say that, the difference is insignificant. This is an idea we will return to later in greater detail.

Now that we have chosen the model without the three-way interaction, can we go further? Do we need the two-way interactions? Let's test

$$H_0: \beta_4 = \beta_5 = \beta_6 = 0.$$

Remember we already chose $\beta_7 = 0$, so,

- Full Model: $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + \beta_6 x_2 x_3 + \epsilon$
- Null Model: $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon$

We fit the null model in R as additive_mod, then use anova() to perform an F-test as usual.

```
additive_mod = lm(mpg ~ disp + hp + domestic, data = autompg)
anova(additive_mod, two_way_int_mod)
```

```
## Analysis of Variance Table
##
## Model 1: mpg ~ disp + hp + domestic
## Model 2: mpg ~ disp * hp + disp * domestic + hp * domestic
## Res.Df RSS Df Sum of Sq F Pr(>F)
## 1 379 7369.7
## 2 376 5673.2 3 1696.5 37.478 < 2.2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1</pre>
```

Here the p-value is small, so we reject the null, and we prefer the full (alternative) model. Of the models we have considered, our final preference is for

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + \beta_6 x_2 x_3 + \epsilon.$$

Bibliography