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Introduction to R



These are course notes for the "Introduction to R" course given by the Monash Bioinformatics Platform¹ for the Proteomics Pre-Lorne workshop. Our teaching style is based on the style of The Carpentries². This course is focussing on the modern Tidyverse³ set of packages. We believe this is currently the quickest route to being productive in R.

- PDF version for printing⁴
- ZIP of data files used in this workshop⁵

During the workshop we will be using the RStudio Cloud to use R over the web:

• RStudio Cloud⁶

You can also install R on your own computer. There are two things to download and install:

- Download R⁷
- Download RStudio⁸

R is the language itself. RStudio provides a convenient environment in which to use R, either on your local computer or on a server.

Source code

This book was created in R using the rmarkdown and bookdown packages!

 $^{^{1}} https://www.monash.edu/researchinfrastructure/bioinformatics$

²https://carpentries.org/

³https://www.tidyverse.org/

 $^{^4 \}rm https://monashbioinformatic$ splatform.github.io/Proteomics-Intro-R-Workshop-2020/r-intro.pdf

 $^{^5 \}rm https://monashbioinformaticsplatform.github.io/Proteomics-Intro-R-Workshop-2020/r-intro-files.zip$

⁶https://rstudio.cloud/

⁷https://cran.rstudio.com/

 $^{^{8} \}rm https://www.rstudio.com/products/rstudio/download/$

• GitHub page⁹

Authors and copyright

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Data files are derived from Gapminder, which has a CC BY-4 license. The attribution is "Free data from www.gapminder.org". The data is given here in a form designed to teach various points about the R language. Refer to the Gapminder site¹¹ for the original form of the data if using it for other uses.

 $^{^9} https://github.com/MonashBioinformaticsPlatform/Proteomics-Intro-R-Workshop-Intro-R-Wo$ $2020/ \\ ^{10} \rm http://creative commons.org/licenses/by/4.0/$

¹¹https://www.gapminder.org

Chapter 1

Starting out in R

R is both a programming language and an interactive environment for data exploration and statistics. Today we will be concentrating on R as an *interactive environment*.

Working with R is primarily text-based. The basic mode of use for R is that the user types in a command in the R language and presses enter, and then R computes and displays the result.

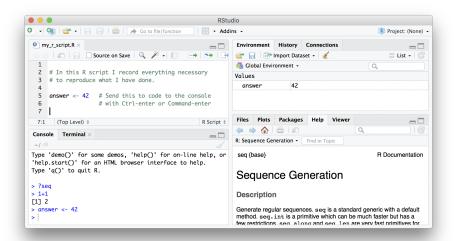
We will be working in RStudio¹. The easiest way to get started is to go to RStudio Cloud² and create a new project. Monash staff and students can log in using their Monash Google account.

The main way of working with R is the *console*, where you enter commands and view results. RStudio surrounds this with various conveniences. In addition to the console panel, RStudio provides panels containing:

- A text editor, where R commands can be recorded for future reference.
- A history of commands that have been typed on the console.
- An "environment" pane with a list of *variables*, which contain values that R has been told to save from previous commands.
- A file manager.
- Help on the functions available in R.
- A panel to show plots.

 $^{^{1} \}rm https://www.rstudio.com/products/rstudio/download/$

²https://rstudio.cloud/



Open RStudio, click on the "Console" pane, type 1+1 and press enter. R displays the result of the calculation. In this document, we will show such an interaction with R as below.

1+1

[1] 2

- + is called an operator. R has the operators you would expect for for basic mathematics: + * / $\hat{}$. It also has operators that do more obscure things.
- * has higher precedence than +. We can use brackets if necessary (). Try 1+2*3 and (1+2)*3.

Spaces can be used to make code easier to read.

We can compare with == < > <= >=. This produces a *logical* value, TRUE or FALSE. Note the double equals, ==, for equality comparison.

```
2 * 2 == 4
```

[1] TRUE

There are also character strings such as "string". A character string must be surrounded by either single or double quotes.

1.1 Variables

A variable is a name for a value. We can create a new variable by assigning a value to it using <-.

```
width <- 5
```

RStudio helpfully shows us the variable in the "Environment" pane. We can also print it by typing the name of the variable and hitting enter. In general, R

will print to the console any object returned by a function or operation *unless* we assign it to a variable.

width

[1] 5

Examples of valid variables names: hello, subject_id, subject.ID, x42. Spaces aren't ok *inside* variable names. Dots (.) are ok in R, unlike in many other languages. Numbers are ok, except as the first character. Punctuation is not allowed, with two exceptions: _ and ..

We can do arithmetic with the variable:

```
# Area of a square
width * width
```

[1] 25

and even save the result in another variable:

```
# Save area in "area" variable
area <- width * width</pre>
```

We can also change a variable's value by assigning it a new value:

```
width <- 10
width
```

[1] 10 area

[1] 25

Notice that the value of area we calculated earlier hasn't been updated. Assigning a new value to one variable does not change the values of other variables. This is different to a spreadsheet, but usual for programming languages.

1.2 Saving code in an R script

Once we've created a few variables, it becomes important to record how they were calculated so we can reproduce them later.

The usual workflow is to save your code in an R script ("R file"). Go to "File/New File/R Script" to create a new R script. Code in your R script can be sent to the console by selecting it or placing the cursor on the correct line, and then pressing **Control-Enter** (**Command-Enter** on a Mac).

Tip

Add comments to code, using lines starting with the # character. This makes it easier for others to follow what the code is doing (and also for us the next time we come back to it).

Challenge: using variables

1. Re-write this calculation so that it doesn't use variables:

```
a <- 4*20
b <- 7
a+b
```

2. Re-write this calcuation over multiple lines, using a variable:

```
2*2+2*2+2*2
```

1.3 Vectors

A *vector* of numbers is a collection of numbers. "Vector" means different things in different fields (mathematics, geometry, biology), but in R it is a fancy name for a collection of numbers. We call the individual numbers *elements* of the vector.

We can make vectors with c(), for example c(1,2,3). c means "combine". R is obsessed with vectors, in R even single numbers are vectors of length one. Many things that can be done with a single number can also be done with a vector. For example arithmetic can be done on vectors as it can be on single numbers.

```
myvec <- c(10,20,30,40,50)
myvec

## [1] 10 20 30 40 50

myvec + 1

## [1] 11 21 31 41 51

myvec + myvec

## [1] 20 40 60 80 100

length(myvec)

## [1] 5

c(60, myvec)

## [1] 60 10 20 30 40 50

c(myvec, myvec)</pre>
```

When we talk about the length of a vector, we are talking about the number of numbers in the vector.

[1] 10 20 30 40 50 10 20 30 40 50

1.4 Types of vector

We will also encounter vectors of character strings, for example "hello" or c("hello", "world"). Also we will encounter "logical" vectors, which contain TRUE and FALSE values. R also has "factors", which are categorical vectors, and behave much like character vectors (think the factors in an experiment).

Challenge: mixing types

Sometimes the best way to understand R is to try some examples and see what it does.

What happens when you try to make a vector containing different types, using c()? Make a vector with some numbers, and some words (eg. character strings like "test", or "hello").

Why does the output show the numbers surrounded by quotes " $\,$ " like character strings are?

Because vectors can only contain one type of thing, R chooses a lowest common denominator type of vector, a type that can contain everything we are trying to put in it. A different language might stop with an error, but R tries to soldier on as best it can. A number can be represented as a character string, but a character string can not be represented as a number, so when we try to put both in the same vector R converts everything to a character string.

1.5 Indexing vectors

Access elements of a vector with [], for example myvec[1] to get the first element. You can also assign to a specific element of a vector.

```
myvec[1]
## [1] 10
myvec[2]
## [1] 20
myvec[2] <- 5
myvec
## [1] 10 5 30 40 50
Can we use a vector to index another vector? Yes!
myind <- c(4,3,2)
myvec[myind]</pre>
```

```
## [1] 40 30 5
```

We could equivalently have written:

```
myvec[c(4,3,2)]
```

```
## [1] 40 30 5
```

Challenge: indexing

We can create and index character vectors as well. A cafe is using R to create their menu.

```
items <- c("spam", "eggs", "beans", "bacon", "sausage")</pre>
```

- 1. What does items[-3] produce? Based on what you find, use indexing to create a version of items without "spam".
- 2. Use indexing to create a vector containing spam, eggs, sausage, spam, and spam.
- 3. Add a new item, "lobster", to items.

1.6 Sequences

Another way to create a vector is with::

```
1:10
```

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

This can be useful when combined with indexing:

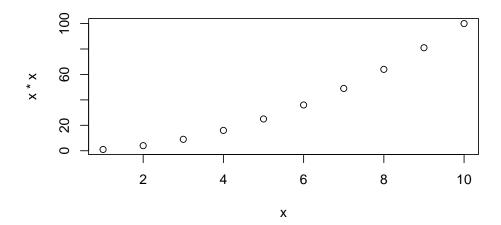
```
items[1:4]
```

```
## [1] "spam" "eggs" "beans" "bacon"
```

Sequences are useful for other things, such as a starting point for calculations:

```
x <- 1:10
x*x
```

```
## [1] 1 4 9 16 25 36 49 64 81 100 plot(x, x*x)
```



1.7 Functions

Functions are the things that do all the work for us in R: calculate, manipulate data, read and write to files, produce plots. R has many built in functions and we will also be loading more specialized functions from "packages".

We've already seen several functions: c(), length(), and plot(). Let's now have a look at sum().

sum(myvec)

[1] 135

We called the function sum with the argument myvec, and it returned the value 135. We can get help on how to use sum with:

?sum

Some functions take more than one argument. Let's look at the function rep, which means "repeat", and which can take a variety of different arguments. In the simplest case, it takes a value and the number of times to repeat that value.

rep(42, 10)

[1] 42 42 42 42 42 42 42 42 42 42

As with many functions in R—which is obsessed with vectors—the thing to be repeated can be a vector with multiple elements.

rep(c(1,2,3), 10)

[1] 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3

So far we have used *positional* arguments, where R determines which argument is which by the order in which they are given. We can also give arguments by *name*. For example, the above is equivalent to

rep(c(1,2,3), times=10)

[1] 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3

```
rep(x=c(1,2,3), 10)
## [1] 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2
```

Arguments can have default values, and a function may have many different possible arguments that make it do obscure things. For example, rep can also take an argument each=. It's typical for a function to be invoked with some number of positional arguments, which are always given, plus some less commonly used arguments, typically given by name.

Challenge: using functions

- 1. Use sum to sum from 1 to 10,000.
- 2. Look at the documentation for the seq function. What does seq do? Give an example of using seq with either the by or length.out argument.

Chapter 2

Data frames

Data frame is R's name for tabular data. We generally want each row in a data frame to represent a unit of observation, and each column to contain a different type of information about the units of observation. Tabular data in this form is called "tidy data".

Today we will be using a collection of modern packages collectively known as the Tidyverse². R and its predecessor S have a history dating back to 1976. The Tidyverse fixes some dubious design decisions baked into "base R", including having its own slightly improved form of data frame, which is called a *tibble*. Sticking to the Tidyverse where possible is generally safer, Tidyverse packages are more willing to generate errors rather than ignore problems.

2.1 Setting up

Our first step is to download the files we need and to install the Tidyverse. This is the one step where we ask you to copy and paste some code:

```
# Download files for this workshop
download.file(
   "https://monashbioinformaticsplatform.github.io/Proteomics-Intro-R-Workshop-2020/r-intro
   destfile="r-intro-files.zip")
unzip("r-intro-files.zip")

# Install Tidyverse
install.packages("tidyverse")
```

If using RStudio Cloud, you might need to switch to R version 3.5.3 to successfully install Tidyverse. Use the drop-down in the top right corner of the page.

People also sometimes have problems installing all the packages in Tidyverse on Windows machines. If you run into problems you may have more success

¹http://vita.had.co.nz/papers/tidy-data.html

²https://www.tidyverse.org/

installing individual packages.

```
install.packages(c("dplyr","readr","tidyr","ggplot2"))
```

We need to load the tidyverse package in order to use it.

```
library(tidyverse)

# OR
library(dplyr)
library(readr)
library(tidyr)
library(ggplot2)
```

The tidyverse package loads various other packages, setting up a modern R environment. In this section we will be using functions from the dplyr, readr and tidyr packages.

R is a language with mini-languages within it that solve specific problem domains. dplyr is such a mini-language, a set of "verbs" (functions) that work well together. dplyr, with the help of tidyr for some more complex operations, provides a way to perform most manipulations on a data frame that you might need.

2.2 Loading data

We will use the read_csv function from readr to load a data set. (See also read.csv in base R.) CSV stands for Comma Separated Values, and is a text format used to store tabular data. The first few lines of the file we are loading are shown below. Conventionally the first line contains column headings.

```
name, region, oecd, g77, lat, long, income2017
Afghanistan, asia, FALSE, TRUE, 33, 66, low
Albania, europe, FALSE, FALSE, 41, 20, upper_mid
Algeria, africa, FALSE, TRUE, 28, 3, upper_mid
Andorra, europe, FALSE, FALSE, 42.50779, 1.52109, high
Angola, africa, FALSE, TRUE, -12.5, 18.5, lower_mid
geo <- read_csv("r-intro-files/geo.csv")</pre>
## Parsed with column specification:
## cols(
     name = col_character(),
##
     region = col_character(),
##
##
     oecd = col_logical(),
##
     g77 = col_logical(),
##
     lat = col_double(),
##
     long = col_double(),
##
     income2017 = col_character()
## )
geo
```

```
## # A tibble: 196 x 7
##
     name
                           region
                                    oecd g77
                                                   lat
                                                         long income2017
##
      <chr>
                           <chr>
                                    <lgl> <lgl> <dbl>
                                                        <dbl> <chr>
##
   1 Afghanistan
                           asia
                                    FALSE TRUE
                                                  33
                                                        66
                                                              low
##
   2 Albania
                                    FALSE FALSE
                                                        20
                           europe
                                                 41
                                                              upper_mid
##
   3 Algeria
                           africa
                                    FALSE TRUE
                                                  28
                                                         3
                                                              upper_mid
##
   4 Andorra
                           europe
                                    FALSE FALSE 42.5
                                                         1.52 high
                                                -12.5
##
   5 Angola
                           africa
                                    FALSE TRUE
                                                        18.5
                                                              lower mid
##
    6 Antigua and Barbuda americas FALSE TRUE
                                                  17.0 -61.8
                                                              high
                                                -34
                                                       -64
##
    7 Argentina
                           americas FALSE TRUE
                                                              upper_mid
##
    8 Armenia
                                    FALSE FALSE
                                                 40.2
                                                        45
                                                              lower_mid
                           europe
##
   9 Australia
                           asia
                                    TRUE
                                         FALSE -25
                                                       135
                                                              high
## 10 Austria
                           europe
                                    TRUE FALSE 47.3
                                                        13.3
                                                              high
## # ... with 186 more rows
```

read_csv has guessed the type of data each column holds:

- <chr> character strings
- <dbl> numerical values. Technically these are "doubles", which is a way of storing numbers with 15 digits precision.
- <lg1> logical values, TRUE or FALSE.

We will also encounter:

- <int> integers, a fancy name for whole numbers.
- <fct> factors, categorical data. We will get to this shortly.

You can also see this data frame referring to itself as "a tibble". This is the Tidyverse's improved form of data frame. Tibbles present themselves more conveniently than base R data frames. Base R data frames don't show the type of each column, and output every row when you try to view them.

Tip

A data frame can also be created from vectors, with the tibble function. (See also data.frame in base R.) For example:

```
tibble(foo=c(10,20,30), bar=c("a","b","c"))

## # A tibble: 3 x 2

## foo bar

## <dbl> <chr>
## 1 10 a

## 2 20 b

## 3 30 c
```

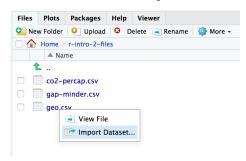
The argument names become column names in the data frame.

Tip

The path to the file on our server is "r-intro-files/geo.csv". This says, starting from your working directory, look in the directory r-intro-files for

the file geo.csv. The steps in the path are separated by /. Your working directory is shown at the top of the console pane. The path needed might be different on your own computer, depending where you downloaded the file.

One way to work out the correct path is to find the file in the file browser pane, click on it and select "Import Dataset...".



2.3 Exploring

The View function gives us a spreadsheet-like view of the data frame.

View(geo)

print with the n argument can be used to show more than the first 10 rows on the console.

```
print(geo, n=200)
```

We can extract details of the data frame with further functions:

```
nrow(geo)
## [1] 196
ncol(geo)
## [1] 7
colnames(geo)
## [1] "name"
                     "region"
                                   "oecd"
                                                 "g77"
                                                               "lat"
## [6] "long"
                     "income2017"
summary(geo)
##
        name
                            region
                                                oecd
                                                                 g77
                        Length: 196
##
    Length: 196
                                             Mode :logical
                                                              Mode :logical
    Class :character
                        Class :character
                                             FALSE:165
                                                              FALSE:65
##
##
    Mode :character
                        Mode :character
                                             TRUE:31
                                                              TRUE :131
##
##
##
##
         lat
                            long
                                            income2017
```

```
##
         :-42.00
                   Min. :-175.000
   Min.
                                     Length: 196
   1st Qu.: 4.00
                   1st Qu.: -5.625
##
                                     Class : character
   Median : 17.42
                   Median : 21.875
                                     Mode :character
   Mean
         : 19.03
                   Mean
                         : 23.004
##
   3rd Qu.: 39.82
                   3rd Qu.: 51.892
  Max. : 65.00
                   Max.
                        : 179.145
```

2.4 Indexing data frames

Data frames can be subset using [row,column] syntax.

```
geo[4,2]
## # A tibble: 1 x 1
##
    region
##
     <chr>>
## 1 europe
```

Note that while this is a single value, it is still wrapped in a data frame. (This is a behaviour specific to Tidyverse data frames.) More on this in a moment.

Columns can be given by name.

```
geo[4, "region"]
## # A tibble: 1 x 1
##
     region
##
     <chr>>
## 1 europe
The column or row may be omitted, thereby retrieving the entire row or column.
geo[4,]
## # A tibble: 1 x 7
##
             region oecd g77
                                   lat long income2017
     name
             <chr> <lgl> <lgl> <dbl> <dbl> <chr>
## 1 Andorra europe FALSE FALSE 42.5 1.52 high
geo[,"region"]
## # A tibble: 196 x 1
##
      region
##
      <chr>
## 1 asia
## 2 europe
   3 africa
##
##
   4 europe
## 5 africa
    6 americas
##
    7 americas
   8 europe
```

```
## 9 asia
## 10 europe
## # ... with 186 more rows
Multiple rows or columns may be retrieved using a vector.
rows_wanted <- c(1,3,5)
geo[rows_wanted,]
## # A tibble: 3 x 7
##
   name
                 region oecd g77
                                       lat long income2017
     <chr>>
                 <chr> <lgl> <lgl> <dbl> <dbl> <chr>
                        FALSE TRUE
## 1 Afghanistan asia
                                      33
                                            66
                                                 low
## 2 Algeria
                 africa FALSE TRUE
                                      28
                                             3
                                                 upper_mid
                 africa FALSE TRUE -12.5 18.5 lower_mid
## 3 Angola
Vector indexing can also be written on a single line.
geo[c(1,3,5),]
## # A tibble: 3 x 7
##
     name
                 region oecd g77
                                       lat long income2017
##
     <chr>
                 <chr> <lgl> <lgl> <dbl> <dbl> <chr>
## 1 Afghanistan asia
                        FALSE TRUE
                                      33
                                            66
                                                 low
                 africa FALSE TRUE
                                      28
                                             3
## 2 Algeria
                                                 upper mid
## 3 Angola
                 africa FALSE TRUE -12.5 18.5 lower_mid
geo[1:7,]
## # A tibble: 7 x 7
##
    name
                         region
                                   oecd g77
                                                        long income2017
                                                 lat
##
     <chr>>
                          <chr>
                                   <lg1> <lg1> <db1>
                                                       <dbl> <chr>
## 1 Afghanistan
                         asia
                                   FALSE TRUE
                                                33
                                                       66
                                                             low
## 2 Albania
                         europe
                                   FALSE FALSE
                                                41
                                                       20
                                                             upper mid
## 3 Algeria
                                   FALSE TRUE
                                                28
                                                        3
                         africa
                                                             upper_mid
## 4 Andorra
                         europe
                                   FALSE FALSE 42.5
                                                        1.52 high
## 5 Angola
                                   FALSE TRUE
                                               -12.5 18.5
                         africa
                                                             lower mid
## 6 Antigua and Barbuda americas FALSE TRUE
                                                17.0 -61.8 high
                         americas FALSE TRUE
## 7 Argentina
                                               -34
                                                      -64
                                                             upper_mid
```

2.5 Columns are vectors

Ok, so how do we actually get data out of a data frame?

Under the hood, a data frame is a list of column vectors. We can use \$ to retrieve columns. Occasionally it is also useful to use [[]] to retrieve columns, for example if the column name we want is stored in a variable.

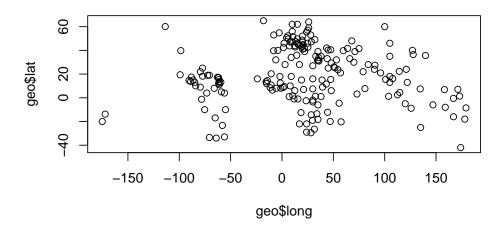
```
head( geo$region )
## [1] "asia"    "europe"    "africa"    "europe"    "africa"    "americas"
```

```
head( geo[["region"]] )
## [1] "asia" "europe" "africa" "europe" "africa" "americas"
To get the "region" value of the 4th row as above, but unwrapped, we can use:
geo$region[4]
```

[1] "europe"

For example, to plot the longitudes and latitudes we could use:

plot(geo\$long, geo\$lat)



2.6 Logical indexing

A method of indexing that we haven't discussed yet is logical indexing. Instead of specifying the row number or numbers that we want, we can give a logical vector which is TRUE for the rows we want and FALSE otherwise. This can also be used with vectors.

We will first do this in a slightly verbose way in order to understand it, then learn a more concise way to do this using the dplyr package.

Southern countries have latitude less than zero.

```
is_southern <- geo$lat < 0
head(is_southern)
## [1] FALSE FALSE FALSE TRUE FALSE
sum(is_southern)
## [1] 40</pre>
```

sum treats TRUE as 1 and FALSE as 0, so it tells us the number of TRUE elements in the vector.

We can use this logical vector to get the southern countries from geo:

geo[is_southern,]

```
## # A tibble: 40 x 7
##
                                            lat long income2017
     name
                      region
                               oecd g77
##
     <chr>
                      <chr>
                               <lgl> <lgl> <dbl> <dbl> <chr>
##
   1 Angola
                      africa FALSE TRUE
                                          -12.5 18.5 lower mid
##
   2 Argentina
                      americas FALSE TRUE -34
                                                -64
                                                      upper_mid
##
   3 Australia
                      asia TRUE FALSE -25
                                                135
                                                      high
##
   4 Bolivia
                      americas FALSE TRUE -17
                                                -65
                                                      lower_mid
   5 Botswana
                      africa FALSE TRUE -22
                                                 24
                                                      upper_mid
##
   6 Brazil
                      americas FALSE TRUE
                                         -10
                                                -55
                                                      upper_mid
   7 Burundi
                      africa FALSE TRUE
##
                                           -3.5 30
                                                      low
## 8 Chile
                      americas TRUE TRUE
                                          -33.5 - 70.6 high
## 9 Comoros
                      africa FALSE TRUE
                                          -12.2 44.4 low
## 10 Congo, Dem. Rep. africa FALSE TRUE
                                           -2.5 23.5 low
## # ... with 30 more rows
```

Comparison operators available are:

```
• x == y - "equal to"
```

- x != y "not equal to"
- x < y "less than"
- x > y "greater than"
- $x \le y -$ "less than or equal to"
- $x \ge y -$ "greater than or equal to"

More complicated conditions can be constructed using logical operators:

- a & b "and", TRUE only if both a and b are TRUE.
- a | b "or", TRUE if either a or b or both are TRUE.
- ! a "not", TRUE if a is FALSE, and FALSE if a is TRUE.

The oecd column of geo tells which countries are in the Organisation for Economic Co-operation and Development, and the g77 column tells which countries are in the Group of 77 (an alliance of developing nations). We could see which OECD countries are in the southern hemisphere with:

```
southern_oecd <- is_southern & geo$oecd
geo[southern_oecd,]</pre>
```

```
## # A tibble: 3 x 7
##
    name
                 region
                          oecd g77
                                        lat long income2017
##
     <chr>
                 <chr>>
                          <lgl> <lgl> <dbl> <dbl> <chr>
## 1 Australia
                 asia
                          TRUE FALSE -25
                                            135
                                                  high
## 2 Chile
                 americas TRUE
                               TRUE -33.5 -70.6 high
## 3 New Zealand asia
                          TRUE FALSE -42
                                            174
```

is_southern seems like it should be kept within our geo data frame for future use. We can add it as a new column of the data frame with:

```
geo$southern <- is_southern
geo
## # A tibble: 196 x 8
##
      name
                           region
                                     oecd g77
                                                    lat
                                                          long income2017 southern
##
      <chr>
                           <chr>
                                     <lg1> <lg1> <db1>
                                                         <dbl> <chr>
                                                                           <1g1>
##
   1 Afghanistan
                                     FALSE TRUE
                                                   33
                                                         66
                                                                low
                                                                           FALSE
                           asia
                                                         20
##
    2 Albania
                                     FALSE FALSE
                                                   41
                                                                upper_mid
                                                                           FALSE
                           europe
    3 Algeria
                                                   28
##
                           africa
                                     FALSE TRUE
                                                          3
                                                                upper_mid
                                                                           FALSE
##
    4 Andorra
                           europe
                                     FALSE FALSE
                                                  42.5
                                                          1.52 high
                                                                           FALSE
##
    5 Angola
                                     FALSE TRUE
                                                  -12.5
                                                         18.5
                                                                lower_mid
                                                                           TRUE
                           africa
                                                   17.0 -61.8
##
    6 Antigua and Barbuda americas FALSE TRUE
                                                               high
                                                                           FALSE
##
    7 Argentina
                           americas FALSE TRUE
                                                  -34
                                                        -64
                                                                upper_mid
                                                                           TRUE
##
    8 Armenia
                           europe
                                     FALSE FALSE
                                                  40.2
                                                                lower mid
                                                                           FALSE
##
   9 Australia
                                     TRUE FALSE -25
                                                        135
                                                                           TRUE
                                                                high
                           asia
## 10 Austria
                                     TRUE FALSE
                                                  47.3
                                                        13.3
                                                               high
                                                                           FALSE
                           europe
## # ... with 186 more rows
```

Challenge: logical indexing

- 1. Which country is in both the OECD and the G77?
- 2. Which countries are in neither the OECD nor the G77?
- 3. Which countries are in the Americas? These have longitudes between -150 and -40.

2.6.1 A dplyr shorthand

The above method is a little laborious. We have to keep mentioning the name of the data frame, and there is a lot of punctuation to keep track of. dplyr provides a slightly magical function called filter which lets us write more concisely. For example:

```
filter(geo, lat < 0 & oecd)
## # A tibble: 3 x 8
##
     name
                                               long income2017 southern
                  region
                            oecd
                                  g77
                                           lat
##
     <chr>
                  <chr>
                            <lgl> <lgl> <dbl> <dbl> <chr>
                                                                  <lgl>
## 1 Australia
                  asia
                            TRUE
                                  FALSE -25
                                                135
                                                                  TRUE
## 2 Chile
                                                                  TRUE
                  americas
                           TRUE
                                  TRUE
                                         -33.5 - 70.6 \text{ high}
## 3 New Zealand asia
                            TRUE
                                  FALSE -42
                                                174
                                                      high
                                                                  TRUE
```

In the second argument, we are able to refer to columns of the data frame as though they were variables. The code is beautiful, but also opaque. It's important to understand that under the hood we are creating and combining logical vectors.

2.7 Factors

income2017

<int>

31

<fct>

##

1 low

The count function from dplyr can help us understand the contents of some of the columns in geo. count is also *magical*, we can refer to columns of the data frame directly in the arguments to count.

```
count(geo, region)
## # A tibble: 4 x 2
##
    region
##
     <chr>
              <int>
## 1 africa
                 54
## 2 americas
                 35
## 3 asia
                 59
## 4 europe
                 48
count(geo, income2017)
## # A tibble: 4 x 2
##
   income2017
##
     <chr>
                <int>
## 1 high
                    58
## 2 low
                    31
## 3 lower_mid
                    52
## 4 upper_mid
                    55
```

One annoyance here is that the different categories in <code>income2017</code> aren't in a sensible order. This comes up quite often, for example when sorting or plotting categorical data. R's solution is a further type of vector called a <code>factor</code> (think a factor of an experimental design). A factor holds categorical data, and has an associated ordered set of <code>levels</code>. It is otherwise quite similar to a character vector.

Any sort of vector can be converted to a factor using the factor function. This function defaults to placing the levels in alphabetical order, but takes a levels argument that can override this.

```
argument that can override this.

head( factor(geo$income2017, levels=c("low","lower_mid","upper_mid","high")))

## [1] low upper_mid upper_mid high lower_mid high

## Levels: low lower_mid upper_mid high

We should modify the income2017 column of the geo table in order to use this:

geo$income2017 <- factor(geo$income2017, levels=c("low","lower_mid","upper_mid","high"))

count now produces the desired order of output:

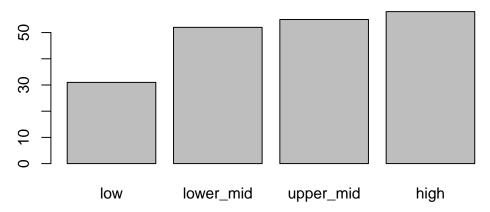
count(geo, income2017)

## # A tibble: 4 x 2
```

```
## 2 lower_mid 52
## 3 upper_mid 55
## 4 high 58
```

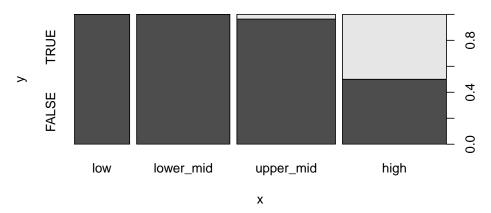
When plot is given a factor, it shows a bar plot:

```
plot(geo$income2017)
```



When given two factors, it shows a mosaic plot:

plot(geo\$income2017, factor(geo\$oecd))



Similarly we can count two categorical columns at once.

```
count(geo, income2017, oecd)
```

```
## # A tibble: 6 x 3
##
     income2017 oecd
                          n
##
     <fct>
                <lgl> <int>
## 1 low
                FALSE
                         31
## 2 lower_mid FALSE
                         52
## 3 upper_mid FALSE
                         53
## 4 upper_mid TRUE
                          2
## 5 high
                FALSE
                         29
## 6 high
                TRUE
                         29
```

2.8 Readability vs tidyness

The counts we obtained counting income2017 vs oecd were properly tidy in the sense of containing a single unit of observation per row. However to view the data, it would be more convenient to have income as columns and OECD membership as rows. We can use the pivot_wider function from tidyr to achieve this. (This is also sometimes also called a "cast" or a "spread".)

```
counts <- count(geo, income2017, oecd)</pre>
pivot wider(counts, names from=income2017, values from=n)
## # A tibble: 2 x 5
##
     oecd
             low lower_mid upper_mid high
##
     <lgl> <int>
                      <int>
                                 <int> <int>
## 1 FALSE
                                    53
               31
                         52
                                           29
## 2 TRUE
               NΑ
                         NΑ
                                     2
                                           29
```

We could further specify values_fill=list(n=0) to fill in the NA values with 0.

Tip

Tidying is often the first step when exploring a data-set. The tidyr³ package contains a number of useful functions that help tidy (or un-tidy!) data. We've just seen pivot_wider which spreads two columns into multiple columns. The inverse of pivot_wider is pivot_longer, which gathers multiple columns into two columns: a column of column names, and a column of values. pivot_longer is often the first step when tidying a dataset you have received from the wild. (This is sometimes also called a "melt" or a "gather".)

Challenge: counting

Investigate how many OECD and non-OECD nations come from the northern and southern hemispheres.

- 1. Using count.
- 2. By making a mosaic plot.

Remember you may need to convert columns to factors for plot to work, and that a southern column could be added to geo with:

```
geo$southern <- geo$lat < 0
```

2.9 Sorting

Data frames can be sorted using the arrange function in dplyr.

³http://tidyr.tidyverse.org/

arrange(geo, lat) ## # A tibble: 196 x 8 ## nameregion oecd g77 lat long income2017 southern ## <chr>> <chr> <lg1> <lg1> <db1> <db1> <fct> <1g1> ## TRUE FALSE -42 TRUE 1 New Zealand asia 174 high

2 Argentina americas FALSE TRUE -34 -64TRUE upper mid -33.5 -70.6 high ## 3 Chile americas TRUE TRUE TRUE ## 4 Uruguay americas FALSE TRUE -33 -56 high TRUE ## 5 Lesotho africa FALSE TRUE -29.528.2 lower_mid TRUE 6 South Africa africa FALSE TRUE -29 24 upper_mid TRUE ## 7 Swaziland FALSE TRUE -26.5 31.5 lower_mid TRUE africa TRUE ## 8 Australia TRUE FALSE -25 135 asia high

9 Paraguay americas FALSE TRUE -23.3 -58 upper_mid TRUE ## 10 Botswana africa FALSE TRUE -22 24 upper_mid TRUE

... with 186 more rows

Numeric columns are sorted in numeric order. Character columns will be sorted in alphabetical order. Factor columns are sorted in order of their levels. The desc helper function can be used to sort in descending order.

```
arrange(geo, desc(name))
```

```
## # A tibble: 196 x 8
##
     name
                                             lat
                                                    long income2017 southern
                     region
                               oecd g77
##
      <chr>
                     <chr>>
                               <lg1> <lg1> <db1>
                                                   <dbl> <fct>
                                                                     <1g1>
##
   1 Zimbabwe
                     africa
                               FALSE TRUE
                                           -19
                                                   29.8
                                                         low
                                                                    TRUE
##
   2 Zambia
                     africa
                               FALSE TRUE
                                           -14.3
                                                  28.5
                                                         lower mid
                                                                    TRUE
##
   3 Yemen
                               FALSE TRUE
                                            15.5 47.5
                                                         lower mid
                                                                    FALSE
                     asia
##
   4 Vietnam
                     asia
                               FALSE TRUE
                                            16.2 108.
                                                         lower mid
                                                                    FALSE
##
   5 Venezuela
                     americas FALSE TRUE
                                             8
                                                  -66
                                                         upper mid
                                                                    FALSE
##
   6 Vanuatu
                               FALSE TRUE
                                           -16
                                                  167
                                                         lower mid
                                                                    TRUE
                     asia
   7 Uzbekistan
##
                     asia
                               FALSE FALSE
                                           41.7
                                                  63.8
                                                         lower_mid
                                                                    FALSE
   8 Uruguay
                     americas FALSE TRUE
                                           -33
                                                  -56
                                                         high
                                                                    TRUE
   9 United States
                     americas TRUE FALSE
                                            39.8 -98.5
                                                         high
                                                                    FALSE
## 10 United Kingdom europe
                               TRUE FALSE
                                           54.8 - 2.70 \text{ high}
                                                                    FALSE
## # ... with 186 more rows
```

2.10 Joining data frames

Let's move on to a larger data set. This is from the Gapminder⁴ project and contains information about countries over time.

⁴https://www.gapminder.org

##		<chr></chr>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>
##	1	Afghanistan	1800	3280000	603	28.2
##	2	Albania	1800	410445	667	35.4
##	3	Algeria	1800	2503218	715	28.8
##	4	Andorra	1800	2654	1197	NA
##	5	Angola	1800	1567028	618	27.0
##	6	Antigua and Barbuda	1800	37000	757	33.5
##	7	Argentina	1800	534000	1507	33.2
##	8	Armenia	1800	413326	514	34
##	9	Australia	1800	351014	814	34.0
##	10	Austria	1800	3205587	1847	34.4
##	#	with 4,302 more	rows			

Quiz

What is the unit of observation in this new data frame?

gap_geo <- left_join(gap, geo, by="name")</pre>

It would be useful to have general information about countries from geo available as columns when we use this data frame. gap and geo share a column called name which can be used to match rows from one to the other.

```
gap_geo
## # A tibble: 4,312 x 12
##
      name
             year population gdp_percap life_exp region oecd g77
                                                                           lat
                                                                                 long
##
      <chr>
            <dbl>
                        <dbl>
                                    <dbl>
                                              <dbl> <chr>
                                                           <lg1> <lg1>
                                                                         <dbl>
                                                                                <dbl>
                                                            FALSE TRUE
##
    1 Afgh~
              1800
                      3280000
                                      603
                                               28.2 asia
                                                                          33
                                                                                66
                                      667
                                                                                20
##
    2 Alba~
              1800
                       410445
                                               35.4 europe FALSE FALSE
                                                                          41
##
    3 Alge~
              1800
                      2503218
                                      715
                                               28.8 africa FALSE TRUE
                                                                          28
                                                                                 3
##
    4 Ando~
              1800
                         2654
                                     1197
                                                    europe FALSE FALSE
                                                                         42.5
                                                                                 1.52
##
    5 Ango~
              1800
                      1567028
                                      618
                                               27.0 africa FALSE TRUE
                                                                         -12.5
                                                                                18.5
##
    6 Anti~
             1800
                        37000
                                      757
                                               33.5 ameri~ FALSE TRUE
                                                                          17.0 -61.8
##
                                     1507
                                               33.2 ameri~ FALSE TRUE
                                                                        -34
                                                                               -64
    7 Arge~
              1800
                       534000
    8 Arme~
##
              1800
                       413326
                                      514
                                                    europe FALSE FALSE
                                                                        40.2
                                                                               45
##
    9 Aust~
             1800
                       351014
                                      814
                                               34.0 asia
                                                            TRUE FALSE -25
                                                                               135
                                               34.4 europe TRUE FALSE 47.3 13.3
## 10 Aust~
             1800
                      3205587
                                     1847
```

southern <1gl>

... with 4,302 more rows, and 2 more variables: income2017 <fct>,

The output contains all ways of pairing up rows by name. In this case each row of geo pairs up with multiple rows of gap.

The "left" in "left join" refers to how rows that can't be paired up are handled. left_join keeps all rows from the first data frame but not the second. This is a good default when the intent is to attaching some extra information to a data frame. inner_join discard all rows that can't be paired up. full_join keeps all rows from both data frames.

2.11 Further reading

We've covered the fundamentals of dplyr and data frames, but there is much more to learn. Notably, we haven't covered the use of the pipe %% to chain dplyr verbs together. The "R for Data Science" book⁵ is an excellent source to learn more. The Monash Data Fluency "Programming and Tidy data analysis in R" course⁶ also covers this.

 $^{^{5} \}mathrm{http://r4ds.had.co.nz/}$

⁶https://monashdatafluency.github.io/r-progtidy/

Chapter 3

Plotting with ggplot2

We already saw some of R's built in plotting facilities with the function plot. A more recent and much more powerful plotting library is ggplot2. ggplot2 is another mini-language within R, a language for creating plots. It implements ideas from a book called "The Grammar of Graphics". The syntax can be a little strange, but there are plenty of examples in the online documentation².

ggplot2 is part of the Tidyverse, so loadinging the tidyverse package will load ggplot2.

```
library(tidyverse)
```

We continue with the Gapminder dataset, which we loaded with:

```
geo <- read_csv("r-intro-files/geo.csv")
gap <- read_csv("r-intro-files/gap-minder.csv")
gap_geo <- left_join(gap, geo, by="name")</pre>
```

3.1 Elements of a ggplot

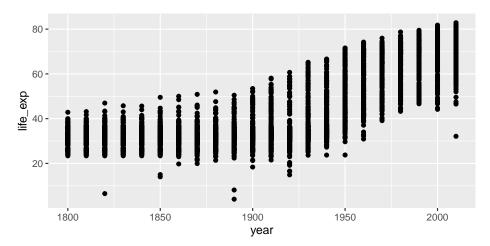
Producing a plot with ggplot2, we must give three things:

- $1.\ {\rm A}$ data frame containing our data.
- 2. How the columns of the data frame can be translated into positions, colors, sizes, and shapes of graphical elements ("aesthetics").
- 3. The actual graphical elements to display ("geometric objects").

Let's make our first ggplot.

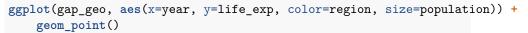
```
ggplot(gap_geo, aes(x=year, y=life_exp)) +
    geom_point()
```

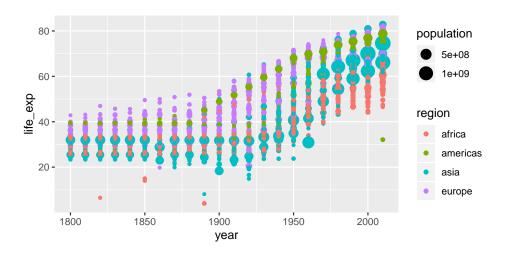
 $^{^1 \}rm https://www.amazon.com/Grammar-Graphics-Statistics-Computing/dp/0387245448$ $^2 \rm http://ggplot2.tidyverse.org/reference/$



The call to ggplot and aes sets up the basics of how we are going to represent the various columns of the data frame. aes defines the "aesthetics", which is how columns of the data frame map to graphical attributes such as x and y position, color, size, etc. aes is another example of magic "non-standard evaluation", arguments to aes may refer to columns of the data frame directly. We then literally add layers of graphics ("geoms") to this.

Further aesthetics can be used. Any aesthetic can be either numeric or categorical, an appropriate scale will be used.





3.1.1 Challenge: make a ggplot

This R code will get the data from the year 2010:

```
gap2010 <- filter(gap_geo, year == 2010)</pre>
```

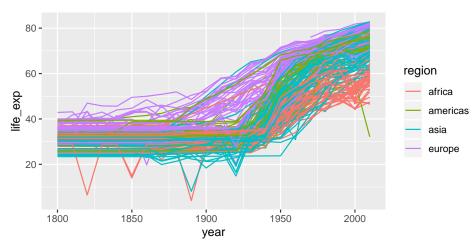
Create a ggplot of this with:

- gdp_percap as x.
- life_exp as y.
- population as the size.
- region as the color.

3.2 Further geoms

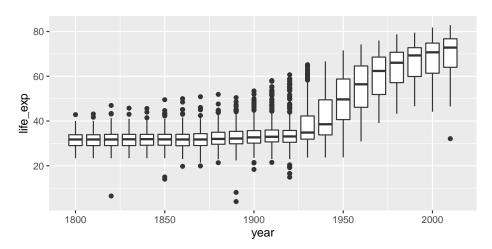
To draw lines, we need to use a "group" aesthetic.

```
ggplot(gap_geo, aes(x=year, y=life_exp, group=name, color=region)) +
    geom_line()
```



A wide variety of geoms are available. Here we show Tukey box-plots. Note again the use of the "group" aesthetic, without this ggplot will just show one big box-plot.

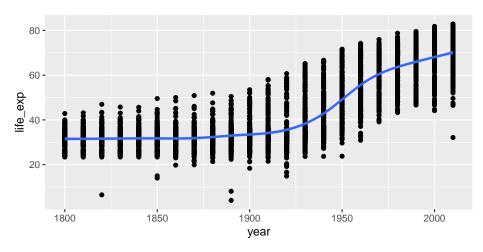
```
ggplot(gap_geo, aes(x=year, y=life_exp, group=year)) +
   geom_boxplot()
```



geom_smooth can be used to show trends.

```
ggplot(gap_geo, aes(x=year, y=life_exp)) +
   geom_point() +
   geom_smooth()
```

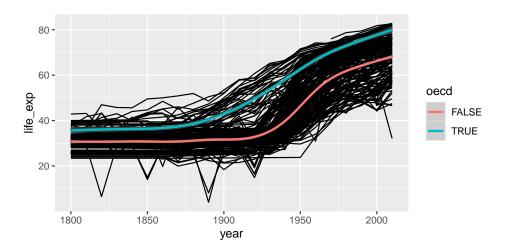
$geom_smooth()$ using method = gam' and formula $y \sim s(x, bs = "cs")'$



Aesthetics can be specified globally in ggplot, or as the first argument to individual geoms. Here, the "group" is applied only to draw the lines, and "color" is used to produce multiple trend lines:

```
ggplot(gap_geo, aes(x=year, y=life_exp)) +
    geom_line(aes(group=name)) +
    geom_smooth(aes(color=oecd))
```

$geom_smooth()$ using method = gam' and formula $y \sim s(x, bs = "cs")'$

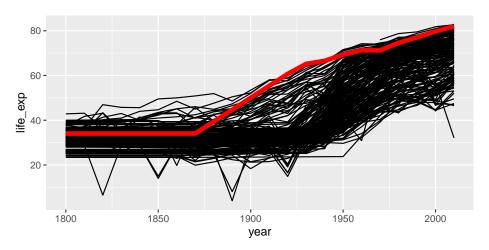


3.3 Highlighting subsets

Geoms can be added that use a different data frame, using the data= argument.

```
gap_australia <- filter(gap_geo, name == "Australia")

ggplot(gap_geo, aes(x=year, y=life_exp, group=name)) +
    geom_line() +
    geom_line(data=gap_australia, color="red", size=2)</pre>
```

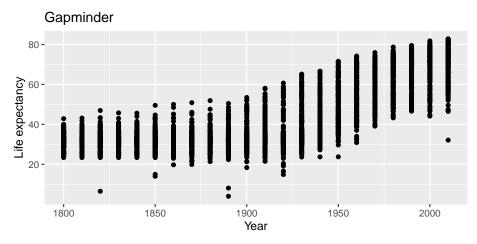


Notice also that the second <code>geom_line</code> has some further arguments controlling its appearance. These are **not** aesthetics, they are not a mapping of data to appearance, but rather a direct specification of the appearance. There isn't an associated scale as when color was an aesthetic.

3.4 Fine-tuning a plot

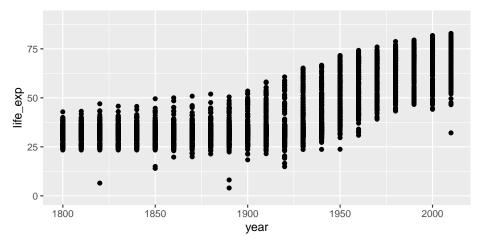
Adding labs to a ggplot adjusts the labels given to the axes and legends. A plot title can also be specified.

```
ggplot(gap_geo, aes(x=year, y=life_exp)) +
    geom_point() +
    labs(x="Year", y="Life expectancy", title="Gapminder")
```



coord_cartesian can be used to set the limits of the x and y axes. Suppose we want our y-axis to start at zero.

```
ggplot(gap_geo, aes(x=year, y=life_exp)) +
    geom_point() +
    coord_cartesian(ylim=c(0,90))
```



Type scale_ and press the tab key. You will see functions giving fine-grained controls over various scales (x, y, color, etc). These allow transformations (eg log10), and manually specified breaks (labelled values). Very fine grained control is possible over the appearance of ggplots, see the ggplot2 documentation for

details and further examples.

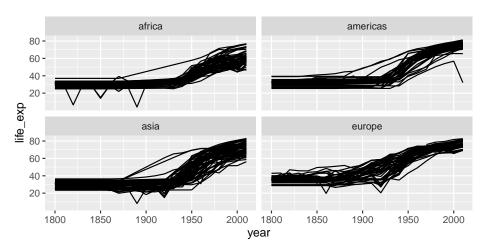
3.4.1 Challenge: refine your ggplot

Continuing with your scatter-plot of the 2010 data, add axis labels to your plot. Give your x axis a log scale by adding scale_x_log10().

3.5 Faceting

Faceting lets us quickly produce a collection of small plots. The plots all have the same scales and the eye can easily compare them.

```
ggplot(gap_geo, aes(x=year, y=life_exp, group=name)) +
    geom_line() +
    facet_wrap(~ region)
```



Note the use of \sim , which we've not seen before. \sim syntax is used in R to specify dependence on some set of variables, for example when specifying a linear model. Here the information in each plot is dependent on the continent.

3.5.1 Challenge: facet your ggplot

Let's return again to your scatter-plot of the 2010 data.

Adjust your plot to now show data from all years, with each year shown in a separate facet, using facet_wrap(~ year).

Advanced: Highlight Australia in your plot.

3.6 Saving ggplots

The act of plotting a ggplot is actually triggered when it is printed. In an interactive session we are automatically printing each value we calculate, but if you are using it with a programming construct such as a for loop or function you might need to explcitly print() the plot.

Ggplots can be saved using ggsave.

```
# Plot created but not shown.
p <- ggplot(gap_geo, aes(x=year, y=life_exp)) + geom_point()

# Only when we try to look at the value p is it shown
p

# Alternatively, we can explicitly print it
print(p)

# To save to a file
ggsave("test.png", p)

# This is an alternative method that works with "base R" plots as well:
png("test.png")
print(p)
dev.off()</pre>
```

3.6.1 Tip about sizing

Figures in papers tend to be quite small. This means text must be proportionately larger than we usually show on screen. Dots should also be proportionately larger, and lines proportionately thicker. The way to achieve this using ggsave is to specify a small width and height, given in inches. To ensure the output also has good resolution, specify a high dots-per-inch, or use a vector-graphics format such as PDF or SVG.

```
ggsave("test2.png", p, width=3, height=3, dpi=600)
```

Chapter 4

Proteomics Data Viz

4.1 Visualizing Proteomics data with ggplot2

Last session we worked on Cross-linking Mass Spectrometry Data. The data consisted of interaction between 300 yeast nuclear proteins. We also learned about concepts behind Grammer of Graphics and plotting using ggplot2.

In this tutorial, we will be working on the data from Yeast Nuclear Protein interaction study using Cross-linking Mass Spectrometry.

```
library(tidyverse)
```

We continue with the Cross-linking Proteomics dataset from Cytoscape tutorial. The data was in excel, therefore we first converted it into Comma separated file (csv) format.

4.1.1 Optional: Reading excel file into R

If you want to load the excel files files directly to R then you can use another library readxl.

```
library(readxl)
nuclear_xl_ms_excel <- readxl::read_excel("r-intro-files/Nuclear_XL_MS.xlsx")</pre>
head(nuclear_xl_ms_excel)
## # A tibble: 6 x 8
     Protein1 Protein2 NameProtein1 NameProtein2 PPINovelty PPIEvidenceInfo~
##
##
     <chr>
              <chr>>
                        <chr>>
                                      <chr>
                                                    <chr>
                                                                <chr>
## 1 P02293
              P04911
                        H2B1
                                      H2A1
                                                    Known
                                                               Structure
## 2 P02293
              P02309
                                      H4
                        H2B1
                                                    Known
                                                               Structure
## 3 P02994
              P32471
                        EF1A
                                      EF1B
                                                    Known
                                                               Structure
## 4 POCX51
              P38011
                        RS16A
                                      GBLP
                                                    Known
                                                               Structure
## 5 P02406
              POCX49
                        RL28
                                      RL18A
                                                    Novel
                                                               STRING
## 6 P33297
              P53549
                        PRS6A
                                      PRS10
                                                    Known
                                                               Structure
## # ... with 2 more variables: TotalNumberOfCSMs <dbl>,
```

NumberUniqueLysLysContacts <dbl>

4.2 Exploring the data

```
library(readxl)
nuclear_xl_ms <- read_csv("r-intro-files/Nuclear_XL_MS.csv")</pre>
head(nuclear xl ms)
## # A tibble: 6 x 8
    Protein1 Protein2 NameProtein1 NameProtein2 PPINovelty PPIEvidenceInfo~
##
    <chr> <chr>
                      <chr>
                                   <chr>
                                                <chr>
                                                           <chr>>
## 1 P02293
                                   H2A1
             P04911
                      H2B1
                                                Known
                                                           Structure
## 2 P02293
             P02309
                      H2B1
                                   Н4
                                                Known
                                                           Structure
## 3 P02994
             P32471
                     EF1A
                                   EF1B
                                                Known
                                                           Structure
## 4 POCX51
             P38011 RS16A
                                   GBLP
                                                Known
                                                           Structure
## 5 P02406
             POCX49 RL28
                                   RL18A
                                                Novel
                                                           STRING
## 6 P33297
             P53549 PRS6A
                                   PRS10
                                                Known
                                                           Structure
## # ... with 2 more variables: TotalNumberOfCSMs <dbl>,
      NumberUniqueLysLysContacts <dbl>
Now lets examine the dataset with two base R functions str and summary
str(nuclear_xl_ms)
## Classes 'spec_tbl_df', 'tbl_df', 'tbl' and 'data.frame': 228 obs. of 8 variables:
## $ Protein1
                               : chr
                                      "P02293" "P02293" "P02994" "P0CX51" ...
## $ Protein2
                                      "P04911" "P02309" "P32471" "P38011" ...
                               : chr
## $ NameProtein1
                                      "H2B1" "H2B1" "EF1A" "RS16A" ...
                               : chr
                                      "H2A1" "H4" "EF1B" "GBLP" ...
## $ NameProtein2
                              : chr
                                      "Known" "Known" "Known" "Known" ...
## $ PPINovelty
                               : chr
                                      "Structure" "Structure" "Structure" ...
## $ PPIEvidenceInfoGroup
                               : chr
   $ TotalNumberOfCSMs
                               : num
                                      36 21 20 13 13 12 12 12 11 10 ...
   $ NumberUniqueLysLysContacts: num 12 6 5 1 2 3 2 3 3 1 ...
   - attr(*, "spec")=
    .. cols(
##
##
         Protein1 = col_character(),
##
         Protein2 = col_character(),
##
         NameProtein1 = col_character(),
         NameProtein2 = col_character(),
##
##
         PPINovelty = col_character(),
##
         PPIEvidenceInfoGroup = col_character(),
         TotalNumberOfCSMs = col_double(),
##
##
         NumberUniqueLysLysContacts = col_double()
     ..)
summary(nuclear_xl_ms)
##
     Protein1
                        Protein2
                                         NameProtein1
                                                            NameProtein2
## Length:228
                      Length:228
                                         Length:228
                                                            Length: 228
## Class:character Class:character Class:character
                                                            Class : character
```

```
##
                       Mode
   Mode
        :character
                            :character
                                          Mode :character
                                                             Mode
                                                                   :character
##
##
##
##
    PPINovelty
                       PPIEvidenceInfoGroup TotalNumberOfCSMs
   Length:228
                                            Min. : 1.000
##
                       Length:228
   Class : character
                       Class : character
                                            1st Qu.: 1.000
   Mode :character
                       Mode :character
                                            Median : 1.000
##
                                            Mean : 2.706
##
                                            3rd Qu.: 3.000
##
                                            Max.
                                                   :36.000
##
   NumberUniqueLysLysContacts
##
   Min.
          : 1.000
##
   1st Qu.: 1.000
   Median : 1.000
         : 1.342
##
   Mean
   3rd Qu.: 1.000
##
##
  Max.
           :12.000
```

While the data in PPINovelty and PPIEvidenceInfoGroup are characters/strings, they can also be thought of as categorical.

We will now look into the unique values for the PPINovelty and PPIEvidenceInfoGroup columns

```
nuclear_xl_ms$PPINovelty %>% unique()

## [1] "Known" "Novel"

nuclear_xl_ms$PPIEvidenceInfoGroup %>% unique()

## [1] "Structure" "STRING" "APID" "Unexplained" "Genetic"
```

R has a class for categorical data known as factors. We can convert these columns to factors and provide an order to those categories (levels). By default, R will order the levels of a factor alphabetically but we can override this behaviour by defining the level order. Here we will order the Evidence based on Strength of evidence for the interaction

```
nuclear_xl_ms <- nuclear_xl_ms %>% mutate(
 PPINovelty = factor(PPINovelty),
  PPIEvidenceInfoGroup = factor(PPIEvidenceInfoGroup, levels = c("Structure", "APID", "STRI
)
nuclear_xl_ms %>% str()
## Classes 'spec_tbl_df', 'tbl_df', 'tbl' and 'data.frame': 228 obs. of 8 variables:
##
   $ Protein1
                                       "P02293" "P02293" "P02994" "P0CX51" ...
                                : chr
   $ Protein2
                                       "P04911" "P02309" "P32471" "P38011" ...
##
                                : chr
                                       "H2B1" "H2B1" "EF1A" "RS16A" ...
##
   $ NameProtein1
```

```
## $ PPINovelty : Factor w/ 2 levels "Known", "Novel": 1 1 1 1 2 1 2 1 1 1
## $ PPIEvidenceInfoGroup : Factor w/ 5 levels "Structure", "APID", ..: 1 1 1 3 1 3
## $ TotalNumberOfCSMs : num 36 21 20 13 13 12 12 12 11 10 ...
```

"H2A1" "H4" "EF1B" "GBLP" ...

: chr

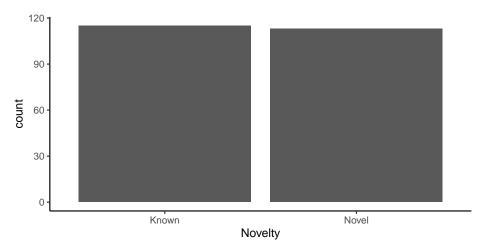
\$ NameProtein2

##

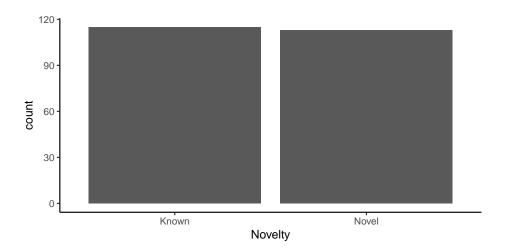
\$ NumberUniqueLysLysContacts: num 12 6 5 1 2 3 2 3 3 1 ...

4.3 Plotting interactions types

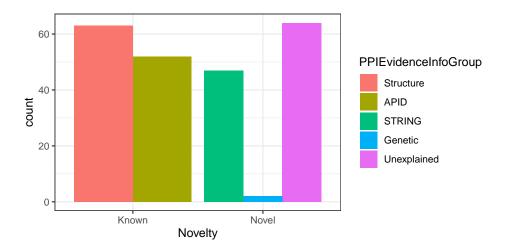
Firstly we will plot the number of Known and novel interactions using with geom_bar



Now, we will rotate the bars to Y-Axis using position="dodge"



Next, step would be to create a stacked bar chart by adding **PPIEvidenceInfoGroup** data on top of each bar



4.4 Individual Proteins

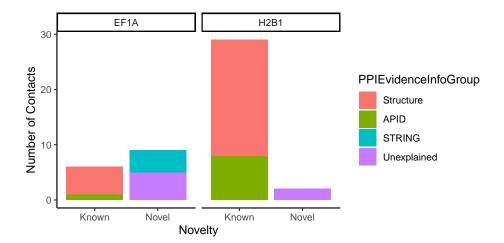
First we will calculate how many times a protein appeared in **NameProtein1** column using **table** function and then sorting by descending order. Next we will use **head()** function to print first five proteins with most observation.

```
table(nuclear_xl_ms$NameProtein1) %>% sort(.,decreasing = TRUE) %>% head()
##
##
    H2B1
         EF1A RL27A
                            EF3A
                                   ODP2
                         НЗ
                          4
We could do same thing for NameProtein2 column as well.
table(nuclear_xl_ms$NameProtein2) %>% sort(.,decreasing = TRUE) %>% head()
##
##
          RS15 NOP56 BFR1 PRS4 RL14A
      Н3
##
                          3
                                3
Now we store the rows containing H2B1 and EF1A proteins in NameProtein1
```

Now we store the rows containing H2B1 and EF1A proteins in **NameProtein1** column in a datafame.

```
two_protein_df<- nuclear_xl_ms %>% filter(NameProtein1 %in% c("H2B1","EF1A"))
ggplot(two_protein_df, aes(x=PPINovelty, y=NumberUniqueLysLysContacts)) +
```

```
geom_col(aes(fill=PPIEvidenceInfoGroup)) +
labs(x= "Novelty",
y= "Number of Contacts") +
facet_wrap(~NameProtein1)+
theme_classic()
```



Chapter 5

Summarizing data

Having loaded and thoroughly explored a data set, we are ready to distill it down to concise conclusions. At its simplest, this involves calculating summary statistics like counts, means, and standard deviations. Beyond this is the fitting of models, and hypothesis testing and confidence interval calculation. R has a huge number of packages devoted to these tasks and this is a large part of its appeal, but is beyond the scope of today.

Loading the data as before, if you have not already done so:

```
library(tidyverse)

geo <- read_csv("r-intro-files/geo.csv")
gap <- read_csv("r-intro-files/gap-minder.csv")
gap_geo <- left_join(gap, geo, by="name")</pre>
```

5.1 Summary functions

R has a variety of functions for summarizing a vector, including: sum, mean, min, max, median, sd.

```
mean( c(1,2,3,4) )
## [1] 2.5
We can use these on the Gapminder data.
gap2010 <- filter(gap_geo, year == 2010)
sum(gap2010$population)
## [1] 6949495061
mean(gap2010$life_exp)
## [1] NA</pre>
```

Missing values 5.2

Why did mean fail? The reason is that life exp contains missing values (NA).

```
gap2010$life_exp
     [1] 56.20 76.31 76.55 82.66 60.08 76.85 75.82 73.34 81.98 80.50 69.13 73.79
    [13] 76.03 70.39 76.68 70.43 79.98 71.38 61.82 72.13 71.64 76.75 57.06 74.19
##
    [25] 77.08 73.86 57.89 57.73 66.12 57.25 81.29 72.45 47.48 56.49 79.12 74.59
    [37] 76.44 65.93 57.53 60.43 80.40 56.34 76.33 78.39 79.88 77.47 79.49 63.69
##
    [49] 73.04 74.60 76.72 70.52 74.11 60.93 61.66 76.00 61.30 65.28 80.00 81.42
    [61] 62.86 65.55 72.82 80.09 62.16 80.41 71.34 71.25 57.99 55.65 65.49 32.11
##
   [73] 71.58 82.61 74.52 82.03 66.20 69.90 74.45 67.24 80.38 81.42 81.69 74.66
##
    [85] 82.85 75.78 68.37 62.76 60.73 70.10 80.13 78.20 68.45 63.80 73.06 79.85
   [97] 46.50 60.77 76.10
                               NA 73.17 81.35 74.01 60.84 53.07 74.46 77.91 59.46
## [109] 80.28 63.72 68.23 73.42 75.47 65.38 69.74
                                                        NA 66.18 76.36 73.55 54.48
                         NA 68.26 80.73 80.90 77.36 58.78 60.53 81.04 76.09 65.33
## [121] 66.84 58.60
            NA 77.85 58.70 74.07 77.92 69.03 76.30 79.84 79.52 73.66 69.24 64.59
## [133]
## [145]
            NA 75.48 71.64 71.46
                                     NA 68.91 75.13 64.01 74.65 73.38 55.05 82.69
## [157] 75.52 79.45 61.71 53.13 54.27 81.94 74.42 66.29 70.32 46.98 81.52 82.21
## [169] 76.15 79.19 69.61 59.30 76.57 71.10 58.74 69.86 72.56 76.89 78.21 67.94
            NA 56.81 70.41 76.51 80.34 78.74 76.36 68.77 63.02 75.41 72.27 73.07
## [181]
## [193] 67.51 52.02 49.57 58.13
R will not ignore these unless we explicitly tell it to with na.rm=TRUE.
mean(gap2010$life_exp, na.rm=TRUE)
## [1] 70.34005
Ideally we should also use weighted.mean here, to take population into account.
weighted.mean(gap2010$life_exp, gap2010$population, na.rm=TRUE)
## [1] 70.96192
NA is a special value. If we try to calculate with NA, the result is NA
NA + 1
## [1] NA
is.na can be used to detect NA values, or na.omit can be used to directly remove
rows of a data frame containing them.
is.na(c(1,2,NA,3))
## [1] FALSE FALSE TRUE FALSE
cleaned <- filter(gap2010, !is.na(life exp))</pre>
weighted.mean(cleaned$life_exp, cleaned$population)
## [1] 70.96192
```

5.3 Grouped summaries

The summarize function in dplyr allows summary functions to be applied to data frames.

```
summarize(gap2010, mean_life_exp=weighted.mean(life_exp, population, na.rm=TRUE))
## # A tibble: 1 x 1
##
     mean_life_exp
##
              <dbl>
## 1
               71.0
So far unremarkable, but summarize comes into its own when the group_by
"adjective" is used.
summarize(
    group_by(gap_geo, year),
    mean_life_exp=weighted.mean(life_exp, population, na.rm=TRUE))
## # A tibble: 22 x 2
##
       year mean_life_exp
##
      <dbl>
                     <dbl>
##
    1 1800
                      30.9
##
    2 1810
                      31.1
    3 1820
                      31.2
##
##
    4 1830
                      31.4
##
    5 1840
                      31.4
##
    6 1850
                      31.6
##
    7
       1860
                      30.3
##
    8
       1870
                      31.5
##
    9
       1880
                      32.0
## 10
       1890
                      32.5
## # ... with 12 more rows
```

Challenge: summarizing

What is the total population for each year? Plot the result.

Advanced: What is the total GDP for each year? For this you will first need to calculate GDP per capita times the population of each country.

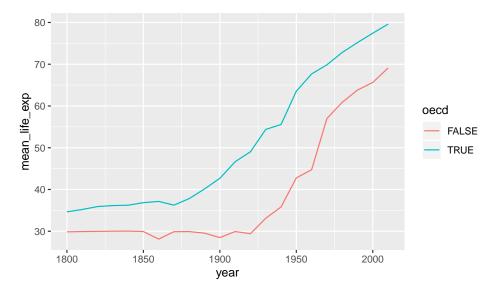
group_by can be used to group by multiple columns, much like count. We can use this to see how the rest of the world is catching up to OECD nations in terms of life expectancy.

```
result <- summarize(
   group_by(gap_geo,year,oecd),</pre>
```

```
mean_life_exp=weighted.mean(life_exp, population, na.rm=TRUE))
result
## # A tibble: 44 x 3
```

```
## # Groups:
               year [22]
       year oecd mean life exp
      <dbl> <lgl>
##
                            <dbl>
##
       1800 FALSE
                             29.9
    2
       1800 TRUE
                             34.7
##
##
    3
       1810 FALSE
                             29.9
                             35.2
##
    4
       1810 TRUE
                             30.0
##
    5
       1820 FALSE
##
    6
       1820 TRUE
                             35.9
##
    7
       1830 FALSE
                             30.0
##
    8
       1830 TRUE
                             36.2
##
       1840 FALSE
                             30.0
    9
       1840 TRUE
## 10
                             36.2
  # ... with 34 more rows
```

ggplot(result, aes(x=year,y=mean_life_exp,color=oecd)) + geom_line()



A similar plot could be produced using <code>geom_smooth</code>. Differences here are that we have full control over the summarization process so we were able to use the exact summarization method we want (<code>weighted.mean</code> for each year), and we have access to the resulting numeric data as well as the plot. We have reduced a large data set down to a smaller one that distills out one of the stories present in this data. However the earlier visualization and exploration activity using <code>ggplot2</code> was essential. It gave us an idea of what sort of variability was present in the data, and any unexpected issues the data might have.

5.4 t-test

We will finish this section by demonstrating a t-test. The main point of this section is to give a flavour of how statistical tests work in R, rather than the details of what a t-test does.

Has life expectancy increased from 2000 to 2010?

```
gap2000 <- filter(gap_geo, year == 2000)
gap2010 <- filter(gap_geo, year == 2010)

t.test(gap2010$life_exp, gap2000$life_exp)

##

## Welch Two Sample t-test

##

## data: gap2010$life_exp and gap2000$life_exp

## t = 3.0341, df = 374.98, p-value = 0.002581

## alternative hypothesis: true difference in means is not equal to 0

## 95 percent confidence interval:

## 1.023455 4.792947

## sample estimates:

## mean of x mean of y

## 70.34005 67.43185</pre>
```

Statistical routines often have many ways to tweak the details of their operation. These are specified by further arguments to the function call, to override the default behaviour. By default, t.test performs an unpaired t-test, but these are repeated observations of the same countries. We can specify paired=TRUE to t.test to perform a paired sample t-test and gain some statistical power. Check this by looking at the help page with ?t.test.

It's important to first check that both data frames are in the same order.

```
all(gap2000$name == gap2010$name)

## [1] TRUE

t.test(gap2010$life_exp, gap2000$life_exp, paired=TRUE)

##

## Paired t-test

##

## data: gap2010$life_exp and gap2000$life_exp

## t = 13.371, df = 188, p-value < 2.2e-16

## alternative hypothesis: true difference in means is not equal to 0

## 95 percent confidence interval:

## 2.479153 3.337249

## sample estimates:

## mean of the differences

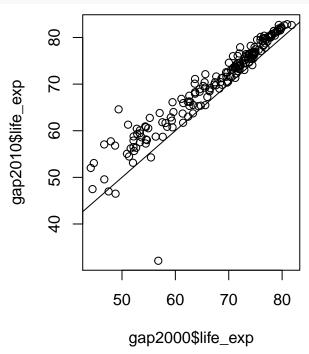
## mean of the differences

## 2.908201</pre>
```

When performing a statistical test, it's good practice to visualize the data to

make sure there is nothing funny going on.

```
plot(gap2000$life_exp, gap2010$life_exp)
abline(0,1)
```



This is a visual confirmation of the t-test result. If there were no difference between the years then points would lie approximately evenly above and below the diagonal line, which is clearly not the case. However the outlier may warrant investigation.

Thinking in R

The result of a t-test is actually a value we can manipulate further. Two functions help us here. class gives the "public face" of a value, and typeof gives its underlying type, the way R thinks of it internally. For example numbers are "numeric" and have some representation in computer memory, either "integer" for whole numbers only, or "double" which can hold fractional numbers (stored in memory in a base-2 version of scientific notation).

class(42)

[1] "numeric"

typeof (42)

[1] "double"

Let's look at the result of a t-test:

```
result <- t.test(gap2010$life_exp, gap2000$life_exp, paired=TRUE)
class(result)
## [1] "htest"
typeof(result)
## [1] "list"
names(result)
    [1] "statistic"
                       "parameter"
                                     "p.value"
                                                    "conf.int"
                                                                  "estimate"
    [6] "null.value"
                                     "alternative" "method"
                       "stderr"
                                                                  "data.name"
result$p.value
## [1] 4.301261e-29
```

In R, a t-test is just another function returning just another type of data, so it can also be a building block. The value it returns is a special type of vector called a "list", but with a public face that presents itself nicely. This is a common pattern in R. Besides printing to the console nicely, this public face may alter the behaviour of generic functions such as plot and summary.

Similarly a data frame is a list of vectors that is able to present itself nicely.

Lists

Lists are vectors that can hold anything as elements (even other lists!). It's possible to create lists with the list function. This becomes especially useful once you get into the programming side of R. For example writing your own function that needs to return multiple values, it could do so in the form of a list.

```
mylist <- list(hello=c("Hello","world"), numbers=c(1,2,3,4))
mylist

## $hello
## [1] "Hello" "world"
##
## $numbers
## [1] 1 2 3 4
class(mylist)

## [1] "list"
typeof(mylist)
## [1] "list"
names(mylist)

## [1] "hello" "numbers"</pre>
```

Accessing lists can be done by name with \$ or by position with [[]].

```
mylist$hello
```

```
## [1] "Hello" "world"
mylist[[2]]
```

[1] 1 2 3 4

Other types not covered here

Matrices are another tabular data type. These come up when doing more mathematical tasks in R. They are also commonly used in bioinformatics, for example to represent RNA-Seq count data. A matrix, as compared to a data frame:

- contains only one type of data, usually numeric (rather than different types in different columns).
- commonly has rownames as well as colnames. (Base R data frames can have rownames too, but it is easier to have any unique identifier as a normal column instead.)
- has individual cells as the unit of observation (rather than rows).

Matrices can be created using as.matrix from a data frame, matrix from a single vector, or using rbind or cbind with several vectors.

You may also encounter "S4 objects", especially if you use Bioconductor¹ packages. The syntax for using these is different again, and uses **2** to access elements.

Programming

Once you have a useful data analysis, you may want to do it again with different data. You may have some task that needs to be done many times over. This is where programming comes in:

- Writing your own functions².
- For-loops³ to do things multiple times.
- If-statements⁴ to make decisions.

The "R for Data Science" book⁵ is an excellent source to learn more. Monash Data Fluency "Programming and Tidy data analysis in R" course⁶ also covers this.

¹http://bioconductor.org/

 $^{^2} http://r4ds.had.co.nz/functions.html \\$

³http://r4ds.had.co.nz/iteration.html

 $^{^4} http://r4ds.had.co.nz/functions.html\#conditional-execution$

⁵http://r4ds.had.co.nz/

 $^{^6} https://monashdata fluency.github.io/r-progtidy/\\$

Chapter 6

R Markdown

6.1 Introduction to markdown

Markdown is a powerful "language" for writing different kinds of documents, such as **PDF** or **HTML** in an efficient way, but markdown documents can also be published as is. The underlying idea for then markdown is that it is easy-to-write and easy-to-read.

You can use any text editor¹ to write your markdown. RStudio² already has an inbuilt text editor and because it also has a few additional things that make markdown writing much easier, we are going to use it's text editor.

There are a few different flavours of markdown around. We're going to mention a few but only focus on one, R $Markdown^3$

- CommonMark⁴
- GitHub Flavored Markdown (GFM)⁵
- R Markdown⁶

R markdown⁷ like most other flavours builds on top of standard markdown. It has some R language⁸ specific features as well as bunch of general enhancers to markdown. When R Markdown⁹ is coupled with Rstudio¹⁰ it creates a powerfull means of documenting your work while you are doing it, which you can then share with colleagues and the public in rapid and clean way.

Let's get right into it. Open **R Markdown file** using these drop down menu steps: **File** -> **New File** -> **R Markdown**. You can put any **title** and any

¹https://en.wikipedia.org/wiki/Text_editor

 $^{^2 {\}rm https://rstudio.com}$

³https://rmarkdown.rstudio.com/

⁴http://commonmark.org/

⁵https://guides.github.com/features/mastering-markdown/

⁶https://rmarkdown.rstudio.com/

 $^{^7 \}mathrm{http://R\%20Markdown.rstudio.com/}$

⁸https://www.r-project.org/

⁹http://R%20Markdown.rstudio.com/

¹⁰https://rstudio.com

author name. For now select Document and Document type HTML. Once you have opened your .Rmd file, click on the Knit HTML button at the top of your pane.

Knitr is an R package that does all the magic of converting and running your R markdown and R code respectively.

These are three main parts to any R markdown document

1. YAML header section (will talk about it at the very end)

title: "Hello world" author: "Kirill" date: "13 July 2016" output: html_document 2. The R code blocks section ```{r} plot(pressure)

3. Everything else is plain old markdown

Have I been Marked Down

6.2 Document types

There are numerous document types that you can turn your markdown into. This all depends on the tool, markdown compiler, but for Rstudio¹¹ at least these a few that a supported.

6.2.0.1 Documents

- html_notebook Interactive R Notebooks
- html_document HTML document w/ Bootstrap CSS
- pdf_document PDF document (via LaTeX template)
- word_document Microsoft Word document (docx)

6.2.0.2 Presentations (slides)

• ioslides_presentation - HTML presentation with ioslides

¹¹https://rstudio.com

6.2.0.3 More

- tufte::tufte_handout PDF handouts in the style of Edward Tufte
- tufte::tufte_html HTML handouts in the style of Edward Tufte
- tufte::tufte_book PDF books in the style of Edward Tufte

More here 12

We are not going to cover all of them, we are mainly going to be working with either html_document or html_notebook both produce very similar results though behave slightly differently. We'll try to touch a little on ioslides_presentation towards the end.

6.3 Vanilla Markdown

There's actually not that much to core (vanilla) markdown. Essentially all of it can be summarised below:

```
# Header1
## Header2
### Header3

Paragraphs are separated
by a blank line.

Two spaces at the end of a line
produces a line break.

Text attributes _italic_,
**bold**, `monospace`.

Horizontal rule:
---
Bullet list:
    * apples
    * oranges
```

* pears

Numbered list:

- 1. wash
- 2. rinse
- repeat

A [link](http://example.com).

 $^{^{12} \}rm https://rmarkdown.rstudio.com/lesson-9.html$

- ![Image](link_to_image)
- > Markdown uses email-style
- > characters for blockquoting.

Which produces:

Chapter 7

Header1

7.1 Header2

7.1.1 Header3

Paragraphs are separated by a blank line.

Two spaces at the end of a line produces a line break.

Text attributes italic, bold, monospace.

Horizontal rule:

Bullet list:

- apples
- oranges
- pears

Numbered list:

- 1. wash
- 2. rinse
- 3. repeat

A $link^{1}$.

Markdown uses email-style > characters for block quoting.

Whenever I need a refresher on markdown basics, I use this cheatsheet².

¹http://example.com

 $^{^2} https://github.com/adam-p/markdown-here/wiki/Markdown-Cheatsheet$

7.1.2 Practice vanilla markdown

Now it's just a matter of learning some of the markdown syntax. Let's delete all current text from the opened document except the YAML header and type this new text in Hello world, I'm learning R markdown! and pressing the Knit HTML button.

Hello world, I'm learning R markdown!

Not much happened. This is because we didn't mark our text in any way. You can put as much text as you want and it will appear as is, unless "specially" marked to look differently.

Now add the # symbol at the start of the line and press the Knit HTML button again. We'll be pressing this button a lot! For those who like keyboard short cuts use ctrl+shift+k instead.

Hello world, I'm learning R markdown!

How about now? A single hash symbol made it whole lot bigger didn't it? We've marked this whole line to be the header line.

Now make three new lines with the same text, but different numbers of # symbols, one, two and three respectively and keep pressing the Knit HTML button

```
### Hello world, I'm learning R markdown!
## Hello world, I'm learning R markdown!
# Hello world, I'm learning R markdown!
```

This is how you can specify different headers type using markdown.

Let's now practice making very short document in markdown with a main topic section and two subsections. We will add short sentences in each section. We will start with main section header and a quote. Let's type the following text and knit our document.

Learning Markdown

> I'm still learning

Now let's add three bullet points summarising what we are going to learn next and then knit the document again.

Learning Markdown

> I'm still learning

Here I'll be learning:

- markdown
- R Markdown
- ggplot2

Now let's add each one of those bullet items as a subsection to the main "Learning Markdown" section. We are going to use ## to mark subsections and don't forget to knit again.

```
# Learning Markdown
> I'm still learning
Here I'll be learning:
- markdown
- R Markdown
- git and github
## Markdown
## R Markdown
## ggplot2
Now let's add a sentence to each section, briefly describing what they are.
# Learning Markdown
> I'm still learning
Here I'll be learning:
- markdown
- R Markdown
- git and github
## Markdown
Here I'll learng vanilla markdown
## R Markdown
```

Whereas here I'll be learning R Markdown

ggplot2

And this section is about plotting

Let's add a emphasis to some of the words in our document. We are going to add *italic* emphasis to the word "vanilla" and we are going to add **bold** emphasis to the capital letter "R" in the word R Markdown. You'll need to knit your document still.

- # Learning Markdown
- > I'm still learning

Here I'll be learning:

- markdown

```
- R Markdown
```

- git and github

Markdown

Here I'll learning _vanilla_ markdown

R Markdown

Whereas here I'll be learning R Markdown

ggplot2

And this section is about plotting

Remember that vanilla markdown³ is comprised entirely of punctuation characters.

7.2 R Markdown

The reason that we are learning R Markdown⁴ is because it gives us a very straightforward way of writing plain text documents with inline R code that will become a very sophisticated document types. The bonus points also come from the fact that R Markdown files are easy to version control (git) and see the difference between versions.

This approach of interleaving analysis code, commentary and description is very explicit, which has direct implication in reproducibility, shareability and collaboration.

7.2.1 Embedding R code

An R chunk is a "special" block within the document that will be read and evaluated by knitr, ultimately converting everything into plain markdown. But for us it means that we can focus on our analysis and embed R code without having to worry about it. Additionally there are large number of chunk options that helps with different aspects of the document including code decoration and evaluation, results and plots rendering and display.

This is how an R code chunk looks like. If you want to include code into your documents it has to be via R chunks. You can further customise the appearance of your code in the final document with chunk options.

```{r}

- - -

<sup>&</sup>lt;sup>3</sup>https://daringfireball.net/projects/markdown/syntax

<sup>&</sup>lt;sup>4</sup>https://rmarkdown.rstudio.com/

The little r there specifies the "engine", basically telling R Markdown how to evaluate the code inside the chunk. Here we are saying use R engine (language) to evaluate the code. The list of languages<sup>5</sup> is rather long, R Markdown can span a much greater area then one might think. In this workshop we are only going to focus on R language.

Let's write our first bit of R code inside the R Markdown document. First we need to start a new R chunk, which we can be done in these ways:

- simply type it out
- press insert button at the top of the window
- ctrl+alt+i

Let's return to our document with the main header section Learning R Markdown. Now let's add simple R code to our chunk, type the following code a <- "Hello world, I'm learning R Markdown!" and press knitr button to build html document. Note that as mentioned above we need to use print() statement to get the content of the variable to the scree/final document.

```
```{r}
a <- 'Hello world, I'm learning R Markdown !'
print(a)</pre>
```

Tip: each chunk can be run independently in the console by pressing ctrl^enter or little green arrow.

7.2.2 Chunk Options

We can tweak many things about your output using different options that we can include inside curly brackets e.g

```
```{r chunk_options, more_chunk_options...}
```

The two rather common options are echo=TRUE and eval=TRUE, both by default are set to true and this is why we didn't have to pass them in previously.

- echo means show what has been typed in i.e show the code in the final document
- eval means evaluate or execute that code

Sometimes we might want to show the code, but not execute it and other times we might just want to execute it and get the results without actually bore audience with the code.

Let's try both of these options one at a time. We start with passing echo=FALSE options first

```
```{r, echo = FALSE}
print("Hello world, I'm learning R Markdown")
```

 $^{^5 \}rm https://bookdown.org/yihui/R\%20Markdown/language-engines.html$

Okay, we shouldn't see our original print() statement in the output document. And now let's pass eval=FALSE options instead

```
```{r eval = FALSE}
print("Hello world, I'm learning R markdown !")
```
```

And now we should only see the result of the print() statement and no output.

Here is a nice reference⁶ that has comprehensive cover of all the options you can pass in.

Let's now try a different example and use the gapminder dataset from the ggplot2 segment for this next example.

```
library(tidyverse)
geo <- readr::read_csv('r-intro-files/geo.csv')
gap <- read_csv('r-intro-files/gap-minder.csv')
gap_geo <- left_join(gap, geo, by='name')
head(gap_geo)
library(tidyverse)
geo <- read_csv("r-intro-files/geo.csv")
gap <- read_csv("r-intro-files/gap-minder.csv")
gap_geo <- left_join(gap, geo, by="name")
head(gap_geo)</pre>
```

```
## # A tibble: 6 x 11
##
     name
            year population gdp_percap life_exp region oecd g77
                                                                        lat
                                                                               long
##
     <chr> <dbl>
                       <dbl>
                                   <dbl>
                                            <dbl> <chr> <lgl> <lgl> <dbl>
                                                                              <dbl>
## 1 Afgh~
                     3280000
                                                                              66
            1800
                                    603
                                             28.2 asia
                                                         FALSE TRUE
                                                                       33
            1800
## 2 Alba~
                                             35.4 europe FALSE FALSE
                                                                       41
                                                                              20
                     410445
                                    667
                                                                       28
                                                                               3
## 3 Alge~
            1800
                     2503218
                                    715
                                             28.8 africa FALSE TRUE
## 4 Ando~
            1800
                        2654
                                    1197
                                                  europe FALSE FALSE
                                                                       42.5
                                                                               1.52
## 5 Ango~
            1800
                     1567028
                                    618
                                             27.0 africa FALSE TRUE
                                                                      -12.5
                                                                              18.5
## 6 Anti~
                                    757
                                             33.5 ameri~ FALSE TRUE
            1800
                       37000
                                                                       17.0 -61.8
## # ... with 1 more variable: income2017 <chr>
```

This table is a bit ugly to look at in your final document. We'll come back to data-frame printing later in the YAML section.

Note: you might be thinking that you've already run library(tidyverse) previously in the session and that you already have tidyverse packages loaded, you shouldn't need to run the command again. When you knit a document, it ignores the state of your RStudio session and runs through the code from start to finish. If your code points to missing files or uses packages that haven't been explicitly loaded somewhere in the document, it will fail to render your document.

 $^{^6 \}rm https://bookdown.org/yihui/rmarkdown/r-code.html$

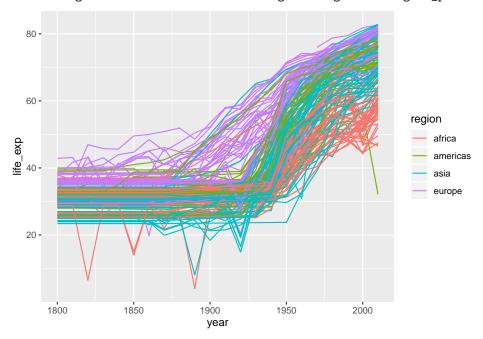
Remember: You can go between R Markdown and *console*, to check your code, at any time. You should see your code block is highlighted differently and you should see a green arrow at the right hand site of that block. Press the green arrow to get an output in the *console*. You can also use ctrl+enter to do the same with the keyboard short cut.

How about little data exploration? From the ggplot2 segment, we can include some plots into our html document, rather than saving the plots to file, moving the plots off the server onto our local computer, then manually including them into a document.

```
color=region)) +
geom_line()
ggplot(gap_geo, aes(x=year, y=life_exp, group=name, color=region)) +
geom_line()
color=region)) +
```



geom_line()

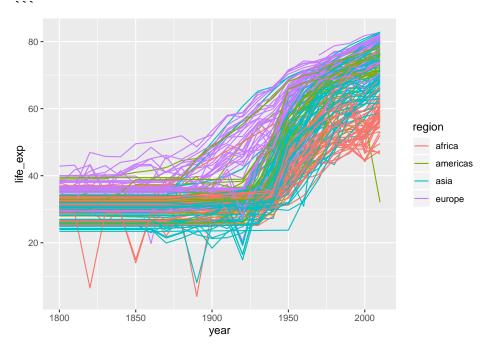


Here is a perfect example where we can hide our code from the viewer, since it isn't most interesting bit about this data. Let's turn echo=FALSE options for all our plots below. We also don't want to get that warning message included in the final document, so we can also include warning=FALSE.

Figure alignment can be done with fig.align options e.g {r fig.align=default}. default means what ever your style sheet has. The other options are, "left", "center" and "right". let's try one out.

```
```{r echo = FALSE, fig.align = 'right', warning=FALSE}
ggplot(gap_geo, aes(x=year, y=life_exp, group=name, color=region)) +
```

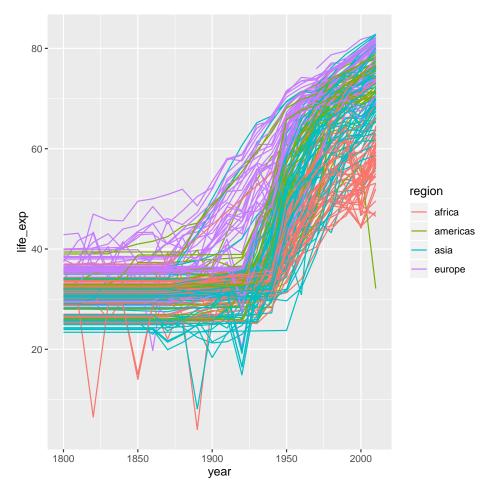
## geom\_line()



Remember that you can you always execute code in the *console* by pressing "green arrow" or using keyborad short cut ctrl+enter

We now know how to align figure to where we want, how about changing the size of it? We can do that with fig.height and fig.width, the units are inches. Let's make  $4 \times 4$  inches figure e.g {r fig.height=6, fig.width=6} . and also align the figure to the center

```{r echo = FALSE, fig.align = 'center', warning=FALSE, fig.height=6, fig.width=6}
ggplot(gap_geo, aes(x=year, y=life_exp, group=name, color=region)) +
geom_line()



One last thing we'd like to share with you is how to add a figure legend or a caption - with fig.cap of course e.g {r, fig.cap="This is my legend"} . Go ahead and add a figure description.

```{r echo = FALSE, fig.align = 'center', warning=FALSE, fig.height=6, fig.width=6, fig.ca
ggplot(gap\_geo, aes(x=year, y=life\_exp, group=name, color=region)) +
geom\_line()

Note that the figure legend follows the same alignment as the figure itself.

There are more chunk options which we encourage you to explore in greater depth in the R Markdown documentation<sup>7</sup>. We have only examined a handful of figure specific options but there are many more options that allow fine control over the behavior of the code and cosmetics of the document.

Lastly, we'll mention that the engine option can be used to specifcy different language types. So you can embed python, BASH, Javascript and a heap of other languages<sup>8</sup> all within the same document.

<sup>&</sup>lt;sup>7</sup>https://bookdown.org/yihui/rmarkdown/r-code.html

 $<sup>^8</sup> https://bookdown.org/yihui/rmarkdown/language-engines.html\\$ 

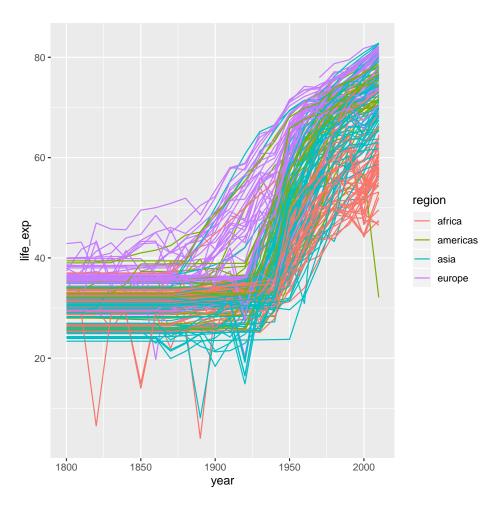


Figure 7.1: This figure illustrates the life expectancy from 1800 to 2000 by region.

#### 7.3 YAML header

At the very top of your .Rmd file you can, optionaly, include a YAML block. In this block you can fine turn your output document, add some metadata and change the document's font and theme. You can also pass additional files such as stylesheet file .css and bibliography file .bib for text citation. We're only going to show you a few possible options and will let you explore the rest on your own.

Navigate to the top of your .Rmd document and find the YAML section there. Just like with the options we passed in to manipulate R code block, YAML block also has  $\mathbf{key} = \mathbf{value}$  pairs, but instead they are separated by colon (:). Now let's add table of content to our document, this will make it easier to navigate your page as well as give nice over view of the content our  $\mathbf{key}$  is  $\mathbf{toc}$  with value  $\mathbf{true}$  or  $\mathbf{yes}$  which one you prefer better.

title: "Hello world"
author: "Kirill"
date: "13 July 2016"
output:
 html\_document:
 toc: true

Note that you need to bring html\_document onto new line and indent it with two spaces. html\_document is a value of output key. output can have other values e.g pdf\_document, word\_document. However html\_document also becomes a key for toc value and toc becames a key for its own value.

Now that we have sort out the initial YAML layout, we can continue adding more options to style our HTML document. The other two useful options that I like to pass in are toc\_depth and number\_sections

title: "Hello world"
author: "Kirill"
date: "13 July 2016"
output:
 html\_document:
 toc: true
 toc\_depth: 4
 number\_sections: yes

Most of those options are self explanatory. The best way to learn what each does, is to pass them in. Note that you can comment lines out inside YAML section with # symbol.

Another two options that can change your document apperance are theme and highlight<sup>9</sup>. There are number of different themes and highlight options. I

 $<sup>^9 \</sup>text{https://bookdown.org/yihui/rmarkdown/html-document.html\#appearance-and-style}$ 

suggest you find the one you like in your own time.

Remember when we printed the gap\_geo, the table rendered wasn't particularly nice to look at? We can control the behavior of tables in html documents in the YAML header<sup>10</sup>. There are a number of options to select one from and pass to df\_print.

```
Try out paged.

output:
 html_document:
 toc: true
 toc_depth: 4
 df_print: paged
```

#### 7.4 Alternate Formats

As mentioned in previous section, output has many options, one of which is ioslides\_presentation. You can simple add:

```
title: "Hello world"
author: "Kirill"
date: "13 July 2016"
output: ioslides_presentation
```

at the top of your document and your .Rmd files will be compiled to a slide presentation instead.

Another way to start with an ioslides\_presentation is select **presentation** options when you were opening R markdown file. Either way you'll notice YAML header reflects your selected output type.

Let's open new R markdown document and let's select presentation instead and let's select HTML (ioslides) option there. You can still save your files as <code>.Rmd</code>, and then press the the <code>Knit HTML</code> button.

The syntax for the document is more or less the same, except ## is now used to mark new slide.

ioslides are fairly basic in terms of slideshow presentations. If you find yourself frustrated with the limitations of ioslides, there are a number of official format options  $^{11}$ , we haven't had much experience with using them. I've been using the xaringan package  $^{12}$ , which isn't an official R Markdown format but I've found it to be quite powerful, though requires a fair degree of familiarity with R Markdown/HTMl/CSS.

 $<sup>^{10} \</sup>rm https://bookdown.org/yihui/rmarkdown/html-document.html\#data-frame-printing$ 

 $<sup>^{11} \</sup>rm https://rmarkdown.rstudio.com/formats.html$ 

 $<sup>^{12} \</sup>rm https://github.com/yihui/xaringan$ 

Alternatively, if you want to produce a PDF document:

---

title: "Hello world" author: "Kirill" date: "13 July 2016" output: pdf\_document

R Markdown documents that render to PDF are compatible with raw LaTeX. The df\_print option is not compatible with paged but will take kable and tibble. If changing document type, it's always important to check which YAML options will carry to the new format and which won't.

The more format specific syntax used in a document, the harder it is to swap a document from one format to another. For example, you can generate a very detailed and customised PDFs from an R Markdown document with heavy usage of LaTeX. However, LaTeX will not be rendered in a HTML document. So it's important to have an idea of how the final document will be used as you work through it.

#### 7.5 Extras

• R Markdown cheatsheet <sup>13</sup>

For a more in-depth R-Markdown tutorial, we recommend:

- R Markdown: The Definitive Guide 14
- bookdown: Authoring Books and Technical Documents with R Markdown<sup>15</sup>
   the bookdown package greatly extends R Markdown
- R for Reproducible Research<sup>16</sup> a workshop delivered by the Monash Bioinformatics Platform focused on R Markdown and reproducible workflows with git.

#### 7.5.1 Code chunk names

You can name code chunks! In your R-Studio session this even adds a little table of contents in the bottom left of your source panel that lets you navigate your R Markdown document via headers and code chunk names.

```
```{r chunk_name, chunk_opts...}
```

¹³https://rstudio.com/wp-content/uploads/2015/02/rmarkdown-cheatsheet.pdf

¹⁴https://bookdown.org/yihui/rmarkdown/

¹⁵https://bookdown.org/yihui/bookdown/

 $^{^{16} \}rm https://monashdata fluency.github.io/r-rep-res/$

7.5.2 html document or html notebook

We've been using the html_document format for most of this tutorial. A very similar looking document is the html_notebook. There's a large overlap in terms of YAML options for both.

```
e.g:
---
output:
  html_notebook:
   toc: true
   toc_depth: 4
   df_print: paged
```

One difference is that a html_notebook will include a button on the rendered webapge to download the .Rmd file that generated the html file. This is one way to easily share the document, in that someone can view your report and then download it and run it on their own machine.

The other difference is that when rendering a html_document, it will ignore the state of the RStudio session and re-run every code block. Variables that have been exist within the environment but have not been defined inside the html_document will cause the render step to fail and must be included for the document to render successfully.

A html_notebook however uses the state of the session. It will only include the output of code blocks that have been run. It's less 'safe' using a notebook, because it doesn't double-check that the document from start to finish is self-contained. It can include variables and functions that were created seperately in the environment but then the document doesn't include instructions on how that variable was generated or what the function is doing.

7.5.3 Cross-referencing

Let's learn how to add external and internal links to your document, remember the syntax for adding links is <code>[DESCRIPTION]</code> (link-address). The external link that we are going to add is going to be this https://rmarkdown.rstudio.com/. Each one of the bullet points above going to become a link to it section. The way you reference internal section is by starting your address with a <code>#</code> symbol then simply using all lower case letters for the section name and all spaces need to be converted to a dash symbol -. Let's add those things in and re-build our document.

```
# Learning Markdown
> I'm still learning
[External resource](https://rmarkdown.rstudio.com/)
Here I'll be learning:
```

- [markdown] (#markdown)
- [R Markdown] (#R Markdown)
- [git and github] (#git-and-github)

Markdown

Here I'll learng _vanilla_ markdown

R Markdown

Whereas here I'll be learning **R**markdown

ggplot2

And this section is about plotting

A bonus exercise is to add logos to each sections. Search internet for:

- Markdown logo, and add the image using syntax
- R Markdown logo, and add the image using syntax
- Git logo, and add the image using syntax
- ggplot2 logo, and add the image using syntax

Note for the external resource that is on internet the address must start with www or https otherwise address will be interpreted as file path.

Chapter 8

Next steps

8.1 Deepen your understanding

Our number one recommendation is to read the book "R for Data Science" by Garrett Grolemund and Hadley Wickham.

Also, statistical tasks such as model fitting, hypothesis testing, confidence interval calculation, and prediction are a large part of R, and one we haven't demonstrated fully today. Linear models, and the linear model formula syntax ~, are core to much of what R has to offer statistically. Many statistical techniques take linear models as their starting point, including limma² for differential gene expression, glm for logistic regression (etc), survival analysis with coxph, and mixed models to characterize variation within populations.

- "Statistical Models in S" by J.M. Chambers and T.J. Hastie is the primary reference for this, although there are some small differences between R and its predecessor S.
- "An Introduction to Statistical Learning" by G. James, D. Witten, T. Hastie and R. Tibshirani can be seen as further development of the ideas in "Statistical Models in S", and is available online. It has more of a machine learning than a statistics flavour to it (the distinction is fuzzy!).
- "Modern Applied Statistics with S" by W.N. Venable and B.D. Ripley is a well respected reference covering R and S.
- "Linear Models with R" and "Extending the Linear Model with R" by J. Faraway⁴ cover linear models, with many practical examples.

¹http://r4ds.had.co.nz/

²https://bioconductor.org/packages/release/bioc/html/limma.html

 $^{^3}$ http://www-bcf.usc.edu/~gareth/ISL/

 $^{^4}$ http://www.maths.bath.ac.uk/~jjf23/

8.2 Expand your vocabulary

Have a look at these cheat sheets to see what is possible with R.

- RStudio's collection of cheat sheets⁵ cover newer packages in R.
- An old-school cheat sheet⁶ for dinosaurs and people wishing to go deeper.
- A Bioconductor cheat sheet⁷ for biological data.

The R Manuals⁸ are the place to look if you need a precise definition of how R behaves.

8.3 Join the community

Join the Data Fluency community at Monash⁹.

- Mailing list for workshop and event announcements.
- Slack for discussion.
- Monthly seminars on Data Science topics.
- Drop-in sessions on Friday afternoon.

Meetups in Melbourne:

- $MelbURN^{10}$
- R-Ladies¹¹

The Carpentries¹² run intensive two day workshops on scientific computing and data science topics worldwide. The style of this present workshop is very much based on theirs. For bioinformatics, COMBINE¹³ is an Australian student and early career researcher organization, and runs Carpentries workshops and similar.

⁵https://www.rstudio.com/resources/cheatsheets/

 $^{{}^6{\}rm https://cran.r-project.org/doc/contrib/Short-refcard.pdf}$

⁷https://github.com/mikelove/bioc-refcard/blob/master/README.Rmd

⁸https://cran.r-project.org/manuals.html

⁹https://www.monash.edu/data-fluency

¹⁰https://www.meetup.com/en-AU/MelbURN-Melbourne-Users-of-R-Network/

¹¹https://www.meetup.com/en-AU/R-Ladies-Melbourne/

¹² https://carpentries.org/

¹³https://combine.org.au/