Appendix D

Reproducible analysis and workflow

The notion that scientific findings can be confirmed repeatedly through *replication* is fundamental to the centuries-old paradigm of science. The underlying logic is that if you have identified a truth about the world, that truth should persist upon further investigation by other observers. In the physical sciences, there are two challenges in replicating a study: replicating the experiment itself, and *reproducing* the subsequent data analysis that led to the conclusion. More concisely, replicability means that different people get the same results with *different* data. Reproducibility means that the same person (or different people) get the same results with the *same* data.

It is easy to imagine why replicating a physical experiment might be difficult, and not being physical scientists ourselves, we won't tackle those issues here. On the other hand, the latter challenge of reproducing the data analysis is most certainly our domain. It seems like a much lower hurdle to clear—isn't this just a matter of following a few steps? Upon review, for a variety of reasons many scientists are in fact tripping over even this low hurdle.

To further explicate the distinction between *replicability* and *reproducibility*, recall that scientists are legendary keepers of lab notebooks. These notebooks are intended to contain all of the information needed to carry out the study again (i.e., replicate): reagents and other supplies, equipment, experimental material, etc. Modern software tools enable scientists to carry this same ethos to data analysis: Everything needed to repeat the analysis (i.e., reproduce) should be recorded in one place.

Even better, modern software tools allow the analysis to be repeated at the push of a button. This provides a proof that the analysis being documented is in fact exactly the same as the analysis that was performed. Moreover, this capability is a boon to those generating the analysis. It enables them to draft and redraft the analysis until they get it exactly right. Even better, when the analysis is written appropriately, it's straightforward to apply the analysis to new data. Spreadsheet software, despite its popularity, is not suitable for this. Spreadsheet software references specific rows and columns of data, and so the analysis commands themselves need to be updated to conform to new data.

The "replication crisis" is a very real problem for modern science. More than ten years ago, John Ioannidis argued that "most published research findings are false." [118] More recently, the journal *Nature* ran a series of editorials bemoaning the lack of replicability in published research [67]. It now appears that even among peer-reviewed, published scientific articles, many of the findings—which are supported by experimental and statistical evidence—do not hold up under the scrutiny of replication. That is, when other researchers try to do the same study, they don't reliably reach the same conclusions.

Some of the issues leading to irreproducibility are hard to understand, let alone solve. Much of the blame involves multiplicity and the "garden of forking paths" introduced in Chapter 7. While we touch upon issues related to null hypothesis testing in Chapter 7, the focus of this chapter is on modern workflows for *reproducible data analysis*, since the ability to regenerate a set of results at a later point in time is a necessary but not sufficient condition for reproducible results.

Reproducible workflows consist of three components: a fully scriptable statistical programming environment (such as R or Python), reproducible analysis (first described as literate programming), and version control (commonly implemented using GitHub).

D.1 Scriptable statistical computing

In order for data analysis to be reproducible, all of the steps taken in the analysis have to be recorded in a linear fashion. Scriptable applications like Python, R, SAS, and Stata do this by default. Even when graphical user interfaces to these programs are used, they add the automatically generated code to the history so that it too can be recorded. Thus, the full series of commands that make up the data analysis can be recorded, reviewed, and transmitted. Contrast this with the behavior of spreadsheet applications like Microsoft Excel and Google Sheets, where it is not always possible to fully retrace one's steps.

D.2 Reproducible analysis with R Markdown

The concept of *literate programming* was introduced by Knuth decades ago [127]. His advice was:

> "Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do."

Central to this prescription is the idea that the relevant documentation for the code—which is understandable not just to the programmer, but to other human beings as well—occurs alongside the code itself. In data analysis, this is manifest as the need to have three kinds of things in one document: the code, the results of that code, and the written analysis. We belong to a growing group of people who find the `rmarkdown` [5] and `knitr` packages [239] to be an environment that is ideally suited to support a reproducible analysis workflow [23].

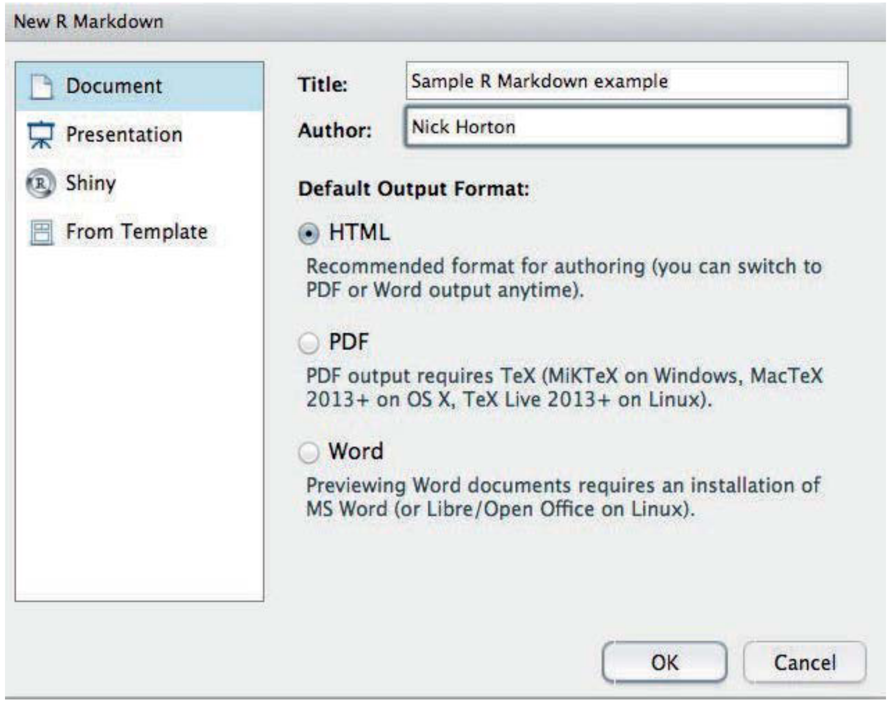
The `rmarkdown` and `knitr` packages use a *source file* and *output file* paradigm. This approach is common in programming, but is fundamentally different than a "what-you-see-is-what-you-get" editor like Microsoft Word or Google Drive. Code is typed into the source document, which is then rendered into an output format that is readable by anyone. The principles of literate programming stipulates that the source file should *also* be readable by anyone.

We favor the simple document markup language R Markdown [4] for most applications. An R Markdown source file can be rendered (by `knitr`, leveraging `pandoc`) into PDF, HTML, and Microsoft Word formats. The resulting document will contain the R code, the results of that code, and the analyst's written analysis.

Markdown is well-integrated with RStudio, and both LaTeX and Markdown source files can be rendered via a single-click mechanism. More details can be found in [239] and [82] as well as the CRAN reproducible research task view [128] (see also `http://yihui.name/knitr`).

As an example of how these systems work, we demonstrate a document written in the Markdown format using data from the `SwimRecords` data frame. Within RStudio, a new template R Markdown file can be generated by selecting `R Markdown` from the `New File` option on the `File` menu. This generates the dialog box displayed in Figure D.1. The default output format is HTML, but other options (PDF or Microsoft Word) are available.

Pro Tip: The R Markdown templates included with the `mosaic` package are useful to set up more appropriate defaults for graph and font size. These can be accessed using the "From Template" option when opening a new R Markdown file.



Title: Sample R Markdown example

Author: Nick Horton

Default Output Format:

(●) HTML

Recommended format for authoring (you can switch to PDF or Word output anytime).

( ) PDF

PDF output requires TeX (MiKTeX on Windows, MacTeX 2013+ on OS X, TeX Live 2013+ on Linux).

( ) Word

Previewing Word documents requires an installation of MS Word (or Libre/Open Office on Linux).

Figure D.1: Generating a new R Markdown file in RStudio

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Figure D.2 displays a modified version of the default R Markdown input file. The file is given a title (`Sample R Markdown example`) with output format set by default to HTML. Simple markup (such as bolding) is added through use of the `**` characters before and after the word `Help`. Blocks of code are begun using the `‘‘‘{r}` command and closed with a `‘‘‘` command (three back quotes).

The formatted output can be generated and displayed by clicking the `Knit HTML` button in RStudio, or by using the commands in the following code block, which can also be used

~~~
---
title: "Sample R Markdown example"
author: "Sample User"
date: "November 8, 2016"
output: html_document
---

```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)
library(mdsr)
```

## R Markdown

This is an R Markdown document. Markdown is a simple formatting syntax for
authoring HTML, PDF, and MS Word documents. For more details on using R
Markdown see http://rmarkdown.rstudio.com.

When you click the **Knit** button a document will be generated that
includes both content as well as the output of any embedded R code chunks
within the document. You can embed an R code chunk like this:

```{r display}
glimpse(SwimRecords)
```

## Including Plots

You can also embed plots, for example:

```{r scatplot, echo=FALSE}
ggplot(data = SwimRecords, aes(x = year, y = time)) +
  geom_point() + aes(colour = sex)  +
  stat_smooth(method = loess, se = FALSE) + theme(legend.position = "right") +
  labs(title = "100m Swimming Records over time")
```

There are n=`r nrow(SwimRecords)` rows in the Swim records dataset.

Note that the `echo = FALSE` parameter was added to the code chunk to
prevent printing of the R code that generated the plot.
~~~

Figure D.2: Sample R Markdown input file.

when running R without the benefit of RStudio.

```
library(rmarkdown)
render("filename.Rmd")   # creates filename.html
browseURL("filename.html")
```

The `render()` function extracts the R commands from a specially formatted R Markdown input file (`filename.Rmd`), evaluates them, and integrates the resulting output, including text and graphics, into an output file (`filename.html`). A screenshot of the results of performing these steps on the `.Rmd` file displayed in Figure D.2 is displayed in Figure D.3. `render()` uses the value of the `output:` option to determine what format to generate. If the `.Rmd` file specified `output: word_document`, then a Microsoft Word document would be created.

Alternatively, a PDF or Microsoft Word document can be generated in RStudio by selecting `New` from the `R Markdown` menu, then clicking on the PDF or Word options.

RStudio also supports the creation of R Presentations using a variant of the R Markdown syntax. Instructions and an example can be found by opening a new `R presentations` document in RStudio.

D.3 Projects and version control

A useful feature of RStudio is projects. A project provides a separate workspace. Selecting a project also reorients your RStudio environment to a specified directory, in the process reorienting the Files tab, the working directory, etc. Once you start working on multiple projects, being able to switch back and forth becomes very helpful.

Given that data science has been called a "team sport," the ability to track changes to files and discuss issues in a collaborative manner is an important prerequisite to reproducible analysis. Projects can be tied to a *version control system*, such as Subversion or Git. These systems help you and your collaborators keep track of changes to files, so that you can go back in time to review changes to previous pieces of code, compare versions, and retrieve older versions as needed.

Pro Tip: While critical for collaboration with others, source code version control systems are also useful for individual projects because they document changes and maintain version histories. In such a setting, the collaboration is with your future self!

GitHub is a cloud-based implementation of Git that is tightly integrated into RStudio. It works efficiently, without cluttering your workspace with duplicate copies of old files or compressed archives. RStudio users can collaborate on projects hosted on GitHub without having to use the command line. This has proven to be an effective way of ensuring a consistent, reproducible workflow, even for beginners. This book was written collaboratively through a private repository on GitHub, just as the `mdsr` package is maintained in a public repository.

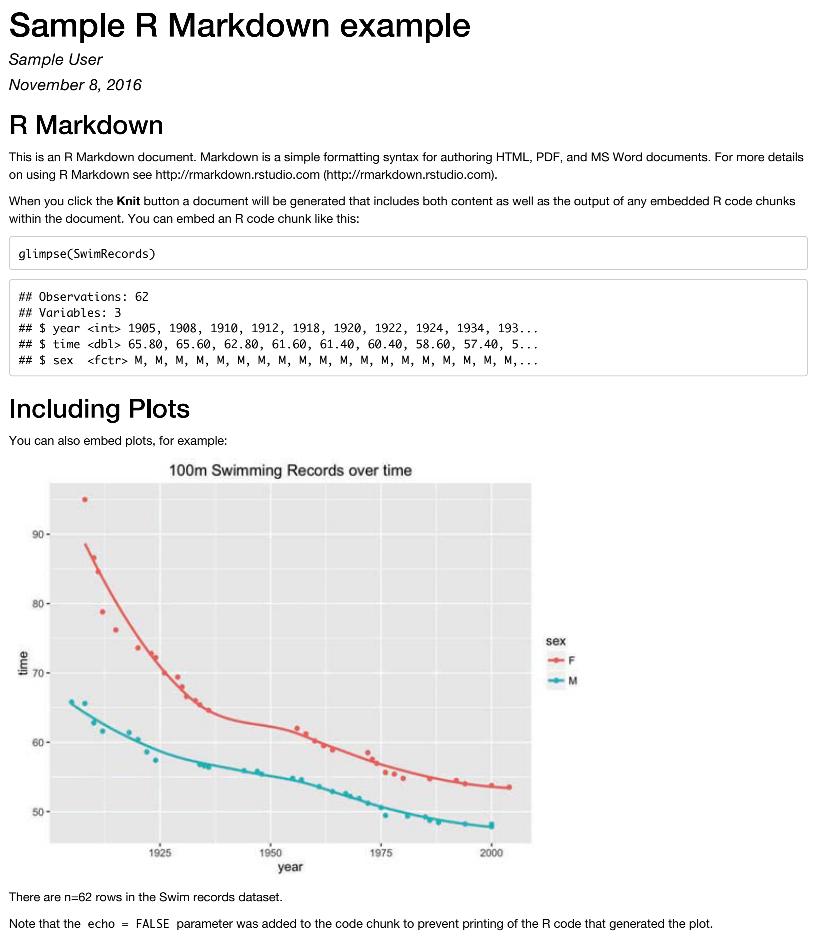
D.4 Further resources

Project TIER is an organization at Haverford College that has developed a protocol [12] for reproducible research. Their efforts originated in the social sciences using Stata, but have since expanded to include R.

R Markdown is under active development. For the latest features see the R Markdown authoring guide at `http://rmarkdown.rstudio.com`. The RStudio cheat sheet serves as a useful reference.

GitHub can be challenging to learn but is now the default in many (most?) data science research settings. Jenny Bryan's resources on "Happy Git and GitHub for the useR" (`http://happygitwithr.com`) are particularly relevant for new data scientists beginning to use GitHub.

Another challenge for reproducible analyses concerns versions of R and other R packages. The `packrat` package helps ensure that projects can maintain a particular version of R and set of packages. This functionality is tied in closely with RStudio.



Sample R Markdown example

Sample User

November 8, 2016

R Markdown

This is an R Markdown document. Markdown is a simple formatting syntax for authoring HTML, PDF, and MS Word documents. For more details on using R Markdown see http://rmarkdown.rstudio.com (http://rmarkdown.rstudio.com).

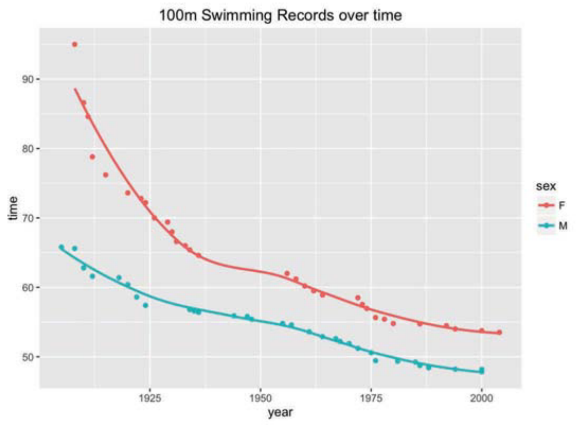
When you click the **Knit** button a document will be generated that includes both content as well as the output of any embedded R code chunks within the document. You can embed an R code chunk like this:

```
glimpse(SwimRecords)
```

```
## Observations: 62
## Variables: 3
## $ year <int> 1905, 1908, 1910, 1912, 1918, 1920, 1922, 1924, 1934, 193...
## $ time <dbl> 65.80, 65.60, 62.80, 61.60, 61.40, 60.40, 58.60, 57.40, 5...
## $ sex  <fctr> M, M, M, M, M, M, M, M, M, M, M, M, M, M, M, M, M, M, M,...
```

Including Plots

You can also embed plots, for example:



There are n=62 rows in the Swim records dataset.

Note that the `echo = FALSE` parameter was added to the code chunk to prevent printing of the R code that generated the plot.

Figure D.3: Formatted output from R Markdown example.

D.5 Exercises

Exercise D.1

The following exercises provide practice with R Markdown files and introduce useful features. Consider an R Markdown file that includes the following code chunks. What will be output when this file is rendered?

~~~
```{r}
x <- 1:5
```

```{r}
x <- x + 1
```

```{r}
x
```
~~~

Exercise D.2

Consider an R Markdown file that includes the following code chunks. What will be output when this file is rendered?

~~~
```{r echo=FALSE}
x <- 1:5
```

```{r echo=FALSE}
x <- x + 1
```

```{r echo=FALSE}
x
```
~~~

Exercise D.3

Consider an R Markdown file that includes the following code chunks. What will be output when the file is rendered?

~~~
```{r echo=FALSE}
x <- 1:5
```

```{r echo=FALSE, eval=FALSE}
x <- x + 1
```

```{r echo=FALSE}
x
```
~~~

Exercise D.4

Consider an R Markdown file that includes the following code chunks. What will be output when the file is rendered?

~~~
```{r echo=FALSE}
x <- 1:5
```

```{r echo=FALSE}
x <- x + 1
```

```{r include=FALSE}
x
```
~~~

Exercise D.5

Describe in words what the following excerpt from an R Markdown file will display when rendered.

~~~
```{r echo=FALSE}
n <- 679
```

The data set has n=`r n` observations.
~~~

Exercise D.6

Describe in words what the following excerpt from an R Markdown file will display when rendered.

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

Exercise D.7

Describe the implications of changing `warning=TRUE` to `warning=FALSE` in the following code chunk.

~~~
```{r warning=TRUE}
sqrt(-1)
```
~~~

Exercise D.8

Why does the `mosaic` package plain R Markdown template include the code chunk option `message=FALSE` when the `mosaic` package is loaded?

Exercise D.9

Describe how the `fig.width` and `fig.height` chunk options can be used to control the size of graphical figures.

Exercise D.10

Explain what the following code chunks will display and why this might be useful for technical reports from a data science project.

~~~~
```{r chunk1, eval=TRUE, include=FALSE}
x <- 15
x
```

```{r chunk2}
x <- x + 3
x
```

```{r chunk1, eval=FALSE, include=TRUE}
```
~~~~

Exercise D.11

The `xtable` package allows the analyst to display nicely formatted tables and results when outputting to pdf files. Use the following code chunks as an example to create a similar display using your own data.

~~~~
```{r results="asis"}
library(xtable)
library(mdsr)
options(xtable.comment = FALSE)
mod <- lm(cesd ~ mcs + sex, data = HELPrct)
xtable(mod)
```
~~~~

Exercise D.12

Insert a chunk in your .Rmd document so that it renders even when there are errors. Some errors are easier to diagnose if you can execute specific R statements during rendering and leave more evidence behind for forensic examination.

Put this chunk near the top of your R Markdown document if you want to soldier on through errors, i.e., turn `foo.Rmd` into `foo.md` and/or `foo.html` no matter what.

~~~~
``{r setup, include = FALSE, cache = FALSE}
knitr::opts_chunk$set(error = TRUE)
```
~~~~

This is also helpful if you are writing a tutorial and want to demo code that throws an error.

It's also possible to set things so that errors are tolerated in a specific chunk.

~~~~
``{r alwaysrun, error = TRUE}
## code goes here
```
~~~~

Use either of these strategies to generate an R Markdown file that includes an error but compiles nonetheless. (Kudos to Jenny Bryan for describing this approach.)