Developing a Workflow to Maximize Reproducibility and Research Impact: Managing Data, Computer Code, and Projects for Success

Althea A. ArchMiller & John R. Fieberg

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Welcome!

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Althea A. ArchMiller *Assistant Professor, Biology, Concordia College, MN*

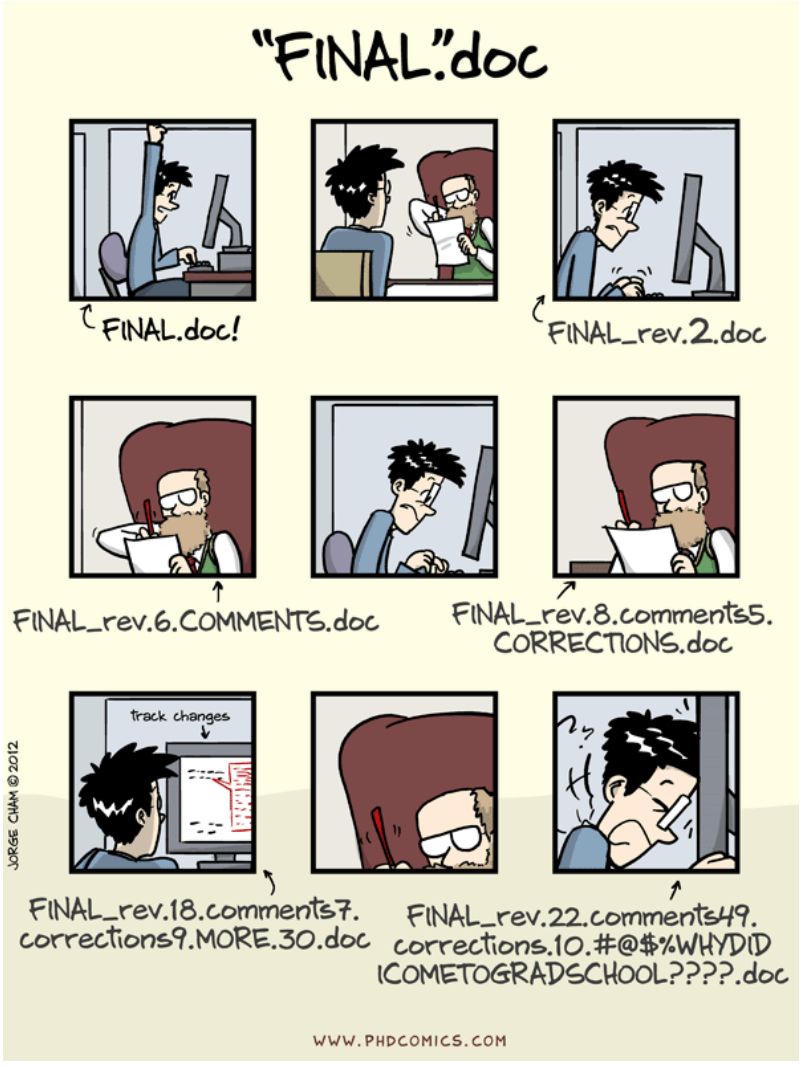
John R. Fieberg *Associate Professor of Quantitative Ecology, University of Minnesota*

Before we begin, please open up the reproducible_workshop repository in RStudio and install these packages:

- knitr
- ezknitr
- devtools

Why worry about reproducibility?

Working towards future reproducibility makes my code easier for my collaborators (and me) to read, run, and debug today,
and that's why I think reproducibility is a **win-win for all researchers**."
-Althea



Why worry about reproducibility?

"[Reproducibility] provides security, saves time, and forces me to be more thoughtful about my workflow." - Ethan Young

- make your life easier! Now, and in the future
- collaborations
- broader research impact
- increased citations
- transparency
- grant and journal requirements

Is my research reproducible?

- What formats are your research documents stored in?

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  - .txt
  - .pdf
  - .html
  - .R/.Rdata
    - YES!

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  - .txt
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  - .html
  - .R/.Rdata
    - YES!
  - .doc/.docx
  - .sas
  - .xls/.xlsx
  - any other proprietary file format
    - NO!

Is my research reproducible?

- Is your code linear?
  - Clear environment often and at beginning of script
  - Don't save .Rdata or history
  - Each program should focus on one main task or analysis
  - Don't rely on manual commenting/uncommenting

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So, what's wrong here?

```
# What variables are significant?
lm.out <- lm(weight ~ height, data = trial.data)
remove(lm.out) # clear previous lm.out for each
               #   new lm() definition above

# Is the relationship significant?
#     (If not, clear and try a new regressor)
summary(lm.out)
```

Is my research reproducible?

- Are your files easily shared with others?
  - Organized directory structure
  - Files relatively linked
  - Well-documented & commented
  - Consistency in coding practices

"The point of having style guidelines is to have a common vocabulary of coding so people can concentrate on *what* you are saying, rather than on *how* you are saying it." - Google's R Style Guide

Workshop Outline

The goal for this workshop is to help you develop the tools to develop a workflow to maximize reproducibility, collaborations, and research impact.

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2. R-Markdown and R-Oxygen for documenting your code and creating reproducible reports

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1. RStudio Projects for organizing data, code, and output
2. R-Markdown and R-Oxygen for documenting your code and creating reproducible reports
3. GitHub for version-control, collaborating and archiving

1. RStudio Projects

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- Raw data
- Processed data
- Analysis scripts
- Paper/Manuscript-related documents
- Sharing documents ("transmittals")
- Metadata
- Maps or other deliverables

RStudio Projects provide an opportunity for you to organize and manage all of these types of folders in **one place** in a way that **relatively links** everything together and **eases sharing**.

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Up next, Activity 1!

Activity 1: Data management and updating

Here, we will read in and process three weeks of experimental data and do some preliminary analysis. Then, we will get a final (4th) week of data, which we will merge with the original data.

The goals are to:

1. Be introduced to RStudio
2. Create a framework for keeping data organized and up-to-date
3. Automatically update our analyses based on the master dataset

Context: Abundance data from ~75 invertebrate species sampled on various beaches along the Dutch coast.

Zuur, A.F., E.N. Ieno, and G.M. Smith (2007) Analysing Ecological Data. Springer, New York.

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Before we begin today, we need sync your individual versions of the workshop documents with Althea's master branch:

1. Open RStudio and your reproducibility_workshop.rproj. (File > Open Project...)
2. Open shell (Tools > Shell...)
3. Type in exactly, then press enter:

```
$ git fetch upstream
```

4. Type in exactly, then press enter:

```
$ git checkout master
```

5. Type in exactly, then press enter:

```
$ git merge upstream/master
```

Activity 1: Data management and updating

Now create a new folder in student_folders/ for all of today's activities. Name the folder after yourself (or an alias).

Open a new R Script file and save it to that new folder as **"activity1a_data_processing.R"**

First, we will read in first three weeks of data and combine them, process the data a little bit, and save the merged/processed data for analysis.

Secondly, we will save another new R Script file as **"activity1b_data_analysis.R"** and do (preliminary) regression analysis.

Finally, we will pretend to have just gotten the final week's data in and update everything in a "reproducible" way.

1. RStudio Projects

Other links

`https://swcarpentry.github.io/r-novice-gapminder/02-project-intro/`

Data Mangement Tips

- Treat data as read-only
  - Don't use Excel, etc, to manipulate raw data
  - Use a single R program for all manipulation
  - Save "cleaned" or "processed" data in easily loadable formats
- Differentiate data types with folders *raw* versus *processed* versus *output* (e.g., linear regression objects, etc)
- Write dates in YYYYMMDD or equivalent format

Why R-Markdown for manuscripts?

"I can do reproducible work in R (making me happy) and format the output report in Word (making my collaborators happy)" - Richard Layton `http://rmarkdown.rstudio.com/articles_docx.html`

Documenting Code

Native R Scripts (.R extensions) (or any analysis code) are generally not designed for reading, but the **knitr** library has been designed for converting R scripts into readable reports, such as Word, PDF, and/or html documents.

Not only do these types of reports help with collaborating, they provide a great framework for archiving your analyses and results.

Example:
`https://conservancy.umn.edu/handle/11299/181607`

Documenting Code

General tips for better coding:

- Consistent and meaningful naming conventions
  - a = b*c
  - weekly.pay = hours.worked*pay.rate (not cross-compatible)
  - weekly_pay = hours_worked*pay_rate
  - weeklyPay = hoursWorked*payRate
- Using YYYYMMDD or equivalent for dates
- When possible, bundle data, code, figures/tables together with **knitr** package using R-Markdown or R-Oxygen languages

Documenting Code: R-Markdown

R-Markdown combines markdown language, which is "an easy-to-write plain text format" and embedded R code chunks that are "run so their output can be included in the final document" [1]

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```
14  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>.
15
16  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:
17
18  ```{r cars}
19  summary(cars)
20  ```
21
```

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.

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```
summary(cars)
```

```
##      speed           dist
##  Min.   : 4.0   Min.   :  2.00
##  1st Qu.:12.0   1st Qu.: 26.00
##  Median :15.0   Median : 36.00
##  Mean   :15.4   Mean   : 42.98
##  3rd Qu.:19.0   3rd Qu.: 56.00
##  Max.   :25.0   Max.   :120.00
```

[1] www.rmarkdown.rstudio.com

Documenting code: R-Markdown

Exercise 2a: Introduction to R-Markdown

- File > New File > R Markdown...
- Choose "html" - optionally put in a title and press "OK"
- This R-Markdown template is ready to "knit" into an html as-is
  - Click the blue Knit button
  - Save in your student_project folder as "activity2a_intro_rmarkdown.Rmd"
  - See the resultant html
- Take a few minutes to modify the .Rmd and view how the changes appear in the knit html document.

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

Documenting code: ezknitr

What folder did the html end up in?

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Now imagine if you wanted to keep the programs/scripts in a folder separate from reports (highly recommended!). You can easily direct the output html file into a different folder using **ezknitr** package.

```
library(ezknitr)
ezknit("student_folders/yours/activity2a_intro_rmarkdown.Rmd",
       out_dir = "student_folders/archmiller_a/reports",
       fig_dir = "figures",
       keep_md = F)
```

Documenting Code: R-Oxygen

Instead of using the R-Markdown language, you can also use **pure R scripts** plus **Roxygen comments** (#') to create fully reproducible reports!

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Additionally, use #+ to define and label R chunks like we did with the "'{r ...} code in the R-Markdown language.

Documenting Code: R-Oxygen

Activity 2b: Introduction to R-Oxygen

Here, we'll quickly convert "activity1b_data_analysis.R" into an html document!

1. Open "activity1b_data_analysis.R"
2. Save As...
   "student_folder/yours/activity2b_intro_roxygen.R"

LaTeX

Another benefit of using knitr/Rmd/Roxygen for creating statistical reports is the nice interface with LaTeX equation syntax.

Activity 3. LaTeX Equations

1. Create a new .Rmd PDF document
2. Save it as "student_folders/yours/activity3_latex.Rmd"
3. Create the following in the output PDF
   - $\alpha + \beta = 2\theta$
   - $\pi^2 = 9.86$
   - $\sum_{i=1}^{n} \sqrt{i} = 42$ (advanced)
4. When you "knit" remember to use ezknitr:

```
library(ezknitr)
ezknit("student_folders/yours/activity3_latex.Rmd",
       out_dir = "student_folders/archmiller_a/reports",
       fig_dir = "figures",
       keep_md = F)
```

https://tobi.oetiker.ch/lshort/lshort.pdf (hint: tables on p75)

Project Workflow w/ RStudio & knitr

Example project directory

- data/
  - raw_data/
  - processed_data/
  - output_data/
- manuscript/
  - ms_figures/
  - transmissions/
  - submission/
- output/
  - figures/
- programs/
- project_file.Rproj

Project Workflow w/ RStudio & knitr

- **data/**
  - **raw_data/**
    - survey_data20161227.csv
    - survey_data20161230.csv
    - survey_data20170103.csv
  - **processed_data/**
    - survey_data_all.Rdata
  - **output_data/**
    - model_out.Rdata

Project Workflow w/ RStudio & knitr

- **programs/**
  - a_data_processing.R
  - b_data_analysis.R
  - c_plots.R

Project Workflow w/ RStudio & knitr

- **output/**
  - a_data_processing.html
  - b_data_analysis.html
  - c_plots.html
  - **figures/**
    - eda1.jpg
    - scatter1.jpg

Project Workflow w/ RStudio & knitr

- **manuscript/**
  - ms.Rmd
  - ms.pdf
  - ms.docx
  - **ms_figures/**
    - fig1.jpg
    - fig2.jpg

Project Workflow w/ RStudio & knitr

- **manuscript/**
  - ms.Rmd
  - ms.pdf
  - ms.docx
  - **ms_figures/**
    - fig1.jpg
    - fig2.jpg
  - **transmittals/**
    - **from_john/**
    - ms20170523.docx
    - ms20170625.docx
    - **from_bob/**
    - ms20170626.docx

Project Workflow w/ RStudio & knitr

- **manuscript/**
  - ms.Rmd
  - ms.pdf
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    - fig1.jpg
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    - ms20170523.docx
    - ms20170625.docx
    - **from_bob/**
    - ms20170626.docx
  - **submission/**
    - ms.pdf
    - fig1.pdf
    - fig2.pdf
    - coverletter.docx

Tips

- Don't use github with large files :-(
- Create new projects in GitHub first, then sync them with RStudio