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

Althea A. ArchMiller & John R. Fieberg

7/12/2017

Welcome!

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

- Althea A. ArchMiller
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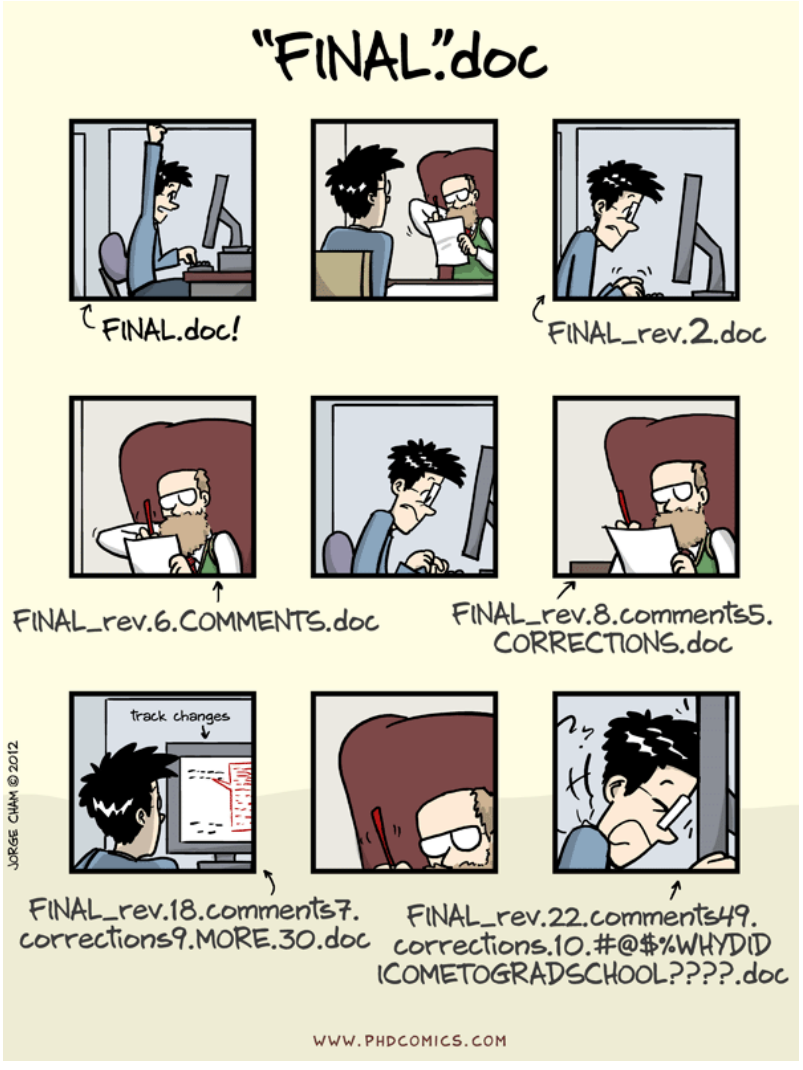
- John R. Fieberg
  - Associate Professor of Quantitative Ecology, College of Fisheries, Wildlife, & Conservation Biology, University of Minnesota

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



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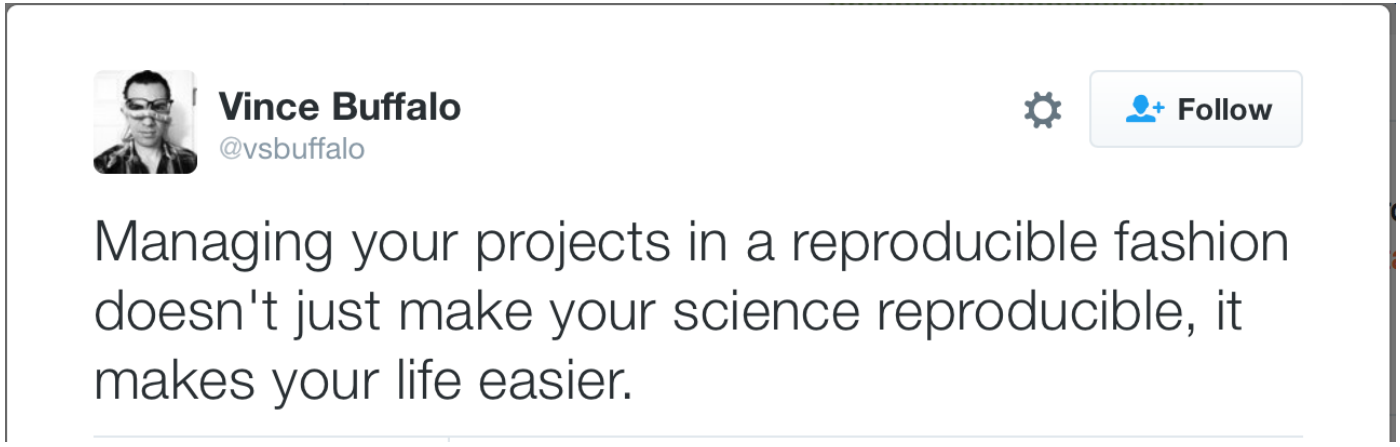

- make your life easier! Now, and in the future
- collaborations
- broader research impact
- increased citations
- transparency
- grant and journal requirements

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

Is my research reproducible?

What formats are your research documents stored in?

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- .pdf
- .html
- .R/.Rdata
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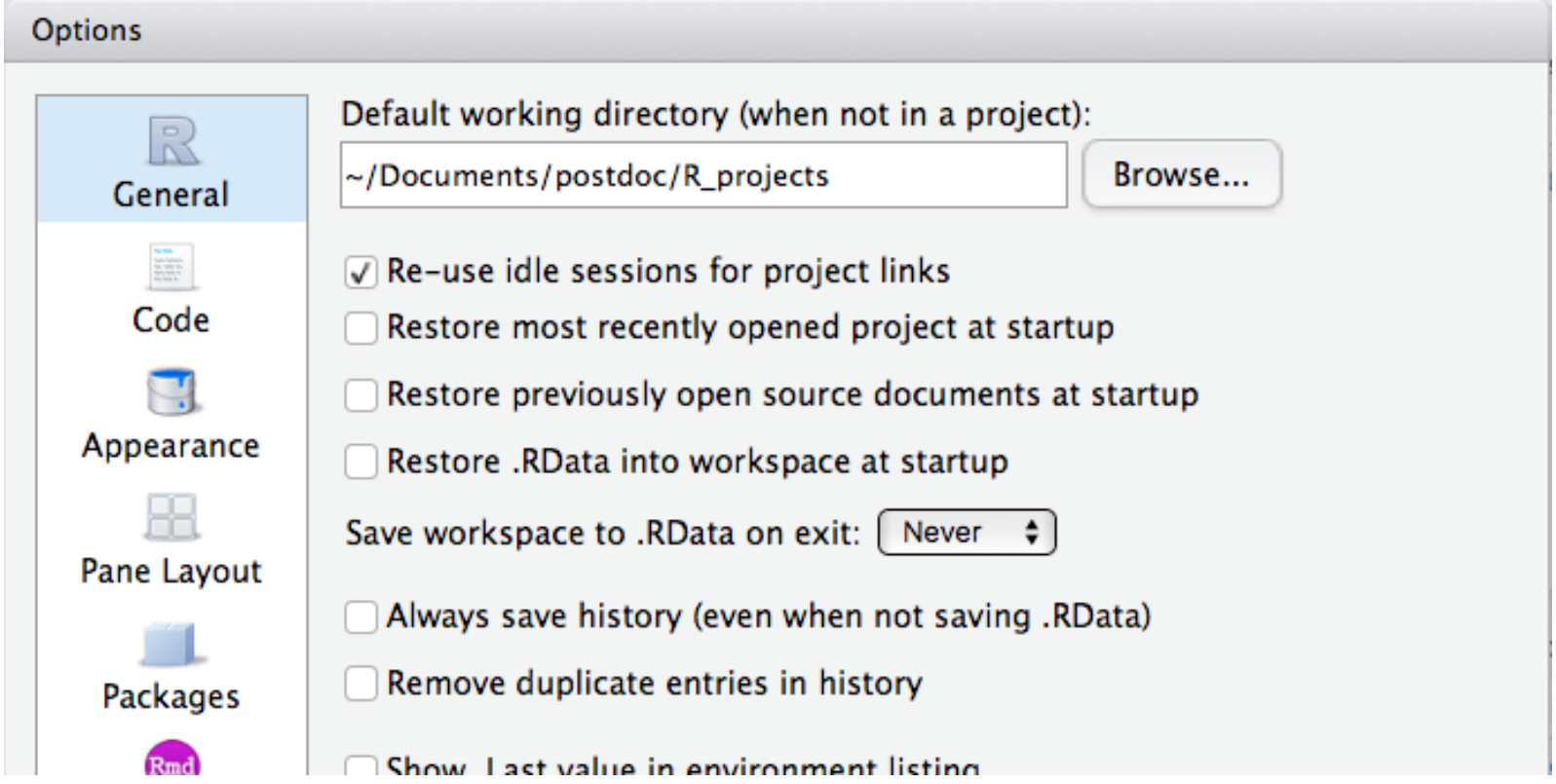
  - YES - these are considered "reproducible"!
- .doc/.docx
- .sas
- .xls/.xlsx
- any other proprietary file format
  - NO - these are not "reproducible"!

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



Is my research reproducible?

So, what's wrong here?

```
# Here, I want to know what variables are significant?
#       I will try each variable in turn
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 variable)
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

Is my research reproducible?

Do you treat your data as read-only?

- Don't use Excel, etc., to manipulate raw data
- Use an R script for data processing
  - Process data in one script, then save for loading into subsequent scripts
- When archiving, provide both raw data and processing code

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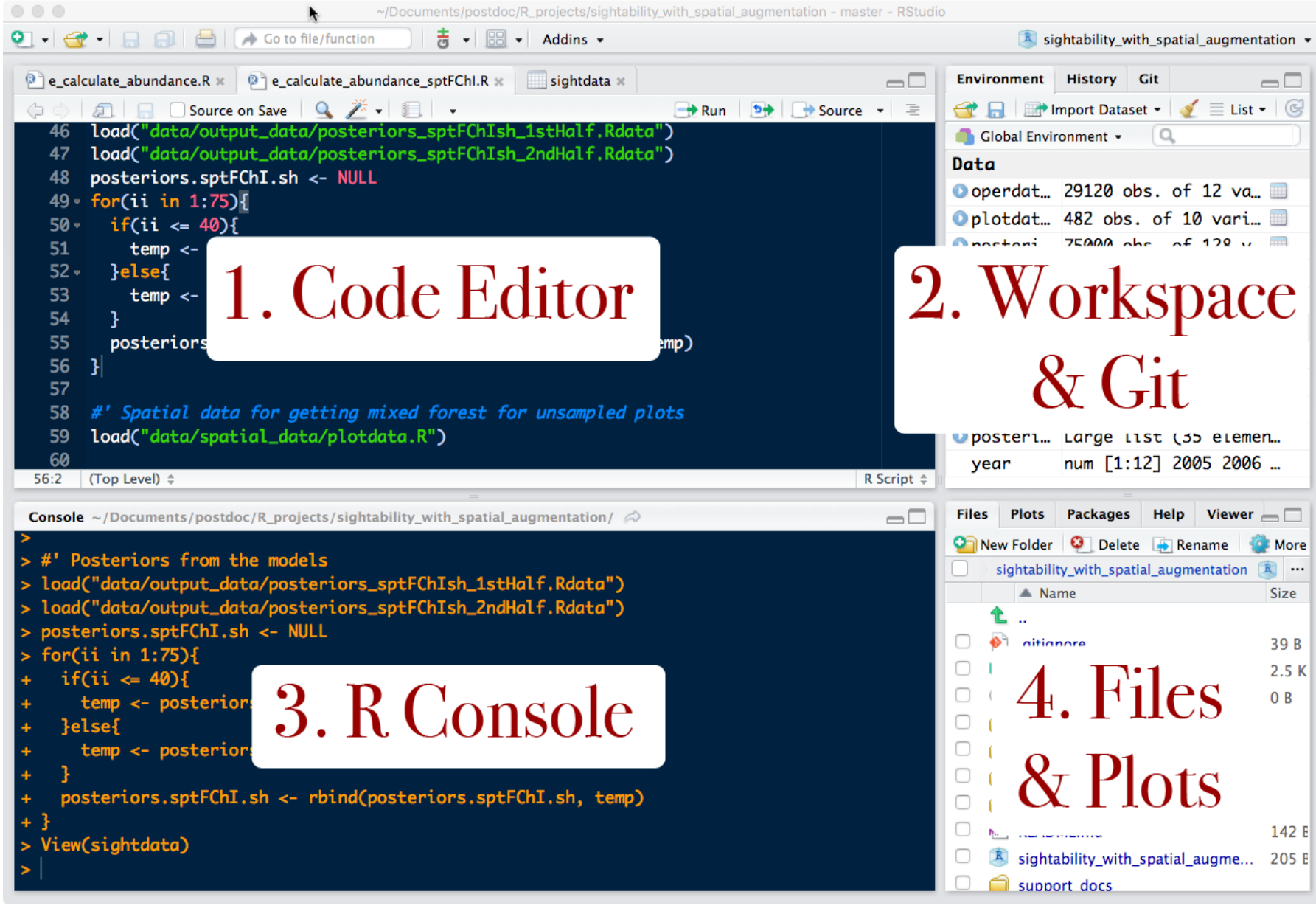
1. RStudio Projects for organizing data, code, and output
2. R-Markdown and R-Oxygen with **knitr** for documenting your code and creating reproducible reports
3. GitHub for version-control, collaborating and archiving

1. RStudio Projects for organizing data, code, and output

1: Introduction to RStudio



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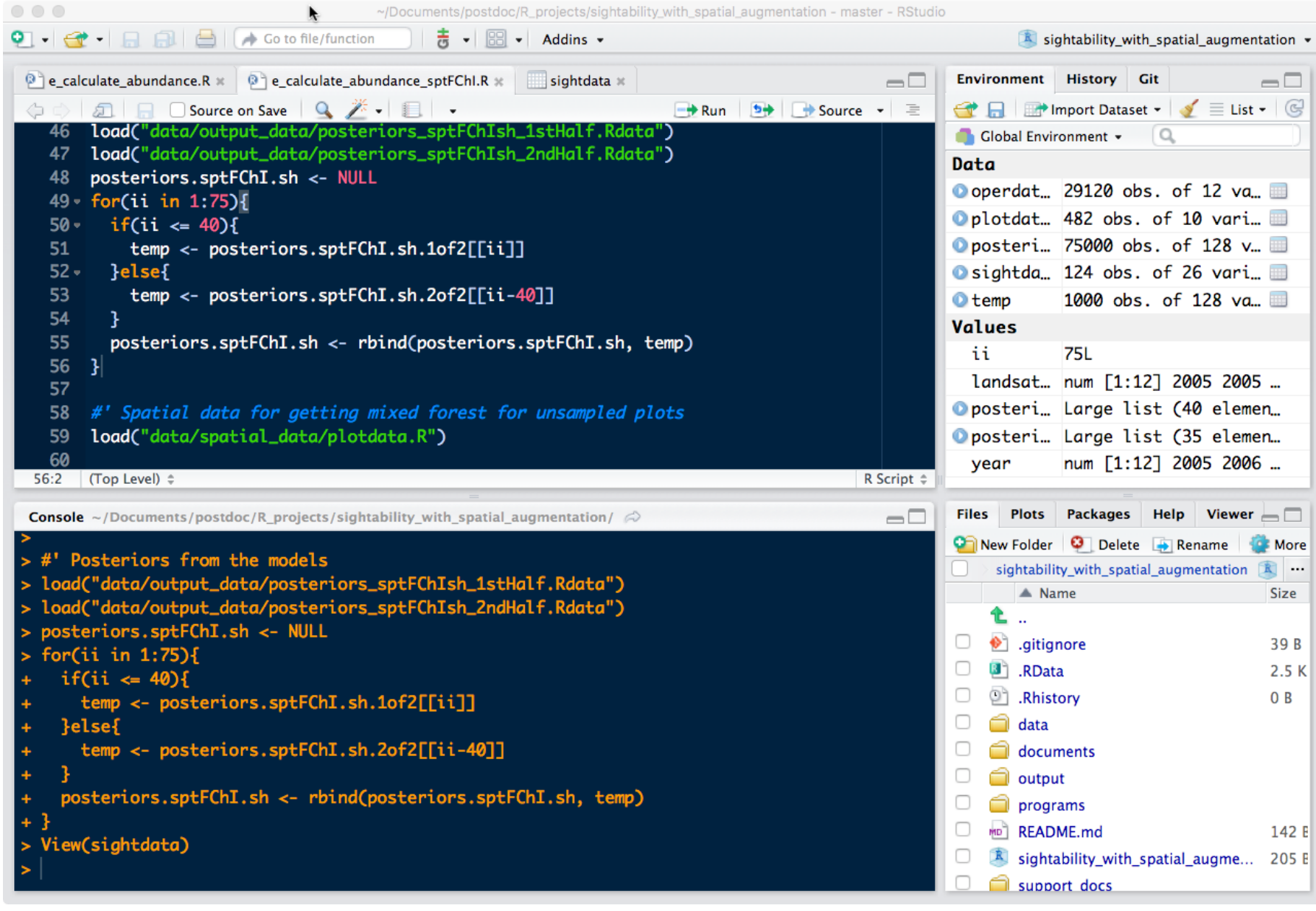


1: Introduction to RStudio

~/Documents/postdoc/R_projects/sightability_with_spatial_augmentation - master - RStudio

Go to file/function | Addins | sightability_with_spatial_augmentation

e_calculate_abundance.R | e_calculate_abundance_sptFChI.R | sightdata | g_plot_results.R

Filter

	year	juldate	plot	offplot	waypoint	observed	pilot	leftseat	rightseat	snowdepth	wind	wdir	tempf	bar	btrend
1	2005	5	58	2	620	1	2	2	3	3	0	0	-10	3049	3
2	2005	5	23	2	80	1	1	1	1	3	0	0	10	3035	3
3	2005	11	105	2	147	0	1	1	4	3	0	0	14	2996	2
4	2005	5	60	2	634	0	2	2	3	3	0	0	-5	3033	2
5	2005	11	100	2	148	0	1	1	4	3	0	0	18	3001	2
6	2005	27	100	2	200	0	1	1	3	3	5	200	21	3037	3
7	2005	11	128	2	138	1	1	1	3	3	0	0	-14	3001	2
8	2005	5	72	2	624	1	2	2	3	3	0	0	-10	3035	2
9	2005	11	72	2	153	1	1	1	4	3	0	0	14	2994	2
10	2005	20	75	2	158	1	1	1	3	3	4	30	9	3010	3
11	2005	5	60	2	636	0	2	2	3	3	0	0	-5	3033	2

Showing 1 to 11 of 124 entries

Environment | History | Git

Diff | Commit | mast

Staged | Status | Path

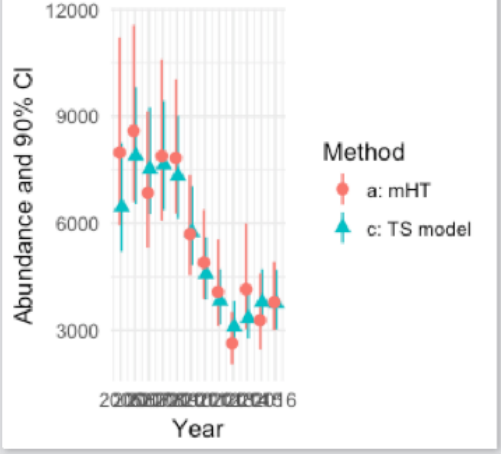
programs/two-step/e_calculate_abundance_sptFChI

Console ~/Documents/postdoc/R_projects/sightability_with_spatial_augmentation/

```
> #' ## Plots
> #'
> #' Abundance
> #+ popnEsts
> ggplot(data = popn.data[popn.data$Method!="b: FE model"&
+                         popn.data$Method!="d:spt FChI (mixed)"&
+                         popn.data$Method!="e:Spt RChI (mixed)"&
+                         popn.data$Method!="e:spt RChI (shrub)"&
+                         popn.data$Method!="f:spt RC (shrub)",],
+        aes(x = Year, y = tauhat, colour=Method, shape=Method))+
+   geom_pointrange(aes(ymin=tau.LL90, ymax=tau.UL90), position=position_dodge(0.3))+
+   ylab("Abundance and 90% CI")+
+   scale_x_continuous(breaks=seq(2004,2016,1))+
+   theme_minimal()
>
```

Files | Plots | Packages | Help | Viewer

Zoom | Export | Pul



1. RStudio Projects

Think about a typical research project, maybe a dissertation chapter or an experiment that you've managed from data collection through publication. What are typical **folders** that you've used?

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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.

Activity 1: Data management and updating

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

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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

1. In the File window of RStudio, copy the **student_folders/student_template** folder. Rename the folder after yourself (or an alias).
2. Open a new R Script file and save it to that new folder as **student_folders/yourname/activity1a_data_processing.R**

Activity 1: Data management and updating

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Activity Overview:

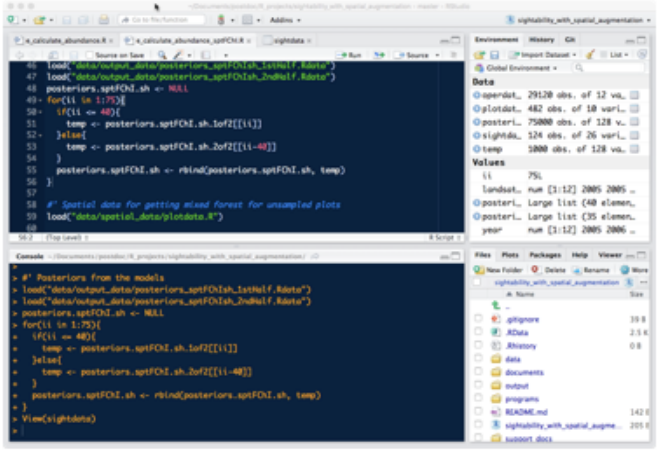
1. We will read in first three weeks of data and combine them, process the data a little bit, and save the merged/processed data for analysis.
2. We will save another new R Script file as **"activity1b_data_analysis.R"** and code/run some preliminary regression analysis.
3. We will pretend to have just gotten the final week's data in and update everything in a "reproducible" way.

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

Overview of **knitr**

R Code

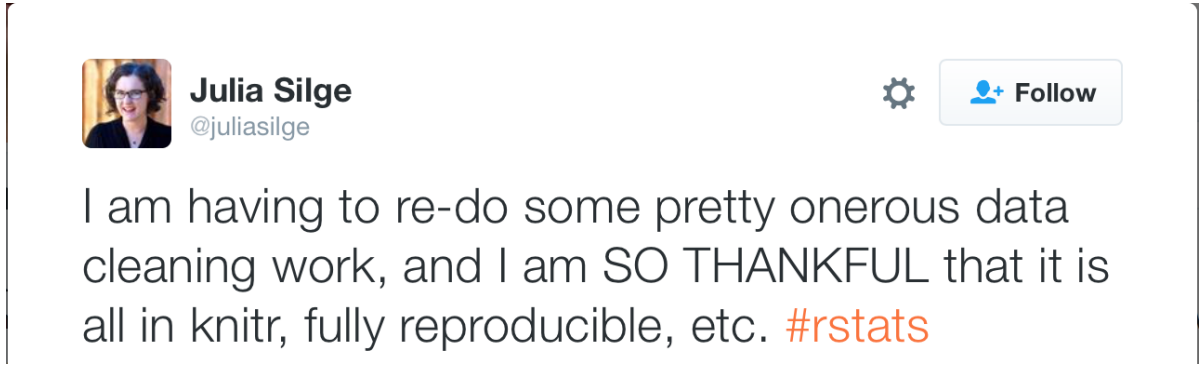
written with
R-Markdown or
R-Oxygen



Report

.html
.doc
.pdf

Why **knitr** 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`

Why **knitr** for manuscripts?

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

- 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

Documenting Code: General tips

- Consistent and meaningful naming conventions
  - a = b*c
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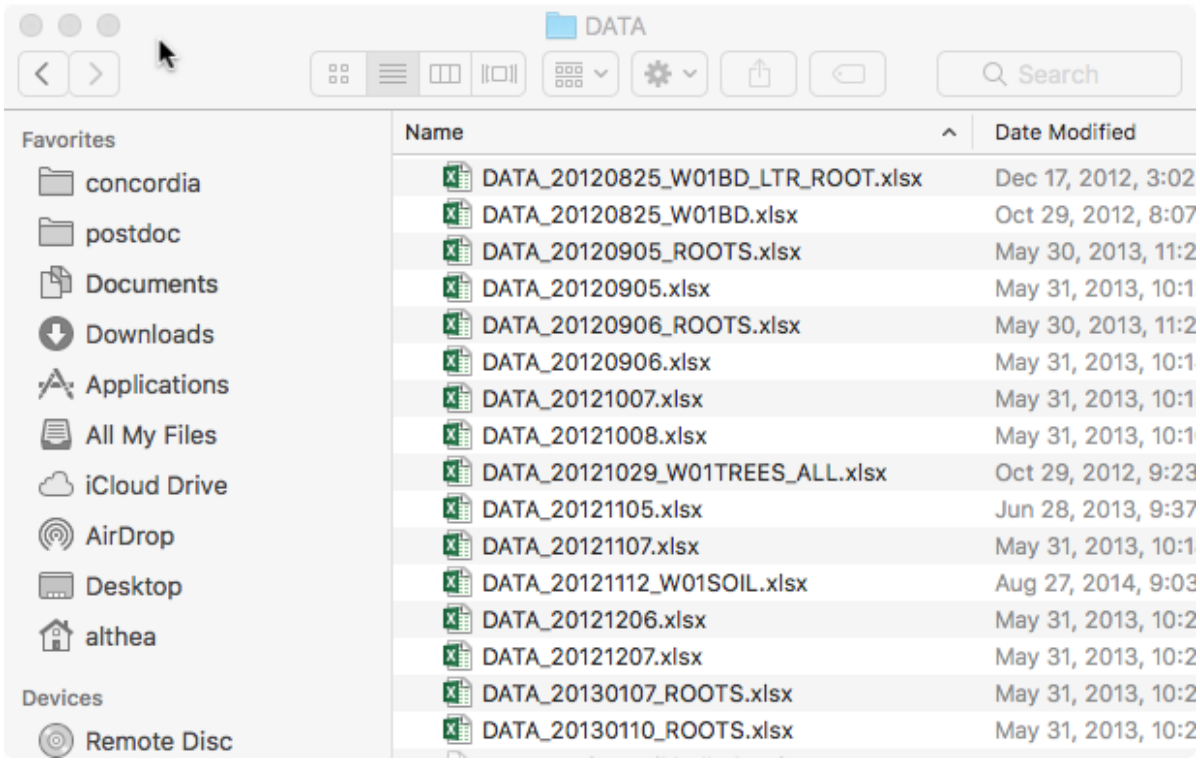
  - weekly_pay = hours_worked*pay_rate
  - weeklyPay = hoursWorked*payRate
- Use YYYYMMDD or equivalent for dates



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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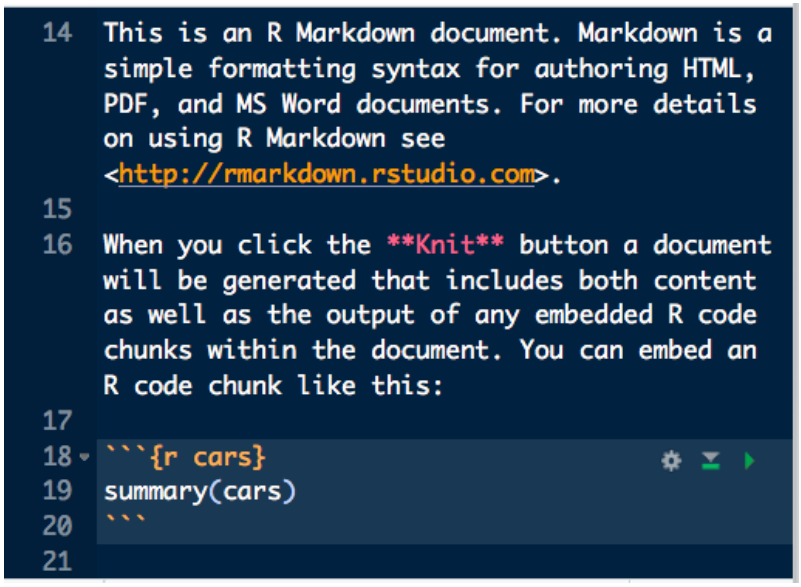

```
14  This is an R Markdown document. Markdown is a
    simple formatting syntax for authoring HTML,
    PDF, and MS Word documents. For more details
    on using R Markdown see
    <http://rmarkdown.rstudio.com>.
15
16  When you click the **Knit** button a document
    will be generated that includes 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
```

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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 as **"student_folders/yourname/activity2a_intro_rmarkdown.Rmd"**
  - View 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.

Documenting code: ezknitr

What folder did the html end up in?

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/yourname/activity2a_intro_rmarkdown.Rmd"
       out_dir = "student_folders/archmiller_a/reports",
       fig_dir = "figures",
       keep_md = F)
```

Note: When using ezknit, must manually save the .Rmd file before knitting!

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

```
library(ezknitr)
ezknit("student_folders/yourname/activity3_latex.Rmd",
       out_dir = "student_folders/yourname/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
  - ms.docx
  - **ms_figures/**
    - fig1.jpg
    - fig2.jpg
  - **transmittals/**
    - **from_john/**
    - ms20170523.docx
    - ms20170625.docx
    - **from_bob/**
    - ms20170626.docx
  - **submission/**
    - ms.pdf
    - fig1.pdf
    - fig2.pdf
    - coverletter.docx

Project Workflow w/ RStudio & knitr

Example of an RStudio project that Althea & John used from conceptualization through publication.

Project Workflow w/ RStudio & knitr

Example of an RStudio project that Althea & John used from conceptualization through publication.

Activity 3: Creating a reproducible report using R-Markdown

Tasks:

1. Knit the rmd as is into a .doc file
2. Add a third week of data and update report
3. Change the formatting using the word-styles-reference-01.docx

3. GitHub for version-control, collaborating and archiving

Introduction to GitHub

GitHub provides a place for you to back-up and version-control your R projects.

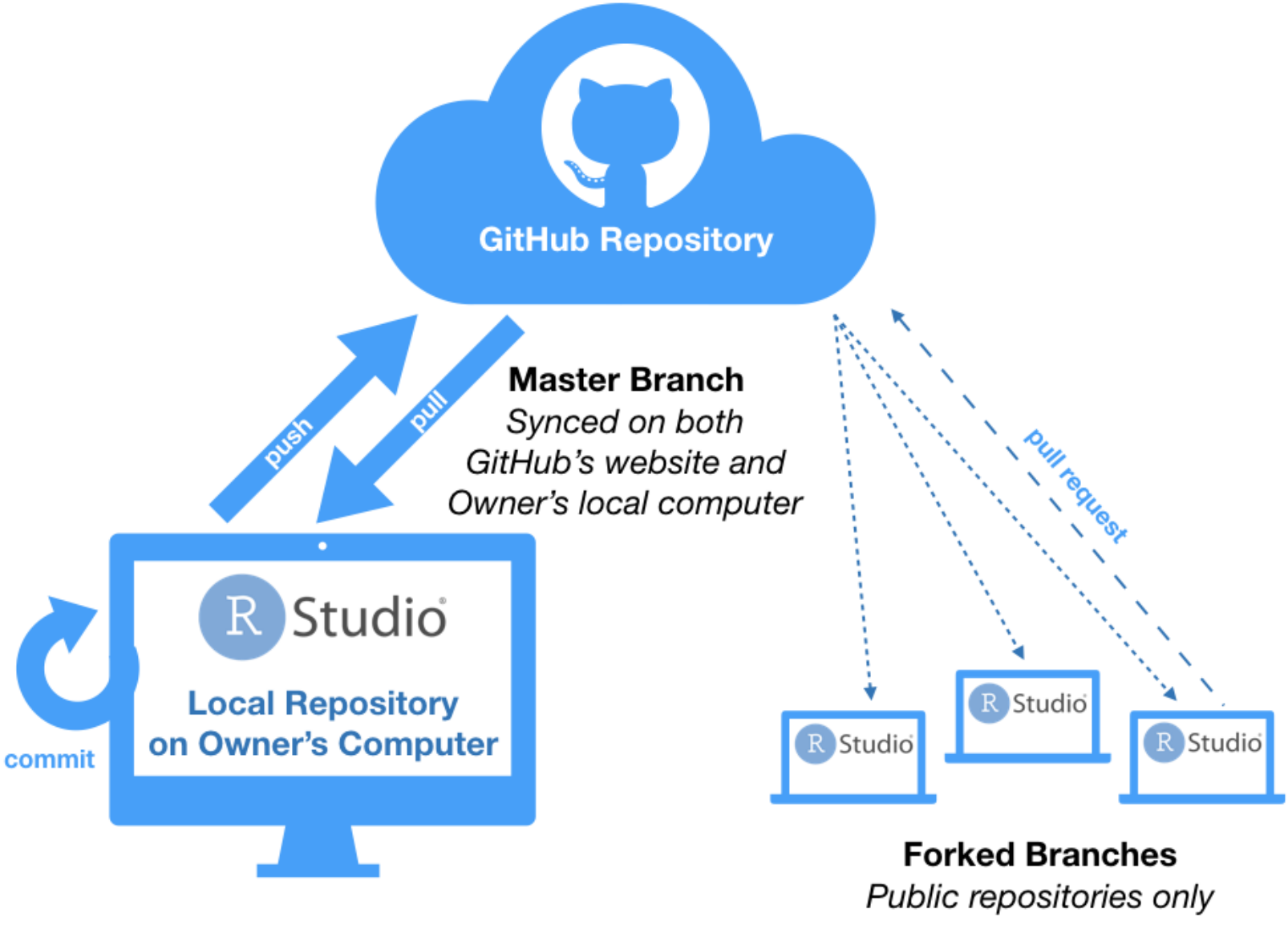
- Interfaces directly with RStudio
- Free (public repositories or with university email) or cheap (private repositories)
- Facilitates collaboration with other co-authors (or the public)
- Can go back to previous code versions (version-control aspect)

Once you're up and running, it's (usually) simple to use!

Introduction to GitHub

Introduction to GitHub

GitHub Overview



Activity 4: GitHub in RStudio

First, we will use the built-in interface for GitHub within RStudio.

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```
git pull origin master # To pull
git add data # add files to a commit
git commit -m "commit message here" #commit
git push origin master # To push commit(s)
```

Additional GitHub Tips

- Don't use github with large files (push limit of 100MB, warning >50MB)
  - If necessary, use git-large-file add on (advanced!)
- Create new projects in GitHub first, then sync them with RStudio (File > New Project > Version Control > Git)

Thanks!

We can use your feedback for the workshop at TWS! Please take a moment or two to fill out our survey.

`https://docs.google.com/forms/d/e/1FAIpQLSdmvePcbb3wztx2JpJUhgTqpjvbR0z3etpnjGrRSRfTBnLpcQ/viewform?usp=sf_link`

Additional resources

- https://swcarpentry.github.io/r-novice-gapminder/02-project-intro/
- knitr documentation and help https://yihui.name/knitr/
- Markdown basics https://daringfireball.net/projects/markdown/basics
- R-Oxygen formatting/tips https://rpubs.com/alobo/spintutorial
- Online Reproducible Research Course http://eriqande.github.io/rep-res-web/