#### Reproducible Science with R

Dr. Matthew K. Lau Class Time: 4.5 hours

#### Overview: Why make your work reproducible and why R? (15 min)

Science is driven by the exchange of information and knowledge. Currently, there is a lot that we can do to make research more transparent and useful. A recent study (Stodden *et al.* 2018) demonstrated that only 26% of studies published in *Science* could be reproduced. This was even more striking given that the study was conducted after the *Science* had instituted it's open data policy.

What this and other studies point to is the need to provide well documented data as well as the software that were needed to conduct the study. Luckily, advances in open-source computer languages, such as **R** and **python**, provide a way to produce computations that can more easily document scientific research in a transparent, easily shared way.

In this course, we will cover how to conduct **reproducible** scientific research using the  $\mathbf{R}$  programming language and supporting software that will enable researchers to more clearly and easily document projects. Participants will gain experience coding in  $\mathbf{R}$  using the RStudio IDE and the git version control system.

Possible additional topics, if time and interest allows: - Shiny Apps - R packages - github

#### Being a good code community member (5 min)

Like science, open-source software development is empowered by community. Everyone participating in this course will follow the Code of Conduct outline by the folks at ROpenSci (https://ropensci.org/coc/).

We all get out of this class what we put into it.

Be considerate and respectiful of each other in speech and actions.

Contribute a safe and effective learning experience for everyone.

https://adainitiative.org/

## Reproducibility Framework (10 min)

#### Max(reproducibility) = Data \* Software \* Documentation

- 1. Setup your project so that there is a clear architecture (RStudio)
- 2. Work so that your computation from initial data to finished results will be coded (wherever possible), including data cleaning and processing steps  $(\mathbf{R})$
- 3. Keep track of versions of your code (git)
- 4. Make initial data available (whenever possible, git)
- 5. Be organized, succinct in style, coding and documentation (**R**, Markdown)

If you're interested in more details on how to conduct reproducible research, see the **TEE** (Transparency in Ecology and Evolution) website http://www.ecoevotransparency.org/ and the **FAIR** reproducible research guide at https://www.go-fair.org/fair-principles/.

#### RStudio Tour (10 min)

Download and install:

- 1. R https://cran.r-project.org/
- 2. RStudio https://www.rstudio.com/products/rstudio/download/#download/

Cheat Sheets

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

https://www.rstudio.com/wp-content/uploads/2016/10/r-cheat-sheet-3.pdf

R is a language, RStudio is an interface to R and other tools.

Parts of RStudio

- "Workbench"
- File system
- Tabs
- Console
- Script(s)
- Help (with RStudio and R)
- Working directory

#### Activity: Example Project (15 min)

Download and open up the example project in RStudio, check your working directory and run the script.

#### Yo, Matt, it's time to take a break! (10 min)

#### Anatomy of an R Script (10 min)

- function anatomy
- objects
- assignments
- basic plotting

#### Activity: Write your own plot code (10 min)

- 1. Open up a new script window
- 2. Write a header
- 3. Comment out your header
- 4. Save your initial script
- 5. Copy the necessary code from the example script
- 6. Make a different plot

#### Tips

Getting help with R:

- ?, ??, help
- Google ("How do I in R?")

• Community (This is not a a test, this is life)

#### Annotate:

• Hashtag hashtag!

## Review and Q/A (10 min)

- 1. Importance of reproducibility
- 2. Max(reproduciblity) = data \* software \* docs
- 3. RStudio
- 4. R language (Arguments, Functions, Scripts)
- 5. Your own script
- 6. Plotting

#### Project Architecture (10 min)

#### Max(reproducibility) = Data \* Software \* Documentation

In this section, we'll go over some project best practices that generally work for computational projects. We'll initiate a new project from RStudio and set up a file system with:

- **README**: describes the project and associated files
- data: folder to collect relevant data files or links
- src: where all of the R scripts should be kept
- results: this is where output from scripts can go
- docs: further documentation and relevant files (e.g. notes, papers)
- bin: ADVANCED if you need to include other associated software

## ACTIVITY: Ecological data project (10 min)

Setup a new project and outline a script that will:

- 1. Import data
- 2. Do some data management
- 3. Do some analyses
- 4. Make a plot

### Data wrangling (15 min)

```
File I/O = read.* and write.*
```

Working directories and relative paths = getwd, setwd, "./../"

Objects and assignments = x < 10 (=, ->, assign)

Mode = Scalars, vectors, matrices, arrays, lists, data.frames

Class = numeric, character, factor, logical, etc.

Indexing = x[1], x[1,1], x[[1]],

Sorting = sort(x), order(x)

Activity: Wrangle those data! (10 min)

Yo, Matt, it's time to take a break! (10 min)

Style: Best Practices and Intro to Packages (5 min)

Hadley Whickam's guide to style http://adv-r.had.co.nz/Style.html

Re-format code in RStudio with:

1. Code -> Reformat Code

#### Data testing (10 min)

Conditional operations Conditional statements Logical type

```
if (!(is.numeric(x[,1]))){warning("Danger Will Robinson!")}else{}
```

#### Activity: Write your own test! (10 min)

#### Review and Q/A (10 min)

- 1. Project organization
- 2. Ecological data
- 3. Data testing

#### Further Study:

- dplyr = reorganize data
- stringr manipulate text (aka. "strings")
- lubridate for handling dates and times
- sp and raster for spatial datasets
- purrr "apply" functions = functions for repeating functions

#### "Backing Up" Version Control (10 min)

#### Max(reproducibility) = Data \* Software \* Documentation

In this module, you'll learn how to use the version control system, known as git, from RStudio. We will cover the basic topics of how to:

- 1. Initiate a project "repository"
- 2. Create, "add" and "commit" changes
- 3. View "diffs" and share a compressed project

We will not cover how to use the online git repository known as *github*. Using *github* provides a central server through which projects can be shared among collaborators in real-time via a system that keeps users from

stepping on each other's "digital toes". To setup a free, private repository through *github.com*, go to their educational program webpage: https://education.github.com

# Activity: Setup your ecological data project as a repository (10 min)

- 1. Using RStudio's menu system, turn on git support
- 2. Make some changes to your script
- 3. Add them to the "stage"
- 4. Review the changes
- 5. Commit them

#### Commit best practices (5 min)

- 1. Commits should represent a task that has progressed or completed
- 2. Files with changes relevant to those tasks should be staged
- 3. In general commit often and describe commits succinctly but informatively

#### Examples:

- "Some changes"
- "Added data import of plant data"

#### Branching (10 min)

• Separates commits

## Activity: Commit! (5 min)

## Activity: Wanna go back in time! (10 min)

Rolling back versions

- 1. View history
- 2. Choose the time point (here's where commit messages are key!)
- 3. Revert

#### Yo, Matt, it's time to take a break!

### Software Dependencies: R Packages and CRAN et al. (5 min)

Functions and other information are grouped into packages and hosted on CRAN (Comprehensive  $\mathbf{R}$  Archive Network). This modular structure allows  $\mathbf{R}$  to grow but still be usable. As of 2016 there were over 8,000 packages on CRAN, an increase of 2,000 from 2015.

https://www.r-bloggers.com/on-the-growth-of-cran-packages/

With regard to reproducibility, this creates an issue as CRAN and  $\mathbf{R}$  are constantly changing. That is why it is imperative to keep track of the "dependencies" of your code. Ways to deal with dependencies:

- 1. Minimize them
- 2. Track them (sessionInfo, packrat, containers/rocker, VM/encapsulator)

https://rviews.rstudio.com/2018/01/18/package-management-for-reproducible-r-code/signal and the state of the control of the

One easy way would be to just record the system and library information using sessionInfo:

```
print(sessionInfo(), locale = FALSE)
```

```
## R version 3.4.4 (2018-03-15)
## Platform: x86_64-apple-darwin15.6.0 (64-bit)
## Running under: macOS High Sierra 10.13.4
## Matrix products: default
## BLAS: /Library/Frameworks/R.framework/Versions/3.4/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/3.4/Resources/lib/libRlapack.dylib
##
## attached base packages:
## [1] stats
                 graphics grDevices utils
                                               datasets
                                                        methods
                                                                   base
## loaded via a namespace (and not attached):
  [1] compiler_3.4.4 backports_1.1.0 magrittr_1.5
##
                                                        rprojroot_1.2
  [5] tools 3.4.4
                        htmltools 0.3.6 Rcpp 0.12.12
                                                        stringi 1.1.6
## [9] rmarkdown_1.9
                                                        digest_0.6.15
                       knitr_1.20
                                        stringr_1.3.0
## [13] packrat 0.4.9-2 evaluate 0.10.1
```

#### packrat (10 min)

Although there are other more sophisticated ways to implement dependency reproducibility, we'll go over packrat, which is implemented in RStudio:

- 1. Tools -> Project Options
- 2. Packrat -> Use packrat for this project
- 3. Use default settings and continue

More info on packrat can be found here: https://rstudio.github.io/packrat/rstudio.html

One handy thing that *packrat* enables is that it can detect what packages your project isn't using and remove them. Use the following bit of code to do this:

```
packrat::clean()
```

**ProTip**: this syntax uses "::" (i.e. a double colon) allowing you to specify the package ("packrat") that contains the function ("clean") that you want to use. This is extremely useful as it means that you don't always have to load (i.e. *library*) the entire package when you just want to use one or a few functions.

## Wrap-up on Reproducibility with R (5 min)

- 1. Max(reproducible) = data \* software \* docs
- 2. Project architecture for better access
- 3. Document (comment, follow style, "Brevity is the soul of wit.")
- 4. Share your results

5. Planned obsolescence: Backup and version

## Possible: Advanced Topics Courses (5 min)

1-hour sessions

Zoom + Slack

Museum or remote locations

- Scientific notebooks with rmarkdown or jupyter
- Advanced command line BASH
- Advanced git and github
- Web apps with *shiny*
- $\bullet$  Advanced plotting with ggplot
- Community analysis with vegan and ecodist
- Matrix operations and linear algebra \*\*%\*\*
- Efficiency with *profVis*
- Network analysis with enaR
- Mapping with googlevis
- ullet Spatial data analysis with sp and raster
- Automated workflow tracking with data provenance RDatatracker
- ullet Code cleaning with Rclean

Survey (5-10 min)