Reproducible Research in R

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FDZ Autumn Academy

Introduction

Introduction

Who are we?

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Introduction

Who are you?

- 1. Occupation, employer?
- 2. Previous knowledge and experience
 - with reproducible research?
 - with R?
- 3. Specific interest/motivation for this workshop?

Agenda

Day 1

- Conceptual Introduction
- Writing Reproducible R Code
- Reproducible Reporting

Day 2

- RMarkdown
- Version Control/git

Reproducible Research

Reproducibilty & Replicability

Reproducibility

- Same research question
- Same analysis
- Same data
- => Same results

Replicability

- Same research question
- Same analysis
- New data
- => Same results

The **replicability** crisis in psychological* research is partly caused by **reproducibility** issues.

- more than 70 percent of the researchers that tried to reproduce other scientist's experiments failed (Baker, 2016).
- more than 50 percent of the researchers that have tried to reproduce their own experiments failed (Baker, 2016).

*Psychology, educational sciences and social work

Baker, M. (2016). Reproducibility crisis. Nature, 533(26), 353-66.

Threats to self-replication (see also Peikert et al., 2021)

- (Silent) Mistakes in data preparation/analysis (e.g., syntax bugs)
- Inconsistent versions of code, data, or both
- Copy-and-paste errors
- ...

Peikert, A., van Lissa, J., Brandmaier, A.M. (2021). Reproducible Research in R: A Tutorial on How to Do the Same Thing More Than Once. Psych 2021, 3, 836–867.

Threats to replication of others

- ...
- Data not available
- Incomplete documentation/reporting
- ..

Proposed solutions (see also Peikert et al., 2021)

- Clean code
- Version control
- Dynamic document generation
- (Independent reproduction)

Workshop Goals

Be able to ...

- ... reproduce your own research (i.e., analyses)
- ... publish your code openly with your research
- ... create research which is reproducible for others
- ... spread the word

RStudio setup

RStudio setup

- 1. Save the course content to a directory on your machine
- 2. Open RStudio
- 3. Choose File < New Project ...
- 4. Choose Existing Directory
- Browse to the directory on your machine where you saved the course content and select the "R-programming" folder as the Project working directory
- 6. Click Open in new session
- 7. Click Create Project

RStudio setup - optional

- 1. Choose Tools < Global options
- 2. Under General
 - DON'T Restore .RData into workspace at startup
 - NEVER Save workspace to .Rdata on exit:
 - Save the code instead!
 - Use saveRDS() and readRDS() for objects that require a long time to computate
- 3. Further personalize RStudio

Writing Reproducible R Scripts

Reproducible Workflow in R & Rstudio

Key Principles:

- 1. Save your code
- 2. Work in projects
 - Use multiple scripts
 - Use multiple projects
- 3. Frequently and completely restart

- Save the code for preprocessing/data manipulation (don't save intermediate data sets)
- Save the code for visualizations (don't save the plots)
- Save the code for analyses (don't save the results)

May the source code be with you!

- Save the code for preprocessing/data manipulation (don't save intermediate data sets)
- Save the code for visualizations (don't save the plots)
- Save the code for analyses (don't save the results)

May the source code be with you!

 Use saveRDS() and readRDS() for objects that require a long time to compute

Within RStudio

- 1. Choose Tools < Global options
- 2. Under General
 - DON'T Restore .RData into workspace at startup
 - NEVER Save workspace to .Rdata on exit:
 - Save your script instead!
 - Use saveRDS() and readRDS() for objects that require a long time to compute
- 3. You can further personalize RStudio
 - Visually (Tools < Global options < appearance)
 - Keyboard shortcuts (Tools < Modify Keyboard Shortcuts...)
 - ...

A typical workflow:

- Write your code in scripts in text editor.
- Execute lines (or chunks) of code by sending them to the R console.
- Add comments using the hash tag #
- Add sections to long scripts (or use multiple scripts)
 - No lines of code are lost when R is shut down or crashes
 - Assures reproducible code/coding
 - Makes it easy to share your code with colleagues or reviewers
 - ...

What is a project?

- One designated folder containing all files related to a single (research) project.
- When necessary, add sub folders for ...
 - data
 - R scripts
 - figures and graphs
 - manuscripts
 - presentations
 - ...
- The folder contains all relevant files, nothing more.

The idea of a project is formalized in an RStudio project.

- Technically it is a small text file with (.Rproj) extension,
- which is associated with RStudio.
- RStudio recognizes the "parent folder" of this file as the project folder

Within an RStudio project...

- the project folder is automatically set as the working directory.

 try getwd() within a project
- Don't use

```
setwd("path\to\your\local\folder")
```

Use relative paths for reading and writing data. Avoid ...

```
cannot open file 'path\that\only\works\on\my-computer': No such file
or directory
```

- With relative paths, code works when ...
 - the project folder is moved (or renamed)
 - you are working on a shared drive
 - you send your project in a ZIP-folder
- useful functions:
 - ?list.dirs
 - ?list.files
- (Or use the here-package)

Keep it clean!

- One folder per project
- No outside code
- No outside computing
- Use separate RStudio projects for each project
- Use separate Rstudio instances for each Rstudio project

How to create an Rstudio project?

- 1. Open Rstudio
- 2. Choose File < New Project ...
- 3. Choose Existing Directory
- 4. Browse to the directory on your machine where you saved the course content and select the "example-project-2" folder as the Project working directory
- 5. Click Open in new session
- 6. Click Create Project

Within a project, use multiple source files (scripts) for:

- 1. Preprocessing data
- 2. Descriptive analysis
- 3. Building models
- 4. Hypothesis testing
- 5. Making graphs
- 6. ...

3. Frequently and Completely Restart

Regularly completely restart your session. Don't use

```
rm(list = ls())
```

- start clean, every time
- restart to make sure everything reproduces
- .rs.restartR()
- Ctrl + Shift + F10

How To?

How to ... read data

To analyse data, you have to *read* the data from some file (or connection) and make it an *object* in R.

Almost any type of file can be read by R, via specific functions and packages (reader, haven, readxl, ...).

- txt → read.table()
- .csv \rightarrow read.csv(), read.csv2()
- .xls → readxl::read_xls()
- .xlsx → readxl::read_xlsx()
- sav → haven::read_sav()
- por → haven::read_por()
- $.sas \rightarrow haven::read_sas()$
- ...

How to ... preproces data

Useful functions in Base R

- ?'[' and ?'[['
- ?merge, ?reshape
- ?apply, ?tapply, ?aggregate,...
- ?sort, ?order
- ...

Useful functions in dplyr

- ?filter, ?select, ?slice
- ?mutate, ?rename
- ?group_by, ?summarize, ?ungroup
- ?arrange
- ?inner_join, ?left_join, ...

How to ... preproces data

For fast and efficient data wrangling with VERY big data, the data.table-package can be helpful.

Never change raw data!

If you made some mistakes while preprocessing raw data \rightarrow change your code and re-run it.

Note that:

- R "reads" the data and loads it in the work space.
- Hence, manipulating data within R(Studio) does not change the data on your machine. Only the loaded data within the work space is changed.

How to ... write data

When the data (a data frame, a fitted model, ..) you want to save is for use in R only, use saveRDS() readRDS().

When the data (a data.frame) is for use by software, several options are available:

- .txt → write.table()
- .csv \rightarrow write.csv(), write.csv2()
- sav → haven::write_sav()
- por → haven::write_por()
- sas → haven::write_sas()
- ...

WARNING:

R does not prompt a warning when you are about to overwrite an existing file.

How to ... save plots

Only use the RStudio "Plot"-window for interactive plot making. Don't use it for saving plots.

For reproducible figures, use pdf(), png(), jpeg(), tiff(), ... instead. See ?jpeg.

Adjust size and aspect ratio using the arguments:

- width = ...
- height = ...
- \bullet units = ... \rightarrow the units for the width and height arguments
- ...

How to ... save plots

```
z_values <- rnorm(1e+4)
sig_z_values <- z_values[pnorm(abs(z_values),</pre>
                                lower.tail = FALSE) < 0.0251
pdf("name_for_this_figure.pdf", width = 10, height = 7)
  # all the code that creates the figure
 hist_data <- hist(z_values,
                    main = "Significant Z-values \n(stupid plot)",
                    xlab = "Z-values")
 hist(sig_z_values,
       breaks = hist_data$breaks,
       add = TRUE,
       col = "skyblue")
dev.off()
```

Reproducible Reporting

Common Workflows

Not very reproducible...

- Perform data preparation via hand/graphical user interfaces (SPSS, Excel)
- Perform data analyses via hand/graphical user interfaces (SPSS, Excel)
- Write a research report/manuscript (Word)
- Insert your results via copy & paste in text or as figures/tables

Reproducible Workflows

Better...

- Perform data preparation via syntax (R, Stata, SPSS)
- Perform data analyses via via syntax (R, Stata, SPSS)
- Write a research report/manuscript via a typesetting system or markup language (Markdown/LaTeX)
- Insert your results via dynamic document generation (RMarkdown/knitr)

Markdown

Lightweight Markup Language

• Pandoc distributed via RStudio

LaTeX

Typesetting System

- Engines (pdflatex, xelatex, lualatex, ...)
- Distributions (OS dependent: Miktex, tinytex, ...)
- Text editors (Texlive, Texmaker, RStudio...)

LaTeX vs. Markdown

Advantages LaTeX

- https://ctan.org/pkg/apa7?lang=en document class
- Better support for formulas
- Looks nicer
- Better customization
- Designated output format: .pdf

https://yihui.org/en/2013/10/markdown-or-latex/

LaTeX vs. Markdown

Advantages Markdown

- Extremely easy to use
- No complicated setup
- Designated output format: .html

https://yihui.org/en/2013/10/markdown-or-latex/

Dynamic Document Generation

Intertwine reporting and data preparation/analyses

- LaTeX \rightarrow knitr (.Rnw)
- ullet Markdown o RMarkdown (.Rmd)

Execute R code during document generation.

LaTeX and knitr

knitr

- substitutes sweave
- allows embedding R chunks in .tex code (.Rnw)
- powerful tool for automated document generation

RMarkdown

See tomorrow!

Semi-Dynamic Document Generation

Unfortunately life is not always easy...

- Limited resources to learn even more tools
- Collaborators insist on using Word
- Journals only accept Word documents for submissions
- ...

However, we can always try to make small improvements!

Semi-Dynamic Document Generation

For Example: Automated APA tables in Word

- → Useful R packages
 - apaTables
 - rempsyc
 - flextable
 - sjPlot
 - stargazer
 - ..

apaTables: Create American Psychological Association (APA) Style Tables

A common task faced by researchers is the creation of APA sayle (i.e., American Psychological Association style) tables from statistical output. In R a large number of function calls are often needed to obtain all of the desired information for a single APA style table. As well, the process of manually creating APA style tables in a word processor is prone to transcription errors. This package creates Word files (doc files) containing APA style tables for several types of analyses. Using this package minimizes transcription errors and reduces the number commands needed by the user.

Version: 2.0.8

Depends: R (> 3.1.2)

Depends: R (≥ 3.1.2)

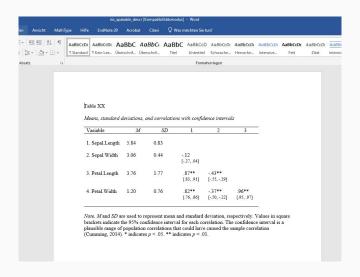
Imports: stats, utils, methods, <u>car</u>, <u>broom</u>, <u>dplyr</u>, <u>boot</u>, <u>tibble</u>, <u>MBESS</u>

Suggests: testthat, knitr
Published: 2021-01-04

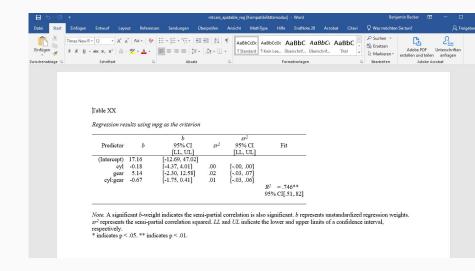
Author: David Stanley [aut, cre]

BugReports: https://github.com/dstanley4/apaTables/issues

Descriptive statistics for a data set



Regression tables



rempsyc

```
rempsyc: Convenience Functions for Psychology
```

Make your workflow faster and easier. Easily customizable plots (via 'ggplot2'), nice APA tables (following the style of the *American Psychological Association*) exportable to Word (via 'flextable'), easily run statistical tests or check assumptions, and automatize various other tasks.

Version: 0.0.9

Depends: R (≥ 3.5)

Depends: R (≥ 3.3)

Imports: boot, car, dplyr (≥ 1.0.4), effectsize, flextable (≥ 0.7.1), ggplot2, ggrepel, ggsignif, lmtest, methods, qqplotr, rlang

Suggests: bootES, broom, correlation, datawizard (≥ 0.5.0), emmeans, ftExtra, ggpubr, interactions, knitr, markdown, openxlsx, openxlsx2,

patchwork, performance ($\geq 0.9.1$), psych, report ($\geq 0.5.1$), markdown, see, testthat ($\geq 3.0.0$), VennDiagram 2022,09.26

Published: 2022-09-26
Author: Rémi Thériault 🙃 [aut. cre]

Maintainer: Rémi Thériault <remi.theriault at mail.mcgill.ca>

BugReports: https://github.com/rempsyc/rempsyc/issues

License: GPL (≥ 3)
URL: https://remr

URL: https://rempsyc.remi-theriault.com

NeedsCompilation: no

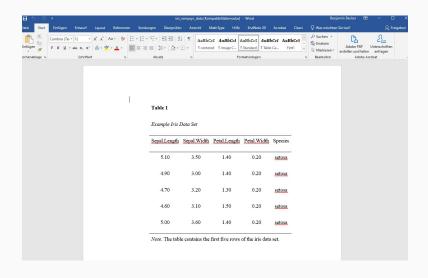
Additional_repositories: https://janmarvin.r-universe.dev

rempsyc

Descriptive statistics for a data set

```
word_table <- rempsyc::nice_table(iris[1:5, ],
   title = c("Table 1", "Example Iris Data Set"),
   footnote = c("The table contains five rows of the iris data set."))
rempsyc::save_as_docx(word_table, path = "iris_rempsyc_data.docx")</pre>
```

rempsyc



Exercises



RMarkdown

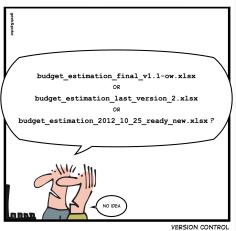
Version Control via Git and Github

Version Controlling

- Motivation
- Setup
- Work Flows
- Recommendations
- Resources

Motivation

SIMPLY EXPLAINED



Motivation 1

Single Author Projects

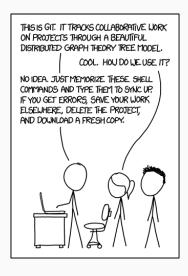
- Implementation of long term change history
 - What has been changed?
 - When was it changed?
- No ridiculous file names
- No archive sub folder
- Accessibility for others ('Open Science')
- Additional safety net
- ..

Motivation 2

Collaborations

- Who has changed what when exactly?
- Clear, current project state
- No annoying mail attachments or file-sharing platforms
- Parallel work easily possible
- Possibility of hierarchical responsibilities
- ...

But...



Prerequisits

- Git-Installation
- RStudio-Installation
 - → Alternatives: Shell, Gitkraken, SmartGit, ...
- Github account
 - → Alternatives: Bitbucket, Gitlab, ...
- Connect everything

Register at Github

https://github.com/



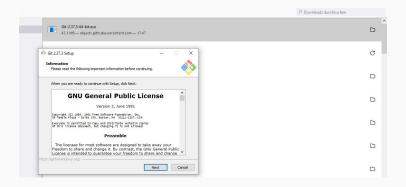
Download git

https://git-scm.com/download/win



Install git

Install git into a folder in which you have sufficient rights (user folder if necessary)



Configure git

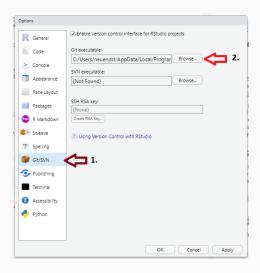
git can be configured for Github via R

Configure git

Check if the configuration was successful via the command line (cmd).

git config -global -list

Connect git and RStudio



RStudio

The RStudio user interface to Git looks like this



Work flow 1

Creating a repository

- Create an online repository (e.g. on Github)
 - Use an R specific .gitignore
 - Initialize with a short readme (.md)
- Clone the repository to your local machine via RStudio as a new project
- An R-Project is added automatically to the existing repository

Excursion: gitignore

- Plain text file
- Which files should not be tracked by git?
 - \rightarrow These then only exist locally in their current version!
- Options
 - Single files
 - Folders
 - Specific data types
 - Combinations of the above
- Use cases
 - Large files (Data, images, ...)
 - Auxiliary files (e.g. created during latex compilation)

Work flow 2

Working with an existing repository

- Before working: Synch your local repo (Pull or clone)
- Perform changes in your local repository
 - \rightarrow Create/modify/delete files
- Stage your changes
- Commit your changes (aka new version)
- Push your commit(s) (online repository is updated)

Excursion: mergen

Conflicts between different updated versions

- Common when working collaboratively
- Discrepancies between your own different local repos → Git communicates these and indicates conflicts
- Select the desired changes
- Stage selection, commit and push

Excursion: Branches

Multiple parallel versions of a project within one repository

- Common e.g. in areas like software development
- e.g. one stable and one development branch
- Only certain modifications should be made in the stable branch
- Note: RStudio GUI has limited support for this

Your impressions?

Recommendations

- Keep it simple!
 - If not necessary, no branches/forks/pull requests
- Have meaningful commits
- Keep it lean (no big files)
- Avoid using the Github homepage working within the repository

Resources

Git + RStudio Resources

- Small Intro (https://r-bio.github.io/intro-git-rstudio/)
- Happy Git with R (https://happygitwithr.com/)
- R Packages and Git (https://r-pkgs.org/git.html)

General Git Resources

• Git Book (http://git-scm.com/book/en/v2)

Exercises



Exercises

- Create an example repository
- Create some descriptive analysis of the mtcars data set
- Version control your work

Good programming practices

"Write code for humans, not for machines!" $\,$

Code Style

Invest time in writing readable R-code.

- It will make collaborations easier
- It will make debugging easier
- It will make your analyses more reproducible

There is a complete *tidyverse* style-guide https://style.tidyverse.org/.

Go easy on your eyes

- with spaces before and after: + / * = <- < == >
- always use <- for assignments
- only use = in function calls
- use indentation (largely automatic in RStudio)
- CamelCaseNames vs snake_case_names
- be consistent!
- wrap long lines at column 70-80 (Rstudio)

White space

```
new_var=(var1*var2/2)-5/(var3+var4)
# versus
new_var <- (var1 * var2 / 2) - 5 / (var3 + var4)</pre>
```

Indentation

```
for(name in names){formula=as.formula(paste0("y~.-",name))
fit<-lm(formula, data=my_data)</pre>
coefs[["name"]]=coef(fit)
print(name)
print(summary(fit))}
 versus
for(name in names){
  formula <- as.formula(paste0("y~.-", name))</pre>
  fit <- lm(formula, data = my_data)</pre>
  coefs[["name"]] <- coef(fit)</pre>
  print(name)
  print(summary(fit))
```

Wrap long lines

```
final_results <- data.frame(first_variable =</pre>
sgrt(results$mean_squared_error), second_variable =
paste0(results$condition, results$class, sep = ":"),
third variable = results$bias)
# versus
final_results <- data.frame(</pre>
  first_variable = sqrt(results$mean_squared_error),
  second_variable = paste0(results$condition,
                            results$class, sep = ":"),
  third_variable = results$bias)
```

Go easy on your mind

- use meaningful names: "self-explainable"
- always write the formal arguments in function calls (except the first)
- benefit from autocompletion (<tab>) => embrace longer names
- use TRUE and FALSE not T and F
- comment, comment, comment
 - NOT what (should be clear from the code)
 - but why
 - explain the reasoning, not the code

Use meaningful names

```
V <- myFun(m1_B)
# versus

RMSE_age_gender <- get_RMSE(lm_age_gender)</pre>
```

Programming advice

Use verbs for functions and nouns for other objects.

Write formal arguments

Benefit from auto completion using tab

Comment, comment

```
## Start every Rscript with a comment that explains
   what the code in the script does, why it does
##
   this, and to which project it belongs.
##
   Your future self will be very thankful!
##
## Mention which packages you are using in this Rscript.
## Use sections to separate chunks -----
## Maybe even subsections =================
## Recode variables so that missings are coded as "NA"
dat[dat %in% c(99, 999)] <- NA # missings coded 99 or 999
```

Keep your code slim

Try to limit your package-dependencies.

Only load library() the packages that you absolutely need. If you are only using dplyr, it does not make sense to load the complete tidyverse.

Controversial: when possible, use the :: operator (and consider not loading the package). ckage::<function>

- explicit dependencies
- less name conflicts

Never Attach

Forget about attach()!

Don't use it, unless you completely understand what happens (see ?attach).

Use with(data.frame, expression) instead.

Testing R code

Writing code is error prone. Incorporate tests and checks in your workflow.

- minimal examples
- write tests and checks
- helpful packages: testthat, RUnit, testit, ...

Computing speed can become an issue. Avoid common pitfalls:

- don't grow, but replace
- vectorize where possible
- check the computing speed

?system.time, microbenchmark or profiling tools

Don't grow!

```
system.time({
  new_data <- NULL
  for(row_nr in seq_len(NROW(data))){
    new_data <- cbind(</pre>
      data[row_nr,],
      result = exp(data$x[row_nr]) /
        log(data$z[row_nr]) +
        5 * sqrt(data$y[row_nr]))
})
           system elapsed
     user
     1.92
             0.00
                      1.94
```

Replace!

```
system.time({
  n_rows <- dim(data)[1]</pre>
  data$result <- rep(NA, n_rows)</pre>
  for(row_nr in seq_len(n_rows)){
    data$result[row_nr] <- exp(data$x[row_nr]) /</pre>
      log(data$z[row_nr]) +
      5 * sqrt(data$y[row_nr])
})
            system elapsed
>
     user
                       0.31
     0.30
              0.02
```

Vectorize!

```
system.time({
  data$result <- exp(data$x) / log(data$z) +
    5 * sqrt(data$y)
})

> user system elapsed
> 0.02  0.00  0.02
```

Compare the speed of different implementations using:

microbenchmark::microbenchmark

```
get_mean1 <- function(x){</pre>
  weight <- 1/length(x)</pre>
  out <- 0
  for(i in seq_along(x)){
    out <- out + x[i] * weight
  return(out)
get_mean2 <- function(x){</pre>
  sum(x)/length(x)
```

Compare the speed of different implementations using:

microbenchmark::microbenchmark

```
x < - rnorm(500)
microbenchmark::microbenchmark(
 mean(x), get_mean1(x), get_mean2(x))
> Unit: nanoseconds
                min
                       lq
                           mean median
                                                max neval
>
          expr
                                         uq
       mean(x) 2100 2300 3631 2400 2600
                                            112300
                                                      100
>
>
  get_mean1(x) 13500 13900 39701 14100 15300 2485100
                                                     100
  get_mean2(x)
                600
                      700 9126
                                   800
                                             824100
                                                    100
                                        900
```

Programming advice

Don't worry about speed before it becomes an issue.

Wrap Up

General Advice

- Investing time in learning R pays off
- It's a steady learning curve
- Learn from masters
- Rewrite important code the first attempt is usually not the best approach

General R Advice

- Document well
- Use a consistent style
- Write functions
- Split long functions in smaller ones
- Write wrappers
- Use Iteration (don't copy paste)
- Use matrix operations and vectorized functions instead of loops
- Use git

Literature Recommendations

R Resources

- Avanced R Ed. 1 (http://adv-r.had.co.nz/)
- Avanced R Ed. 2 (https://adv-r.hadley.nz/)
- R Inferno (https: //www.burns-stat.com/pages/Tutor/R_inferno.pdf)
- R Packages (https://r-pkgs.org/)
- Clean Code (https://mooc.aptikom.or.id/pluginfile. php/1174/mod_resource/content/1/Clean%20Code_%20A% 20Handbook%20of%20Agile%20Software%20C%20-% 20Robert%20C.%20Martin.pdf)



Thank you for your attention!

Questions? Remarks?