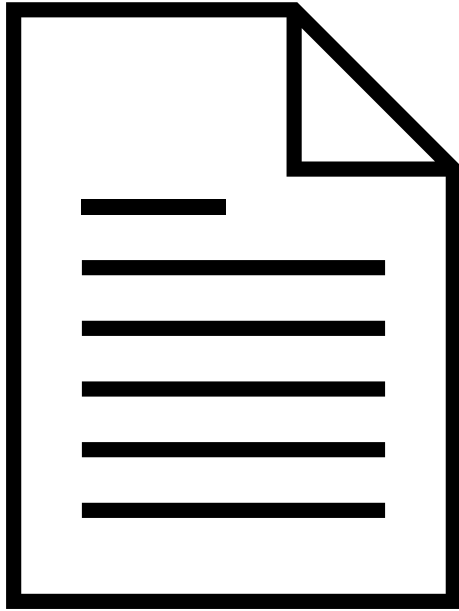


Lessons Learned Registering Simulation Studies

Lindsay Alley and Mairead Shaw

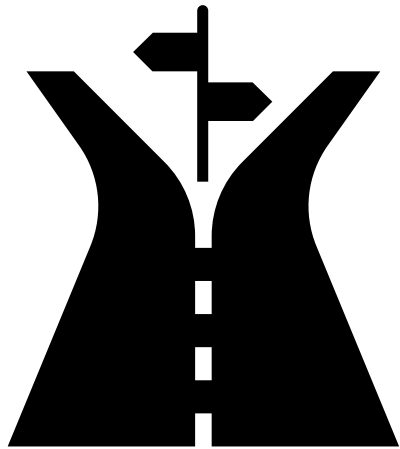
McGill University



Study Planning and Justification

- RR vs traditional simulation:
 - Stage 1 reviews!
 - Can't make choices based on results
 - Injects rigour
- Justify your study conditions
- Describe your expected results

Justify Study Conditions



- What's different?
 - Can't use results
 - Locked in (mostly)
 - Reviewers can request changes at Stage 1, but not Stage 2!
- Justify using:
 - Your research questions
 - A previous simulation
 - A review of:
 - Common practice
 - Simulations



Describe Expected Results

Research Question	Hypotheses	Analysis Plan	Interpretations
How does sample size affect type 1 error rates?	Lower type 1 error rates with increasing sample size	ANOVA comparing Type 1 Error rates between sample size conditions	If we find support... If we don't...



Describe Expected Results

- More results than you know what to do with!
- Which results will you present?
 - Consider decision rules in advance
- How will you organize results?
 - Example tables and plots

The collage contains the following elements:

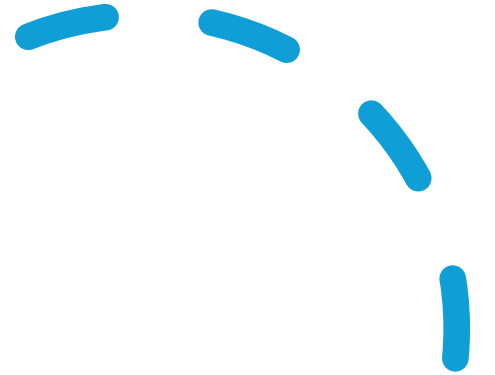
- Circle:** A diagram of a circle with radius r .
Formulas: $A = \pi r^2$ and $C = 2\pi r$.
- Cone:** A diagram of a cone with height h and radius r .
Formula: $V = \frac{1}{3} \pi r^2 h$.
- Cylinder:** A diagram of a cylinder with radius r .
Formula: $V = \pi r^2 h$.
- Trigonometry Table:**

	30°	45°	60°
sin	$\frac{1}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{3}}{2}$
cos	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{1}{2}$
tan	$\frac{\sqrt{3}}{3}$	1	$\sqrt{3}$
- Right Triangle:** A right-angled triangle with angles 30°, 45°, and 60°. The sides are labeled $2x$, x , and $x\sqrt{3}$.
- Integration Formulas:**
 - $\int \sin x dx = -\cos x + C$
 - $\int \frac{dx}{\cos^2 x} = \tan x + C$
 - $\int \tan x dx = -\ln|\cos x| + C$
 - $\int \frac{dx}{\sin x} = \ln\left|\frac{x}{2}\right| + C$
 - $\frac{dx}{a^2 + x^2} = \frac{1}{a} \arctg \frac{x}{a}$
 - $\frac{dx}{x^2 - a^2} = \frac{1}{2a} \ln\left|\frac{x-a}{x+a}\right| + C$
- Graphs:** A graph of the tangent function $\tan(\theta)$ with θ in radians, showing vertical asymptotes at $\pm \frac{\pi}{2}$.
- Quadratic Equations:**
 - $ax^2 + bx + c = 0$
 - $a(x^2 + \frac{b}{a}x + \frac{c}{a}) = 0$
 - $x^2 + 2\frac{b}{2a}x + (\frac{b}{2a})^2 - (\frac{b}{2a})^2 + \frac{c}{a} = 0$
 - $(x + \frac{b}{2a})^2 - \frac{b^2 - 4ac}{4a^2} = 0$



Reproducibility

- Is it reproducible?
- Is it easy to check reproducibility?



Stage 1 Simulation Code

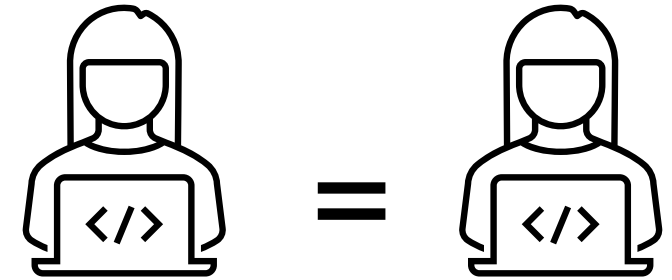
- In a simulation study, you're simulating your data, but don't want to know actual results
- Option 1: small number of fake datasets
 - Saves computing time and keeps results unstable

```
c_options <- c(10, 10, 10)
n_options <- c(10, 10, 10)
effect_size_options <- c("null", "small", "medium")
ndat_options <- 5
# ndat_options <- 1000
```

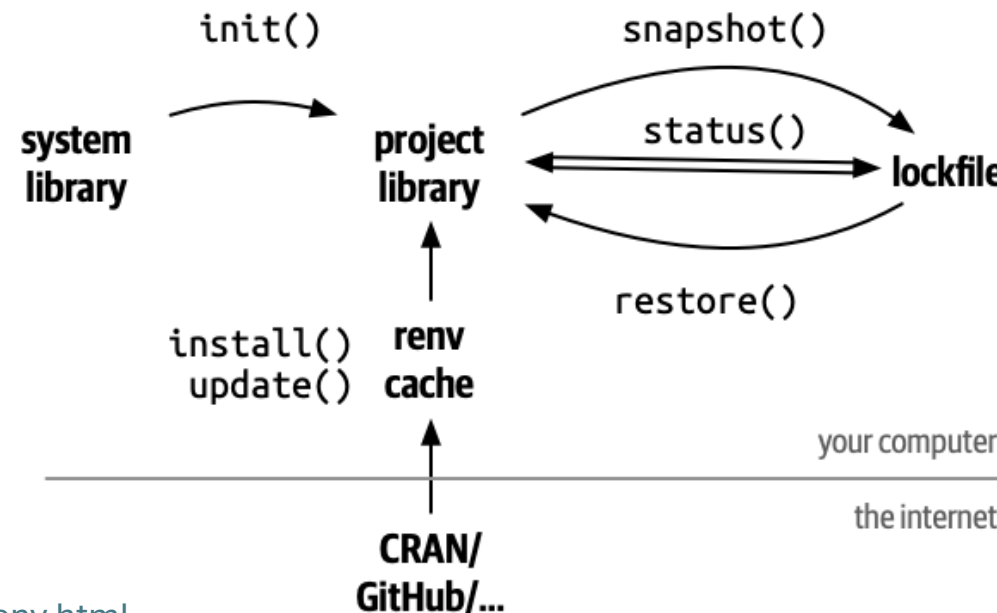
- Option 2: simulate data that has the structure you want, but fake starting values

```
# TEST EFFECTS
if (effect_size == "null") {
  effect <- 0.1
} else if (effect_size == "small") {
  effect <- 0.1
} else if (effect_size == "medium") {
  effect <- 0.1
} else {
  stop("Error in effect size condition")
}
```

Reproducibility: Package and Software

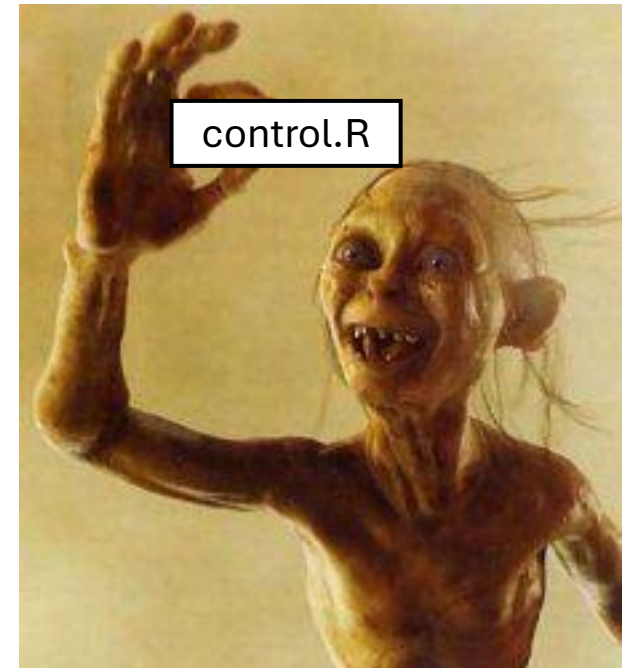
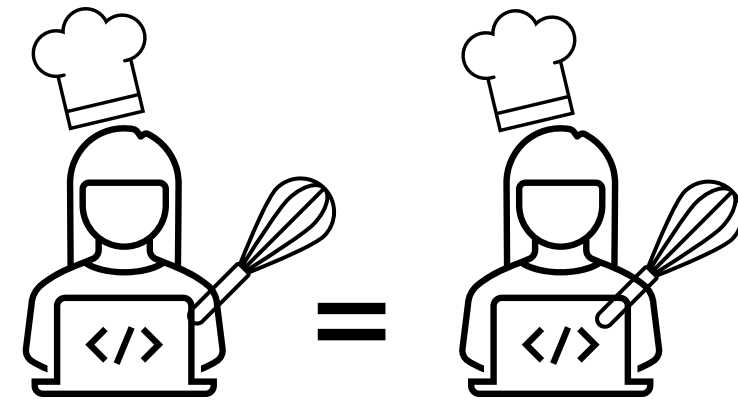


- List software and package versions in your paper
- renv automatically tracks your package versions and installs them on a reproducer's machine with the call `renv::restore()`



Reproducibility: Control File

- Many manual changes = recipe for disaster
- Implementing some kind of “control file” can help manage files: one file that manages all conditions and runs the entire simulation, calling separate function-specific files
- More effort up front, way easier in the long run



Control File Structure (for latest project)

```
# control.R

# Load dependencies
library(lme4)

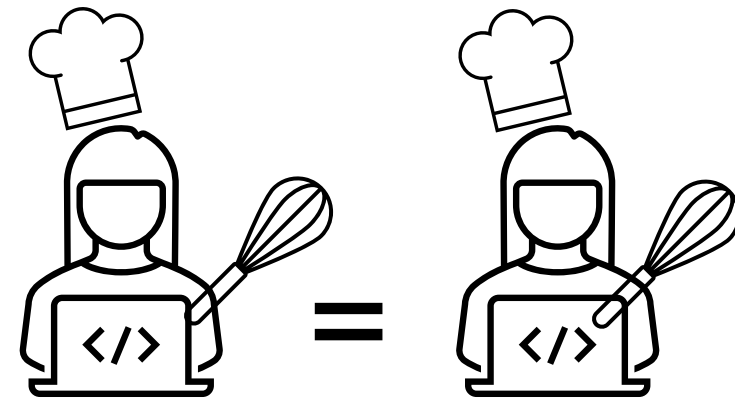
# Load functions written in other files
source("R/generate_data.R")
source("R/run_models.R")
source("R/calculate_results.R")

# Specify variables you manipulate
c_options <- c(10, 20, 30)
n_options <- c(10, 20, 30)
effect_size_options <- c("null", "small", "medium")
ndat_options <- 1000

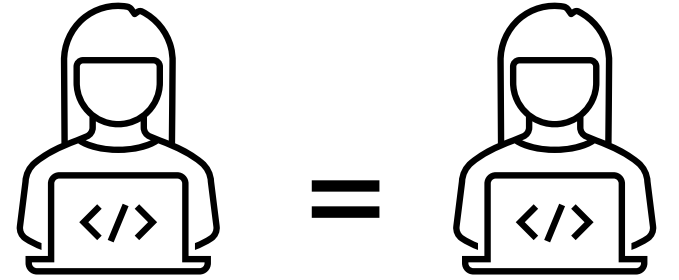
# Create population data
datasets <- generate_data(c_options, n_options, effect_size_options, ndat_options)

# Run models of interest
raw_values <- run_models(datasets)

# Calculate final results
results <- calculate_results(raw_values)
```

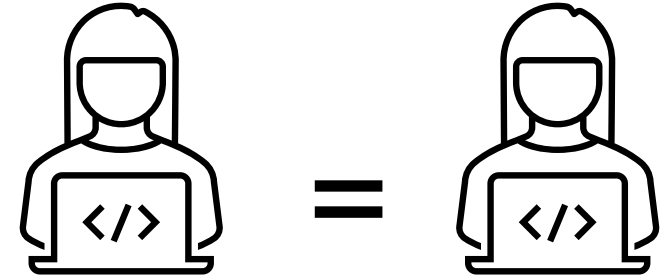


Reproducibility: Make Reproducers' Lives Easier



- Implement ways for reviewers to check that they're on the right track without running the entire simulation
- We're often simulating hundreds or thousands of datasets; manually exporting some allows reviewers to check theirs match ours early on
- If something doesn't reproduce, can help narrow down why

Reproducibility: Make Reproducers' Lives Easier



CODE

```
# create datasets
datasets <- simulate_data(ndat = 1000)

# save out two datasets
write.csv(datasets[[1]], "tests/df1.csv")

write.csv(datasets[[2]], "tests/df2.csv")
```

GITHUB README

Step 1.1. Check the generated "df1" dataset for reproducibility. The first five rows of data should be:

```
X_id      y      x1      z1
1  1 13.085108  0.005631125  0.6302638
2  1  6.031263 -0.638537285  0.6302638
3  1 18.820961  0.263297987  0.6302638
4  1 16.852893 -1.448011439  0.6302638
5  1 10.133860  0.230134755  0.6302638
```

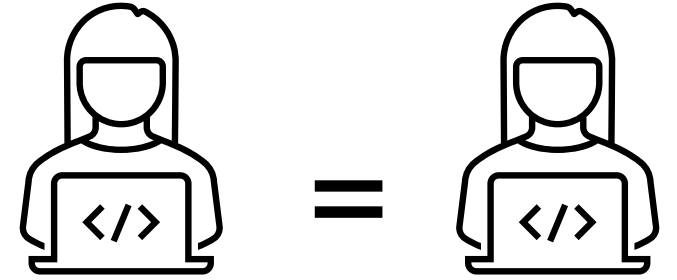


Step 1.2. Check the second generated "df2" dataset. The first five rows of data should be:

```
X_id      y      x1      z1
1  1  9.956949  1.2972483  0.09844718
2  1 12.188077  1.3861479  0.09844718
3  1  9.065660 -0.9633913  0.09844718
4  1 12.261863 -1.3337259  0.09844718
5  1  9.805620 -0.5786500  0.09844718
```



Reproducibility: Make Reproducers' Lives Easier

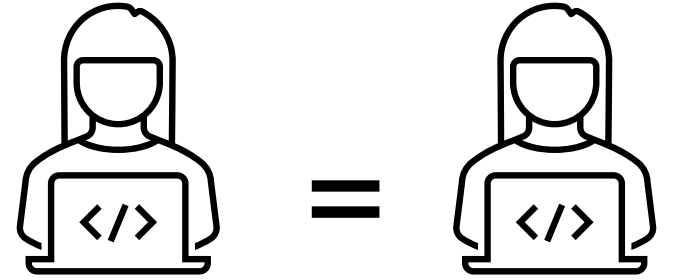


Reference your code in
your paper

- Clearly labelled files
- Create numbered sections or use line numbers
 - “Simulated data were generated from a standard normal distribution (data_generation.R, 2.2)”

```
68 ▾ ### 1.2 Demographics
69
70 ▾ ```{r 1.2.1}
71 # descriptives by sample group
72
```

Reproducibility: Odds and Ends



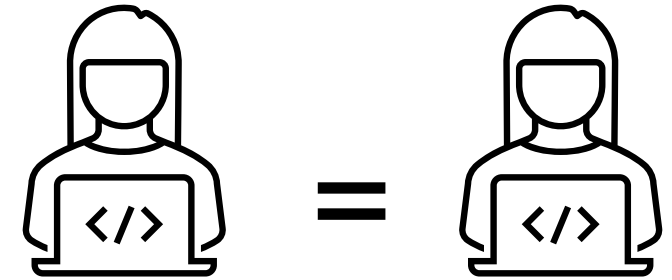
- Set seed
- Store your code publicly
 - OSF, GitHub
 - If you're worried about releasing the code before running the study, you can make a read-only option
 - GitHub read-only mirror of repository: <https://gitfront.io>

Reproducibility: Odds and Ends

GITHUB

The screenshot shows the GitHub interface for a repository named 'multimlm'. At the top, it indicates the repository is 'Private' and has '1 Branch' and '0 Tags'. Below this, there are navigation options for 'master', '1 Branch', and '0 Tags', along with a search bar and buttons for 'Add file' and 'Code'. The main content area displays a commit history table with columns for the commit message, commit hash, time ago, and number of commits. Below the table, there is a 'README' section with the title 'Multilevel Modelling Multiverse Simulation'.

Commit Message	Commit Hash	Time Ago	Commits
Add coding sheet for review of papers.	6e2ac50	2 weeks ago	31
Updates PLCI with explicit instruction, updates data files f...		last month	
Adds renv for session and package info, closes #13.		3 months ago	
Add coding sheet for review of papers.		2 weeks ago	
Updates PLCI with explicit instruction, updates data files f...		last month	
Adds renv for session and package info, closes #13.		3 months ago	
Updates PLCI with explicit instruction, updates data files f...		last month	
Updates estimator to Nelder-Mead. Close #1.		2 months ago	
Starts reproducibility readme, #19, #20.		3 months ago	
Centers generated datasets and updates renv with appro...		3 months ago	



READ-ONLY MIRROR

The screenshot shows a GitHub repository page for 'multimlm' that has been mirrored. The repository name 'multimlm' is at the top, with a 'Clone' button. Below this, a list of files and folders is shown, including 'R', 'renv', 'review of papers', 'tests', '.Rprofile', 'README.md', 'final_results.csv', 'multimlm.Rproj', and 'renv.lock'. Below the file list, the 'README.md' file is expanded, showing the title 'Multilevel Modelling Multiverse Simulation'.

Closing Thoughts

- A lot of these things apply generally as good practices. Preregistration just makes it unavoidable
- Reviewers are with you along the way, which can help catch your oversights
- Preregistration frontloads the work – you do more reading and planning up front, and once results are in you have identified contingent paths
- Future you is the one following the map, so make it as detailed as possible