Benjamin-Chung Lab Manual

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Welcome to the Benjamin-Chung Lab!

1.1 About the lab

Welcome to the lab of Dr. Jade Benjamin-Chung, Assistant Professor in Epidemiology & Population Health at Stanford University. Our mission is to improve population health by creating high quality evidence about what health interventions work in whom and where, when, and how to implement them. Most of our research is focused on infectious diseases, including malaria, diarrhea, soil-transmitted helminths, and influenza. Our focus is on improving the health of vulnerable populations from low-resource settings, both domestically and internationally. We use a variety of epidemiologic, computational, and statistical methods, including causal inference and machine learning methods, in pursuit of our mission. To learn more about the lab, visit jadebc.net.

1.2 About this lab manual

This lab manual covers our communication strategy, code of conduct, and best practices for reproducibility of computational workflows. It is a living document that is updated regularly.

This manual was created with input from a large number of team members and with inspiration from other scientists' lab manuals. Contributors include Jade Benjamin-Chung, Kunal Mishra, Stephanie Djajadi, Nolan Pokpongkiat, Anna Nguyen, Iris Tong, and Gabby Barratt Heitmann.

Feel free to draw from this manual (and please cite it if you do!).

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4.0 International License.

Culture and conduct

by Jade Benjamin-Chung

2.1 Lab culture

We are committed to a lab culture that is collaborative, supportive, inclusive, open, and free from discrimination and harassment.

We encourage students / staff of all experience levels to respectfully share their honest opinions and ideas on any topic. Our group has thrived upon such respectful honest input from team members over the years, and this document is a product of years of student and staff input (and even debate) that has gradually improved our productivity and overall quality of our work.

2.2 Diversity, equity, and inclusion

The Benjamin-Chung lab recognizes the importance of and is committed to cultivating a culture of diversity, equity, and inclusion. This means being a safe, supportive, and anti-racist environment in which students from diverse backgrounds are equally and inclusively supported in their education and training. Diversity takes many forms, and includes, but is not limited to, differences in race, ethnicity, gender, sexuality, socioeconomic status, religion, disability, and political affiliation.

2.3 Protecting human subjects

All lab members must complete CITI Human Subjects Biomedical Group 1 training and share their certificate with Jade. She will add team members to

relevant Institutional Review Board protocols prior to their start date to ensure they have permission to work with identifiable datasets.

One of the most relevant aspects of protecting human subjects in our work is maintaining confidentiality. For students supporting our data science efforts, in practice this means:

- Be sure to understand and comply with project-specific policies about where data can be saved, particularly if the data include personal identifiers.
- Do not share data with anyone without permission, including to other members of the group, who might not be on the same IRB protocol as you (check with Jade first).

Remember, data that looks like it does not contain identifiers to you might still be classified as data that requires special protection by our IRB or under HIPAA, so always proceed with caution and ask for help if you have any concerns about how to maintain study participant confidentiality.

2.4 Authorship

We adhere to the ICMJE Definition of authorship and are happy for team members who meet the definition of authorship to be included as co-authors on scientific manuscripts.

Communication and coordination

by Jade Benjamin-Chung

One benefit of the academic environment is its schedule flexibility. This means that lab members may choose to work in the early morning, evening, or weekends. That said, we do not expect lab members to respond outside of business hours (unless there are special circumstances).

3.1 Slack

- Use Slack for scheduling, coding related questions, quick check ins, etc. If your Slack message exceeds 200 words, it might be time to use email.
- Use channels instead of direct messages unless you need to discuss something private.
- Please make an effort to respond to messages that message you (e.g., @jade) as quickly as possible and always within 24 hours.
- If you are unusually busy (e.g., taking MCAT/GRE, taking many exams)
 or on vacation please alert the team in advance so we can expect you not
 to respond at all / as quickly as usual and also set your status in Slack
 (e.g., it could say "On vacation") so we know not to expect to see you
 online.
- Please thread messages in Slack as much as possible.

3.2 Email

Use email for longer messages (>200 words) or messages that merit preservation.

• Generally, strive to respond within 24 hours hours. As noted above, if you are unusually busy or on vacation please alert the team in advance so we can expect you not to respond at all / as quickly as usual.

3.3 Trello

- Jade will add new cards within our shared Trello board that outline your tasks
- The higher a card is within your list, the higher priority it is.
- Generally, strive to complete the tasks in your card by the date listed.
- Use checklists to break down a task into smaller chunks. Sometimes Jade will write this for you, but you can also add this yourself.
- Jade will move your card to the "Completed" list when it is done.

3.4 Google Drives

• We mostly use Google Drive to create shared documents with longer descriptions of tasks. These documents are linked to in Trello. Jade often shares these with the whole team since tasks are overlapping, and even if a task is assigned to one person, others may have valuable insights.

3.5 Meetings

- Our meetings start on the hour.
- If you are going to be late, please send a message in our Slack channel.
- If you are regularly not able to come on the hour, notify the team and we might choose the modify the agenda order or the start time.

Reproducibility

by Jade Benjamin-Chung

Our lab adopts the following practices to maximize the reproducibility of our work.

- 1. Design studies with appropriate methodology and adherence to best practices in epidemiology and biostatistics
- 2. Register study protocols
- 3. Write and register pre-analysis plans
- 4. Create reproducible workflows
- 5. Process and analyze data with internal replication and masking
- 6. Use reporting checklists with manuscripts
- 7. Publish preprints
- 8. Publish data (when possible) and replication scripts

4.1 What is the reproducibility crisis?

In the past decade, an increasing number of studies have found that published study findings could not be reproduced. Researchers found that it was not possible to reproduce estimates from published studies: 1) with the same data and same or similar code and 2) with newly collected data using the same (or similar) study design. These "failures" of reproducibility were frequent enough and broad enough in scope, occurring across a range of disciplines (epidemiology, psychology, economics, and others) to be deeply troubling. Program and policy decisions based on erroneous research findings could lead to wasted resources, and at worst, could harm intended beneficiaries. This crisis has motivated new practices in reproducibility, transparency, and openness. Our lab is committed to adopting these best practices, and much of the remainder of the lab manual focuses on how to do so.

Recommended readings on the "reproducibility crisis":

- Nuzzo R. How scientists fool themselves and how they can stop. 2015. https://www.nature.com/articles/526182a
- Stoddart C. Is there a reproducibility crisis in science? 2016. https://www.nature.com/articles/d41586-019-00067-3
- Munafo MR, et al. A manifesto for reproducible science. *Nature Human Behavior* 2017 http://dx.doi.org/10.1038/s41562-016-0021

4.2 Study design

Appropriate study design is beyond the scope of this lab manual and is something trainees develop through their coursework and mentoring.

4.3 Register study protocols

We register all randomized trials on clinical trials gov, and in some cases register observational studies as well.

4.4 Write and register pre-analysis plans

We write pre-analysis plans for most original research projects that are not exploratory in nature, although in some cases, we write pre-analysis plans for exploratory studies as well. The format and content of pre-analysis plans can vary from project to project. Here is an example of one: https://osf.io/tgbxr/. Generally, these include:

- 1. Brief background on the study (a condensed version of the introduction section of the paper)
- 2. Hypotheses / objectives
- 3. Study design
- 4. Description of data
- 5. Definition of outcomes
- 6. Definition of interventions / exposures
- 7. Definition of covariates
- 8. Statistical power calculation
- 9. Statistical analysis:
- · Type of model
- Covariate selection / screening
- Standard error estimation method
- Missing data analysis
- Assessment of effect modification / subgroup analyses
- Sensitivity analyses

• Negative control analyses

4.5 Create reproducible workflows

Reproducible workflows allow a user to reproduce study estimates and ideally figures and tables with a "single click". In practice, this typically means running a single bash script that sources all replication scripts in a repository. These replication scripts complete data processing, data analysis, and figure/table generation. The following chapters provide detailed guidance on this topic:

- Chapter 5: Code repositories
- Chapter 6: Coding practices
- Chapter 7: Coding style
- Chapter 8: Code publication
- Chapter 9: Working with big data
- Chapter 10: Github
- Chapter 11: Unix

4.6 Process and analyze data with internal replication and masking

See my video on this topic: https://www.youtube.com/watch?v=WoYkY9MkbRE

4.7 Use reporting checklists with manuscripts

Using reporting checklists helps ensure that peer-reviewed articles contain the information needed for readers to assess the validity of your work and/or attempt to reproduce it. A collection of reporting checklists is available here: https://www.equator-network.org/about-us/what-is-a-reporting-guideline/)

4.8 Publish preprints

A preprint is a scientific manuscript that has not been peer reviewed. Preprint servers create digital object identifiers (DOIs) and can be cited in other articles and in grant applications. Because the peer review process can take many months, publishing preprints prior to or during peer review enables other scientists to immediately learn from and build on your work. Importantly, NIH allows applicants to include preprint citations in their biosketches. In most cases, we publish preprints on medRxiv.

4.9 Publish data (when possible) and replication scripts

Publishing data and replication scripts allows other scientists to reproduce your work and to build upon it. We typically publish data on Open Science Framework, share links to Github repositories, and archive code on Zenodo.

Code repositories

By Kunal Mishra, Jade Benjamin-Chung, and Stephanie Djajadi

Each study has at least one code repository that typically holds R code, shell scripts with Unix code, and research outputs (results .RDS files, tables, figures). Repositories may also include datasets. This chapter outlines how to organize these files. Adhering to a standard format makes it easier for us to efficiently collaborate across projects.

5.1 Project Structure

We recommend the following directory structure:

```
0-run-project.sh
0-config.R
1 - Data-Management/
    0-prep-data.sh
    1-prep-cdph-fluseas.R
    2a-prep-absentee.R
    2b-prep-absentee-weighted.R
    3a-prep-absentee-adj.R
    3b-prep-absentee-adj-weighted.R
2 - Analysis/
   0-run-analysis.sh
    1 - Absentee-Mean/
        1-absentee-mean-primary.R
        2-absentee-mean-negative-control.R
        3-absentee-mean-CDC.R
        4-absentee-mean-peakwk.R
        5-absentee-mean-cdph2.R
        6-absentee-mean-cdph3.R
```

```
2 - Absentee-Positivity-Check/
    3 - Absentee-P1/
    4 - Absentee-P2/
3 - Figures/
    0-run-figures.sh
4 - Tables/
    0-run-tables.sh
5 - Results/
    1 - Absentee-Mean/
        1-absentee-mean-primary.RDS
        2-absentee-mean-negative-control.RDS
        3-absentee-mean-CDC.RDS
        4-absentee-mean-peakwk.RDS
        5-absentee-mean-cdph2.RDS
        6-absentee-mean-cdph3.RDS
.gitignore
.Rproj
```

For brevity, not every directory is "expanded", but we can glean some important takeaways from what we do see.

5.2 . Rproj files

An "R Project" can be created within RStudio by going to File >> New Project. Depending on where you are with your research, choose the most appropriate option. This will save preferences, working directories, and even the results of running code/data (though I'd recommend starting from scratch each time you open your project, in general). Then, ensure that whenever you are working on that specific research project, you open your created project to enable the full utility of .Rproj files. This also automatically sets the directory to the top level of the project.

5.3 Configuration ('config') File

This is the single most important file for your project. It will be responsible for a variety of common tasks, declare global variables, load functions, declare paths, and more. Every other file in the project will begin with source("0-config"), and its role is to reduce redundancy and create an abstraction layer that allows you to make changes in one place (0-config.R) rather than 5 different files. To this end, paths which will be reference in multiple scripts (i.e. a merged_data_path) can be declared in 0-config.R and simply referred to by its variable name in scripts. If you ever want to change things, rename them,

or even switch from a downsample to the full data, all you would then to need to do is modify the path in one place and the change will automatically update throughout your project. See the example config file for more details. The paths defined in the O-config.R file assume that users have opened the .Rproj file, which sets the directory to the top level of the project.

5.4 Order Files and Directories

This makes the jumble of alphabetized filenames much more coherent and places similar code and files next to one another. This also helps us understand how data flows from start to finish and allows us to easily map a script to its output (i.e. 2 - Analysis/1 - Absentee-Mean/1-absentee-mean-primary.RDS). If you take nothing else away from this guide, this is the single most helpful suggestion to make your workflow more coherent. Often the particular order of files will be in flux until an analysis is close to completion. At that time it is important to review file order and naming and reproduce everything prior to drafting a manuscript.

5.5 Using Bash scripts to ensure reproducibility

Bash scripts are useful components of a reproducible workflow. At many of the directory levels (i.e. in 3 - Analysis), there is a bash script that runs each of the analysis scripts. This is exceptionally useful when data "upstream" changes – you simply run the bash script. See the Unix Chapter for further details.

After running bash scripts, .Rout log files will be generated for each script that has been executed. It is important to check these files. Scripts may appear to have run correctly in the terminal, but checking the log files is the only way to ensure that everything has run completely.

Coding practices

by Kunal Mishra, Jade Benjamin-Chung, Stephanie Djajadi, and Iris Tong

6.1 Organizing scripts

Just as your data "flows" through your project, data should flow naturally through a script. Very generally, you want to:

- 1. describe the work completed in the script in a comment header
- 2. source your configuration file (0-config.R)
- 3. load all your data
- 4. do all your analysis/computation
- 5. save your data.

Each of these sections should be "chunked together" using comments. See this file for a good example of how to cleanly organize a file in a way that follows this "flow" and functionally separate pieces of code that are doing different things.

6.2 Documenting your code

6.2.1 File headers

Every file in a project should have a header that allows it to be interpreted on its own. It should include the name of the project and a short description for what this file (among the many in your project) does specifically. You may optionally wish to include the inputs and outputs of the script as well, though the next section makes this significantly less necessary.

- # @Organization Example Organization
- # @Project Example Project

6.2.2 Sections and subsections

Rstudio (v1.4 or more recent) supports the use of Sections and Subsections. You can easily navigate through longer scripts using the navigation pane in RStudio, as shown on the right below.

```
## Subsection -----
### Sub-subsection ------
```

6.2.3 Code folding

Consider using RStudio's code folding feature to collapse and expand different sections of your code. Any comment line with at least four trailing dashes (-), equal signs (=), or pound signs (#) automatically creates a code section. For example:

6.2.4 Comments in the body of your script

Commenting your code is an important part of reproducibility and helps document your code for the future. When things change or break, you'll be thankful for comments. There's no need to comment excessively or unnecessarily, but a comment describing what a large or complex chunk of code does is always helpful. See this file for an example of how to comment your code and notice that comments are always in the form of:

This is a comment -- first letter is capitalized and spaced away from the pound sign

6.2.5 Function documentation

Every function you write must include a header to document its purpose, inputs, and outputs. For any reproducible workflows, they are essential, because R is dynamically typed. This means, you can pass a string into an argument that is meant to be a data.table, or a list into an argument meant for a tibble. It is the responsibility of a function's author to document what each argument is meant to do and its basic type. This is an example for documenting a function (inspired by JavaDocs and R's Plumber API docs):

Usage: calc_fluseas_mean(data, yname)

```
# Description: Make a dataframe with rows for flu season and site
# and the number of patients with an outcome, the total patients,
# and the percent of patients with the outcome

# Args/Options:
# data: a data frame with variables flu_season, site, studyID, and yname
# yname: a string for the outcome name
# silent: a boolean specifying whether the function shouldn't output anything to the console (DEF
# Returns: the dataframe as described above
# Output: prints the data frame described above if silent is not True

calc_fluseas_mean = function(data, yname, silent = TRUE) {
    ### function code here
}
```

The header tells you what the function does, its various inputs, and how you might go about using the function to do what you want. Also notice that all optional arguments (i.e. ones with pre-specified defaults) follow arguments that require user input.

- Note: As someone trying to call a function, it is possible to access a function's documentation (and internal code) by CMD-Left-Clicking the function's name in RStudio
- Note: Depending on how important your function is, the complexity of your function code, and the complexity of different types of data in your project, you can also add "type-checking" to your function with the assertthat::assert_that() function. You can, for example, assert_that(is.data.frame(statistical_input)), which will ensure that collaborators or reviewers of your project attempting to use your function are using it in the way that it is intended by calling it with (at the minimum) the correct type of arguments. You can extend this to ensure that certain assumptions regarding the inputs are fulfilled as well (i.e. that time_column, location_column, value_column, and population_column all exist within the statistical_input tibble).

6.3 Object naming

Generally we recommend using nouns for objects and verbs for functions. This is because functions are performing actions, while objects are not.

Try to make your variable names both more expressive and more explicit. Being a bit more verbose is useful and easy in the age of autocompletion! For example, instead of naming a variable vaxcov_1718, try naming it vaccination_coverage_2017_18. Similarly, flu_res could be named

absentee_flu_residuals, making your code more readable and explicit.

• For more help, check out Be Expressive: How to Give Your Variables Better Names

We recommend you use Snake_Case.

- Base R allows . in variable names and functions (such as read.csv()), but this goes against best practices for variable naming in many other coding languages. For consistency's sake, snake_case has been adopted across languages, and modern packages and functions typically use it (i.e. readr::read_csv()). As a very general rule of thumb, if a package you're using doesn't use snake_case, there may be an updated version or more modern package that does, bringing with it the variety of performance improvements and bug fixes inherent in more mature and modern software.
- Note: you may also see camelCase throughout the R code you come across. This is *okay* but not ideal try to stay consistent across all your code with snake_case.
- Note: again, its also worth noting there's nothing inherently wrong with using . in variable names, just that it goes against style best practices that are cropping up in data science, so its worth getting rid of these bad habits now.

6.4 Function calls

In a function call, use "named arguments" and put each argument on a separate line to make your code more readable.

Here's an example of what not to do when calling the function a function calc_fluseas_mean (defined above):

```
mean_Y = calc_fluseas_mean(flu_data, "maari_yn", FALSE)
And here it is again using the best practices we've outlined:
mean_Y = calc_fluseas_mean(
  data = flu_data,
   yname = "maari_yn",
   silent = FALSE
)
```

6.5 The here package

The here package is one great R package that helps multiple collaborators deal with the mess that is working directories within an R project structure. Let's

say we have an R project at the path /home/oski/Some-R-Project. My collaborator might clone the repository and work with it at some other path, such as /home/bear/R-Code/Some-R-Project. Dealing with working directories and paths explicitly can be a very large pain, and as you might imagine, setting up a Config with paths requires those paths to flexibly work for all contributors to a project. This is where the here package comes in and this a great vignette describing it.

6.6 Reading/Saving Data

6.6.1 .RDS vs .RData Files

One of the most common ways to load and save data in Base R is with the load() and save() functions to serialize multiple objects in a single .RData file. The biggest problems with this practice include an inability to control the names of things getting loaded in, the inherent confusion this creates in understanding older code, and the inability to load individual elements of a saved file. For this, we recommend using the RDS format to save R objects.

• Note: if you have many related R objects you would have otherwise saved all together using the save function, the functional equivalent with RDS would be to create a (named) list containing each of these objects, and saving it.

6.6.2 CSVs

Once again, the readr package as part of the Tidvyerse is great, with a much faster read_csv() than Base R's read.csv(). For massive CSVs (> 5 GB), you'll find data.table::fread() to be the fastest CSV reader in any data science language out there. For writing CSVs, readr::write_csv() and data.table::fwrite() outclass Base R's write.csv() by a significant margin as well.

6.7 Integrating Box and Dropbox

Box and Dropbox are cloud-based file sharing systems that are useful when dealing with large files. When our scripts generate large output files, the files can slow down the workflow if they are pushed to GitHub. This makes collaboration difficult when not everyone has a copy of the file, unless we decide to duplicate files and share them manually. The files might also take up a lot of local storage. Box and Dropbox help us avoid these issues by automatically storing the files, reading data, and writing data back to the cloud.

Box and Dropbox are separate platforms, but we can use either one to store and share files. To use them, we can install the packages that have been created to integrate Box and Dropbox into R. The set-up instructions are detailed below.

Make sure to authenticate before reading and writing from either Box or Dropbox. The authentication commands should go in the configuration file; it only needs to be done once. This will prompt you to give your login credentials for Box and Dropbox and will allow your application to access your shared folders.

6.7.1 Box

Follow the instructions in this section to use the boxr package. Note that there are a few setup steps that need to be done on the box website before you can use the boxr package, explained here in the section "Creating an Interactive App." This gets the authentication keys that must be put in box. Once that is done, add the authentication keys to your code in the configuration file, with box_auth(client_id = "<your_client_id>", client_secret = "<your_client_secret_id>"). It is also important to set the default working directory so that the code can reference the correct folder in box: box_setwd(<folder_id>). The folder ID is the sequence of digits at the end of the URL.

Further details can be found here.

6.7.2 Dropbox

first time only

Follow the instructions at this link to use the rdrop2 package. Similar to the boxr package, you must authenticate before reading and writing from Dropbox, which can be done by adding drop_auth() to the configuration file.

Saving the authentication token is not required, although it may be useful if you plan on using Dropbox frequently. To do so, save the token with the following commands. Tokens are valid until they are manually revoked.

```
# save the output of drop_auth to an RDS file
token <- drop_auth()
# this token only has to be generated once, it is valid until revoked
saveRDS(token, "/path/to/tokenfile.RDS")
# all future usages
# to use a stored token, provide the rdstoken argument
drop_auth(rdstoken = "/path/to/tokenfile.RDS")</pre>
```

6.8 Tidyverse

Throughout this document there have been references to the Tidyverse, but this section is to explicitly show you how to transform your Base R tendencies to Tidyverse (or Data.Table, Tidyverse's performance-optimized competitor). For most of our work that does not utilize very large datasets, we recommend that you code in Tidyverse rather than Base R. Tidyverse is quickly becoming the

6.8. TIDYVERSE 27

gold standard in R data analysis and modern data science packages and code should use Tidyverse style and packages unless there's a significant reason not to (i.e. big data pipelines that would benefit from Data. Table's performance optimizations).

The package author has published a great textbook on R for Data Science, which leans heavily on many Tidyverse packages and may be worth checking out.

The following list is not exhaustive, but is a compact overview to begin to translate Base R into something better:

Base R	Better Style, Performance, and Utility
read.csv()	readr::read_csv() or
	<pre>data.table::fread()</pre>
write.csv()	readr::write_csv() or
	<pre>data.table::fwrite()</pre>
readRDS	readr::read_rds()
saveRDS()	readr::write_rds()
data.frame()	tibble::tibble() or
	<pre>data.table::data.table()</pre>
rbind()	<pre>dplyr::bind_rows()</pre>
cbind()	<pre>dplyr::bind_cols()</pre>
df\$some_column	<pre>df %>% dplyr::pull(some_column)</pre>
<pre>df\$some_column =</pre>	df %>%
	<pre>dplyr::mutate(some_column =)</pre>
<pre>df[get_rows_condition,]</pre>	df %>%
_	dplyr::filter(get_rows_condition)
df[,c(col1, col2)]	df %>% dplyr::select(col1,
	col2)
merge(df1, df2, by =, all.x	<pre>df1 %>% dplyr::left_join(df2,</pre>
=, all.y =)	<pre>by =) or dplyr::full_join or</pre>
•	dplyr::inner_join or
	dplyr::right_join
	1 0 -0
str()	dplyr::glimpse()
<pre>grep(pattern, x)</pre>	stringr::str_which(string,
	pattern)
<pre>gsub(pattern, replacement, x)</pre>	stringr::str_replace(string,
	pattern, replacement)
<pre>ifelse(test_expression, yes, no)</pre>	<pre>if_else(condition, true, false)</pre>

Base R	Better Style, Performance, and Utility
Nested: ifelse(test_expression1, yes1, ifelse(test_expression2, yes2, ifelse(test_expression3, yes3, no))) proc.time() stopifnot()	<pre>case_when(test_expression1 ~ yes1, test_expression2 ~ yes2, test_expression3 ~ yes3, TRUE ~ no) tictoc::tic() and tictoc::toc() assertthat::assert_that() or assertthat::see_if() or assertthat::validate_that()</pre>

For a more extensive set of syntactical translations to Tidyverse, you can check out this document.

Working with Tidyverse within functions can be somewhat of a pain due to non-standard evaluation (NSE) semantics. If you're an avid function writer, we'd recommend checking out the following resources:

- Tidy Eval in 5 Minutes (video)
- Tidy Evaluation (e-book)
- Data Frame Columns as Arguments to Dplyr Functions (blog)
- Standard Evaluation for *_join (stackoverflow)
- Programming with dplyr (package vignette)

6.9 Coding with R and Python

If you're using both R and Python, you may wish to check out the Feather package for exchanging data between the two languages extremely quickly.

6.10 Repeating analyses with different variations

In many cases, we will need to apply our modeling on different combinations of interests (outcomes, exposures, etc.). We can certainly use a for loop to repeat the execution of a wrapper function, but generally, for loops request high memory usage and produce the results in long computation time.

Fortunately, R has some functions which implement looping in a compact form to help repeating your analyses with different variations (subgroups, outcomes, covariate sets, etc.) with better performances.

6.10.1 lapply() and sapply()

lapply() is a function in the base R package that applies a function to each element of a list and returns a list. It's typically faster than for. Here is a

simple generic example:

```
result <- lapply(X = mylist, FUN = func)
```

There is another very similar function called sapply(). It also takes a list as its input, but if the output of the func is of the same length for each element in the input list, then sapply() will simplify the output to the simplest data structure possible, which will usually be a vector.

6.10.2 mapply() and pmap()

Sometimes, we'd like to employ a wrapper function that takes arguments from multiple different lists/vectors. Then, we can consider using mapply() from the base R package or pmap() from the purr package.

Please see the simple specific example below where the two input lists are of the same length and we are doing a pairwise calculation:

```
mylist1 = list(0:3)
mylist2 = list(6:9)
mylists = list(mylist1, mylist2)

square_sum <- function(x, y) {
    x^2 + y^2
}

#Use `mapply()`
result1 <- mapply(FUN = square_sum, mylist1, mylist2)

#Use `pmap()`
library(purrr)
result2 <- pmap(.1 = mylists, .f = square_sum)

#unlist(as.list(result1)) = result2 = [36 50 68 90]</pre>
```

There are two major differences between mapply() and pmap(). The first difference is that mapply() takes seperate lists as its input arguments, while pmap() takes a list of list. Secondly, the output of mapply() will be in the form of a matrix or an array, but pmap() produces a list directly.

However, when the input lists are of different lengths AND/OR the wrapper function doesn't take arguments in pairs, mapply() and pmap() may not give the preferable results.

Both mapply() and pmap() will recycle shorter input lists to match the length of the longest input list. Assume that now mylist2 = list(6:12). Then, pmap(mylists, square_sum) will generate [36 50 68 90 100 122 148] where elements 0, 1, and 2 are recycled to match 10, 11, and 12. And it will

return an error message that "longer object length is not a multiple of shorter object length."

Thus, unless the recycling pattern described above is desirable feature for a certain experiment design, when the input lists are of different lengths, the best practice is probably to use lapply() and then combine the results.

Here is an example where we'd like to find the square_sum for every element combination of mylist1 and mylist2.

```
mylist1 <- list(0:3)
mylist2 <- list(6:12)

square_sum <- function(x, y) {
    x^2 + y^2
}

results <- list()

for (i in seq_along(mylist1[[1]])) {
    result <- lapply(X = mylist2, FUN = function(y) square_sum(mylist1[[1]][i], y))
    results[[i]] <- result
}</pre>
```

This example doesn't work in the way that 0 is paired to 6, 1 is paired to 7, and so on. Instead, every element in mylist1 will be paired with every element in mylist2. Thus, the "unlisted" results from the example will have 4*7=28 elements.

We can use flatten() or unlist() functions to decrease the depths of our results. If the results are data frames, then we will need to use bind_rows() to combine them.

6.10.3 Parallel processing with parallel and future packages

One big drawback of lapply() is its long computation time, especially when the list length is long. Fortunately, computers nowadays must have multiple cores which makes parallel processing possible to help make computation much faster.

Assume you have a list called mylist of length 1000, and lapply(X = mylist, FUN = func) applies the function to each of the 1000 elements one by one in T seconds. If we could execute the func in n processors simultaneously, then ideally, we would shrink the computation time to T/n seconds.

In practice, using functions under the parallel and the future packages, we can split mylist into smaller chunks and apply the function to each element of

the several chunks in parallel in different cores to significantly reduce the run time.

6.10.3.1 parLapply()

stopCluster(cl)

```
Below is a generic example of parLapply():
library(parallel)

# Set how many processors will be used to process the list and make cluster n_cores <- 4
cl <- makeCluster(n_cores)

#Use parLapply() to apply func to each element in mylist
result <- parLapply(cl = cl, x = mylist, FUN = func)

#Stop the parallel processing
```

Let's still assume mylist is of length 1000. The parLapply above splits mylist into 4 sub-lists each of length 250 and applies the function to the elements of each sub-list in parallel. To be more specific, first apply the function to element 1, 251, 501, 751; second apply to element 2, 252, 502, 752; so on and so forth. As such, the computation time will be greatly reduced.

You can use parallel::detectCores() to test how many cores your machine has and to help decide what to put for n_cores. It would be a good idea to leave at least one core free for the operating system to use.

We will always start parLapply() with makeCluster(). stopCluster() is not fully necessary but follows the best practices. If not stopped, the processing will continue in the back end and consuming the computation capacity for other software in your machine. But keep in mind that stopping the cluster is similar quitting R, meaning that you will need to re-load the packages needed when you need to do parallel processing use parLapply() again.

6.10.3.2 future.lapply()

```
Below is a generic example of future.lapply():
library(future)
library(future.apply)

# First, plan how the future_lapply() will be resolved
future::plan(
   multisession, workers = future::availableCores() - 1
)

# Use future_lapply() to apply func to each element in mylist
```

```
future_lapply(x = mylist, FUN = func)
```

Here, future::availableCores() checks how many cores your machine has. Similar to parLapply() showed above, future_lapply() parallelizes the computation of lapply() by executing the function func simultaneously on different sub-lists of mylist.

6.11 Reviewing Code

Before publishing new changes, it is important to ensure that the code has been tested and well-documented. GitHub makes it possible to document all of these changes in a pull request. Pull requests can be used to describe changes in a branch that are ready to be merged with the base branch (more information in the GitHub section). Github allows users to create a pull request template in a repository to standardize and customize the information in a pull request. When you add a pull request template to your repository, everyone will automatically see the template's contents in the pull request body.

6.11.1 Creating a Pull Request Template

Follow the instructions below to add a pull request template to a repository. More details can be found at this GitHub link.

- 1. On GitHub, navigate to the main page of the repository.
- 2. Above the file list, click Create new file.
- 3. Name the file pull_request_template.md. GitHub will not recognize this as the template if it is named anything else. The file must be on the master branch.
 - 1. To store the file in a hidden directory instead of the main directory, name the file .github/pull_request_template.md.
- 4. In the body of the new file, add your pull request template. This could include:
 - A summary of the changes proposed in the pull request
 - How the change has been tested
 - @mentions of the person or team responsible for reviewing proposed changes

Here is an example pull request template.

```
# Description
## Summary of change
Please include a summary of the change, including any new functions added and example ## Link to Spec
```

Please include a link to the Trello card or Google document with details of the task.

```
## Who should review the pull request? \boldsymbol{\sigma}
```

Coding style

by Kunal Mishra, Jade Benjamin-Chung, and Stephanie Djajadi

7.1 Comments

1. **File Headers** - Every file in a project should have a header that allows it to be interpreted on its own. It should include the name of the project and a short description for what this file (among the many in your project) does specifically. You may optionally wish to include the inputs and outputs of the script as well, though the next section makes this significantly less necessary.

- # @Organization Example Organization
- # @Project Example Project
- # @Description This file is responsible for [...]

- 2. File Structure Just as your data "flows" through your project, data should flow naturally through a script. Very generally, you want to 1) source your config => 2) load all your data => 3) do all your analysis/computation => save your data. Each of these sections should be "chunked together" using comments. See this file for a good example of how to cleanly organize a file in a way that follows this "flow" and functionally separate pieces of code that are doing different things.
 - Note: If your computer isn't able to handle this workflow due to RAM or requirements, modifying the ordering of your code to accomodate it won't be ultimately helpful and your code will be fragile, not to mention less readable and messy. You need to look into high-performance computing (HPC) resources in this case.

- 3. Single-Line Comments Commenting your code is an important part of reproducibility and helps document your code for the future. When things change or break, you'll be thankful for comments. There's no need to comment excessively or unnecessarily, but a comment describing what a large or complex chunk of code does is always helpful. See this file for an example of how to comment your code and notice that comments are always in the form of:
- # This is a comment -- first letter is capitalized and spaced away from the pound sign
 - 4. Multi-Line Comments Occasionally, multi-line comments are necessary. Don't add line breaks manually to a single-line comment for the purpose of making it "fit" on the screen. Instead, in RStudio > Tools > Global Options > Code > "Soft-wrap R source files" to have lines wrap around. Format your multi-line comments like the file header from above.

7.2 Line breaks

• For ggplot calls and dplyr pipelines, do not crowd single lines. Here are some nontrivial examples of "beautiful" pipelines, where beauty is defined by coherence:

```
# Example 1
school_names = list(
  OUSD_school_names = absentee_all %>%
    filter(dist.n == 1) %>%
    pull(school) %>%
    unique %>%
    sort,
  WCCSD_school_names = absentee_all %>%
    filter(dist.n == 0) %>%
    pull(school) %>%
    unique %>%
    sort
)
# Example 2
absentee_all = fread(file = raw_data_path) %>%
  mutate(program = case_when(schoolyr %in% pre_program_schoolyrs ~ 0,
                             schoolyr %in% program_schoolyrs ~ 1)) %>%
  mutate(period = case_when(schoolyr %in% pre_program_schoolyrs ~ 0,
                            schoolyr %in% LAIV schoolyrs ~ 1,
                            schoolyr %in% IIV schoolyrs ~ 2)) %>%
  filter(schoolyr != "2017-18")
```

And of a complex ggplot call: # Example 3 ggplot(data=data, mapping=aes_string(x="year", y="rd", group=group)) + geom_point(mapping=aes_string(col=group, shape=group), position=position_dodge(width=0.2), size=2.5) +geom_errorbar(mapping=aes_string(ymin="lb", ymax="ub", col=group), position=position dodge(width=0.2), width=0.2) +geom_point(position=position_dodge(width=0.2), size=2.5) +geom_errorbar(mapping=aes(ymin=lb, ymax=ub), position=position_dodge(width=0.2), width=0.1) +scale_y_continuous(limits=limits, breaks=breaks, labels=breaks) + scale_color_manual(std_legend_title,values=cols,labels=legend_label) + scale_shape_manual(std_legend_title,values=shapes, labels=legend_label) + geom_hline(yintercept=0, linetype="dashed") + xlab("Program year") + ylab(yaxis_lab) + theme complete bw() + theme(strip.text.x = element_text(size = 14), axis.text.x = element_text(size = 12)) +

Imagine (or perhaps mournfully recall) the mess that can occur when you don't strictly style a complicated ggplot call. Trying to fix bugs and ensure your code is working can be a nightmare. Now imagine trying to do it with the same code 6 months after you've written it. Invest the time now and reap the rewards as the code practically explains itself, line by line.

ggtitle(title)

7.3 Automated Tools for Style and Project Workflow

7.3.1 Styling

- 1. Code Autoformatting RStudio includes a fantastic built-in utility (keyboard shortcut: CMD-Shift-A) for autoformatting highlighted chunks of code to fit many of the best practices listed here. It generally makes code more readable and fixes a lot of the small things you may not feel like fixing yourself. Try it out as a "first pass" on some code of yours that doesn't follow many of these best practices!
- 2. Assignment Aligner A cool R package allows you to very powerfully format large chunks of assignment code to be much cleaner and much more readable. Follow the linked instructions and create a keyboard shortcut of your choosing (recommendation: CMD-Shift-Z). Here is an example of how assignment aligning can dramatically improve code readability:

```
# Before
OUSD_not_found_aliases = list(
    "Brookfield Village Elementary" = str_subset(string = OUSD_school_shapes$schnam, pat
    "Carl Munck Elementary" = str_subset(string = OUSD_school_shapes$schnam, pattern = "!
    "Community United Elementary School" = str_subset(string = OUSD_school_shapes$schnam
    "East Oakland PRIDE Elementary" = str_subset(string = OUSD_school_shapes$schnam, pat
    "EnCompass Academy" = str_subset(string = OUSD_school_shapes$schnam, pattern = "EnCompass Academy" = str_subset(string = OUSD_school_shapes$school_shapes$schnam, pattern = "EnCompass Academy" = str_subset(string = OUSD_school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes$school_shapes
    "Global Family School" = str_subset(string = OUSD_school_shapes$schnam, pattern = "G
    "International Community School" = str_subset(string = OUSD_school_shapes$schnam, pa
    "Madison Park Lower Campus" = "Madison Park Academy TK-5",
    "Manzanita Community School" = str_subset(string = OUSD_school_shapes$schnam, patter:
    "Martin Luther King Jr Elementary" = str_subset(string = OUSD_school_shapes$schnam,
    "PLACE @ Prescott" = "Preparatory Literary Academy of Cultural Excellence",
    "RISE Community School" = str_subset(string = OUSD_school_shapes$schnam, pattern = "
)
# After
OUSD_not_found_aliases = list(
    "Brookfield Village Elementary"
                                                                               = str_subset(string = OUSD_school_shapes$schnam
    "Carl Munck Elementary"
                                                                               = str_subset(string = OUSD_school_shapes$schnam
    "Community United Elementary School" = str subset(string = OUSD school shapes$schnam
    "East Oakland PRIDE Elementary"
                                                                               = str_subset(string = OUSD_school_shapes$schnam
    "EnCompass Academy"
                                                                               = str_subset(string = OUSD_school_shapes$schnam
    "Global Family School"
                                                                               = str_subset(string = OUSD_school_shapes$schnam
    "International Community School"
                                                                               = str_subset(string = OUSD_school_shapes$schnam
    "Madison Park Lower Campus"
                                                                               = "Madison Park Academy TK-5",
    "Manzanita Community School"
                                                                               = str_subset(string = OUSD_school_shapes$schnam
    "Martin Luther King Jr Elementary"
                                                                              = str_subset(string = OUSD_school_shapes$schnam
    "PLACE @ Prescott"
                                                                               = "Preparatory Literary Academy of Cultural Exc
    "RISE Community School"
                                                                               = str_subset(string = OUSD_school_shapes$schnam
```

3. StyleR - Another cool R package from the Tidyverse that can be powerful

and used as a first pass on entire projects that need refactoring. The most useful function of the package is the style_dir function, which will style all files within a given directory. See the function's documentation and the vignette linked above for more details.

- Note: The default Tidyverse styler is subtly different from some of the things we've advocated for in this document. Most notably we differ with regards to the assignment operator (<- vs =) and number of spaces before/after "tokens" (i.e. Assignment Aligner add spaces before = signs to align them properly). For this reason, we'd recommend the following: style_dir(path = ..., scope = "line_breaks", strict = FALSE). You can also customize StyleR even more if you're really hardcore.
- Note: As is mentioned in the package vignette linked above, StyleR modifies things *in-place*, meaning it overwrites your existing code and replaces it with the updated, properly styled code. This makes it a good fit on projects with version control, but if you don't have backups or a good way to revert back to the intial code, I wouldn't recommend going this route.
- 4. Linter Linters are programming tools that check adherence to a given style, syntax errors, and possible semantic issues. The R linter, called lintr, can be found in this package. It helps keep files consistent across different authors and even different organizations. For example, it notifies you if you have unused variables, global variables with no visible binding, not enough or superflous whitespace, and improper use of parentheses or brackets. A list of its other purposes can be found in this link, and most guidelines are based on Hadley Wickham's R Style Guide.
 - **Note**: You can customize your settings to set defaults or to exclude files. More details can be found here.
 - Note: The lintr package goes hand in hand with the styler package. The styler can be used to automatically fix the problems that the lintr catches.

Working with Big Data

by Kunal Mishra and Jade Benjamin-Chung

8.1 The data.table package

It may also be the case that you're working with very large datasets. Generally I would define this as 10+ million rows. As is outlined in this document, the 3 main players in the data analysis space are Base R, Tidvyerse (more specificially, dplyr), and data.table. For a majority of things, Base R is inferior to both dplyr and data.table, with concise but less clear syntax and less speed. Dplyr is architected for medium and smaller data, and while its very fast for everyday usage, it trades off maximum performance for ease of use and syntax compared to data.table. An overview of the dplyr vs data.table debate can be found in this stackoverflow post and all 3 answers are worth a read.

You can also achieve a performance boost by running dplyr commands on data.tables, which I find to be the best of both worlds, given that a data.table is a special type of data.frame and fairly easy to convert with the as.data.table() function. The speedup is due to dplyr's use of the data.table backend and in the future this coupling should become even more natural.

If you want to test whether using a certain coding approach increases speed, consider the tictoc package. Run tic() before a code chunk and toc() after to measure the amount of system time it takes to run the chunk. For example, you might use this to decide if you really need to switch a code chunk from dplyr to data.table.

8.2 Using downsampled data

In our studies with very large datasets, we save "downsampled" data that usually includes a 1% random sample stratified by any important variables, such as year or household id. This allows us to efficiently write and test our code without having to load in large, slow datasets that can cause RStudio to freeze. Be very careful to be sure which dataset you are working with and to label results output accordingly.

8.3 Optimal RStudio set up

Using the following settings will help ensure a smooth experience when working with big data. In RStudio, go to the "Tools" menu, then select "Global Options". Under "General":

Workspace

- Uncheck Restore RData into workspace at startup
- Save workspace to RData on exit choose **never**

History

• Uncheck Always save history

Unfortunately RStudio often gets slow and/or freezes after hours working with big datasets. Sometimes it is much more efficient to just use Terminal / gitbash to run code and make updates in git.

Github

by Stephanie Djajadi and Nolan Pokpongkiat

9.1 Basics

- A detailed tutorial of Git can be found here on the CS61B website.
- If you are already familiar with Git, you can reference the summary at the end of Section B.
- If you have made a mistake in Git, you can refer to this article to undo, fix, or remove commits in git.

9.2 Github Desktop

While knowing how to use Git on the command line will always be useful since the full power of Git and its customizations and flexibilty is designed for use with the command line, Github also provides Github Desktop as an graphical interface to do basic git commands; you can do all of the basic functions of Git using this desktop app. Feel free to use this as an alternative to Git on the command line if you prefer.

9.3 Git Branching

Branches allow you to keep track of multiple versions of your work simultaneously, and you can easily switch between versions and merge branches together once you've finished working on a section and want it to join the rest of your code. Here are some cases when it may be a good idea to branch:

• You may want to make a dramatic change to your existing code (called refactoring) but it will break other parts of your project. But you want

- to be able to simultaneously work on other parts or you are collaborating with others, and you don't want to break the code for them.
- You want to start working on a new part of the project, but you aren't sure yet if your changes will work and make it to the final product.
- You are working with others and don't want to mix up your current work with theirs, even if you want to bring your work together later in the future.

A detailed tutorial on Git Branching can be found here. You can also find instructions on how to handle merge conflicts when joining branches together.

9.4 Example Workflow

A standard workflow when starting on a new project and contributing code looks like this:

Command	Description
SETUP: FIRST TIME	Clone the repo. This copies of all the project
ONLY: git clone <url></url>	files in its current state on Github to your local
<directory_name></directory_name>	computer.
1. git pull origin	update the state of your files to match the most
master	current version on GitHub
2. git checkout -b	create new branch that you'll be working on and
<new_branch_name></new_branch_name>	go to it
3. Make some file changes	work on your feature/implementation
4. git add -p	add changes to stage for commit, going through changes line by line
5. git commit -m	commit files with a message
<pre><commit message=""></commit></pre>	
6. git push -u origin	push branch to remote and set to track (-u only
<pre><branch_name></branch_name></pre>	needed if this is first push)
7. Repeat step 4-5.	work and commit often
8. git push	push work to remote branch for others to view
9. Follow the link given	PR merges in work from your branch into
from the git push	master
command to submit a pull	
request (PR) on GitHub	
online	
(10.) Your changes and PR	
get approved, your	
reviewer deletes your	
remote branch upon	
merging	
11. git fetchall	clean up your local git by untracking deleted
prune	remote branches

Other helpful commands are listed below.

9.5 Commonly Used Git Commands

Command	Description
<pre>git clone <url> <directory_name></directory_name></url></pre>	clone a repository, only needs to be done the first time
git pull origin master	pull from master before making any changes
git branch	check what branch you are on
git branch -a	check what branch you are on + all remote
	branches
git checkout -b	create new branch and go to it (only necessary
<new_branch_name></new_branch_name>	when you create a new branch)
<pre>git checkout <branch name=""></branch></pre>	switch to branch
git add <file name=""></file>	add file to stage for commit
git add -p	adds changes to commit, showing you changes
-	one by one
git commit -m <commit< td=""><td>commit file with a message</td></commit<>	commit file with a message
message>	
git push -u origin	push branch to remote and set to track (-u only
<pre><branch_name></branch_name></pre>	works if this is first push)
git branch	set upstream to origin/ <branch_name> (use if</branch_name>
set-upstream-to	you forgot -u on first push)
origin <branch_name></branch_name>	
git push origin	push work to branch
<pre><branch_name></branch_name></pre>	
git checkout	switch to branch and merge changes from
<pre><branch_name> git</branch_name></pre>	<pre>master into <branch_name> (two commands)</branch_name></pre>
merge master	
git merge	switch to branch and merge changes from
<pre><branch_name> master</branch_name></pre>	<pre>master into <branch_name> (one command)</branch_name></pre>
git checkouttrack	pulls a remote branch and creates a local branch
origin/ <branch_name></branch_name>	to track it (use when trying to pull someone
	else's branch onto your local computer)
git pushdelete	delete remote branch
<remote_name></remote_name>	
 branch_name>	
git branch -d	deletes local branch, -D to force
 branch_name>	
git fetchall	untrack deleted remote branches
prune	

9.6 How often should I commit?

It is good practice to commit every 15 minutes, or every time you make a significant change. It is better to commit more rather than less.

9.7 What should be pushed to Github?

Never push .Rout files! If someone else runs an R script and creates an .Rout file at the same time and both of you try to push to github, it is incredibly difficult to reconcile these two logs. If you run logs, keep them on your own system or (preferably) set up a shared directory where all logs are name and date timestamped.

There is a standardized .gitignore for R which you can download and add to your project. This ensures you're not committing log files or things that would otherwise best be left ignored to GitHub. This is a great discussion of project-oriented workflows, extolling the virtues of a self-contained, portable projects, for your reference.

Unix commands

by Stephanie Djajadi, Kunal Mishra, Anna Nguyen, and Jade Benjamin-Chung

We typically use Unix commands in Terminal (for Mac users) or Git Bash (for Windows users) to

- Run a series of scripts in parallel or in a specific order to reproduce our work
- 2. To check on the progress of a batch of jobs
- 3. To use git and push to github

10.1 Basics

On the computer, there is a desktop with two folders, folder1 and folder2, and a file called file1. Inside folder1, we have a file called file2. Mac users can run these commands on their terminal; it is recommended that Windows users use Git Bash, not Windows PowerShell.

10.2 Syntax for both Mac/Windows

When typing in directories or file names, quotes are necessary if the name includes spaces.

Command	Description
cd desktop/folder1 pwd ls cp "file2" "newfile2"	Change directory to folder1 Print working directory List files in the directory Copy file (remember to include file
	extensions when typing in file names like $.pdf$ or $.R)$

Command	Description
mv "newfile2" "file3"	Rename newfile2 to file3
cd	Go to parent of the working directory (in
	this case, desktop)
mv "file1" folder2	Move file1 to folder2
mkdir folder3	Make a new folder in folder2
rm <filename></filename>	Remove files
rm -rf folder3	Remove directories (-r will attempt to
	remove the directory recursively, -rf will
	force removal of the directory)
clear	Clear terminal screen of all previous
	commands

10.3 Running Bash Scripts

Windows	Mac / Linux	Description
chmod +750 <filename.sh></filename.sh>	chmod +x <filename.sh></filename.sh>	Change access permissions for a file (only needs to be done once)
./ <filename.sh></filename.sh>	./ <filename.sh></filename.sh>	Run file (./ to run any executable file)
<pre>bash bash_script_name &</pre>	bash shash_script_name.sh &	Run shell script in the background

10.4 Running Rscripts in Windows

Note: This code seems to work only with Windows Command Prompt, not with Git Bash.

When R is installed, it comes with a utility called Rscript. This allows you to run R commands from the command line. If Rscript is in your PATH, then typing Rscript into the command line, and pressing enter, will not error. Otherwise, to use Rscript, you will either need to add it to your PATH (as an environment variable), or append the full directory of the location of Rscript on your machine. To find the full directory, search for where R is installed your computer. For instance, it may be something like below (this will vary depending on what version of R you have installed):

C:\Program Files\R\R-3.6.0\bin

For appending the PATH variable, please view this link. I strongly recommend

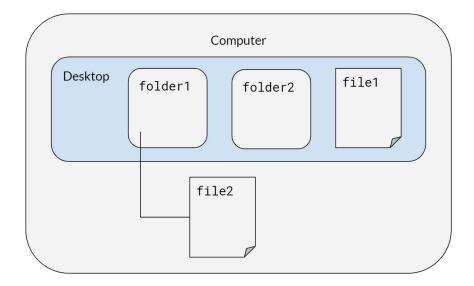


Figure 10.1: Here is our example desktop.

completing this option.

If you add the PATH as an environment variable, then you can run this line of code to test: Rscript -e "cat('this is a test')", where the -e flag refers to the expression that will be executed.

If you do not add the PATH as an environment variable, then you can run this line of code to replicate the results from above: "C:\Program Files\R\R-3.6.0\bin" -e "cat('this is a test')"

To run an R script from the command line, we can say: Rscript -e "source('C:/path/to/script/some_code.R')"

10.4.1 Common Mistakes

- Remember to include all of the quotation marks around file paths that have a spaces.
- If you attempt to run an R script but run into Error: '\U' used without hex digits in character string starting "'C:\U", try replacing all \ with \\ or /.

10.5 Checking tasks and killing jobs

```
MINGW64:/c/Users/Stephanie Djajadi/desktop/folder2
  cd ~/desktop
 Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop
$ pwd
/c/Users/Stephanie Djajadi/desktop
 Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop
desktop.ini file1.txt folder1/ folder2/
Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop
$ cd folder1
 Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder1
file2.txt
 Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder1
$ cp file2.txt newfile2.txt
 stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder1
file2.txt newfile2.txt
Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder1
$ mv newfile2.txt file3.txt
 Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder1
file2.txt file3.txt
Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder1 $ cd ..
 stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop
$ ls
desktop.ini file1.txt folder1/ folder2/
Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop
$ mv file1.txt folder2
 Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop
 cd folder2
Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder2
file1.txt
Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder2
$ mkdir folder3
 tephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder2
$ ls
file1.txt folder3/
 Stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder2
  rm file1.txt
 stephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder2
  rm -rf folder3
 tephanie Djajadi@DESKTOP-LOH5VOO MINGW64 ~/desktop/folder2
  1s
```

Figure 10.2: Here is an example of what your terminal might look like after executing the commands in the order listed above.

Windows	Mac / Linux	Description
tasklist	ps -v	List all processes on the command line
	top -o [cpu/rsize]	List all running processes, sorted by CPU or memory usage
taskkill /F /PID pid_number	kill <pid_number></pid_number>	Kill a process by its process ID
taskkill /IM "process name" /F		Kill a process by its name
start /b program.exe		Runs jobs in the background (exclude /b if you want the program to run in a new console)
	nohup	Prevents jobs from stopping
	disown	Keeps jobs running in the background even if you close R
taskkill /?		Help, lists out other commands

To kill a task in Windows, you can also go to Task Manager > More details > Select your desired app > Click on End Task.

10.6 Running big jobs

For big data workflows, the concept of "backgrounding" a bash script allows you to start a "job" (i.e. run the script) and leave it overnight to run. At the top level, a bash script (0-run-project.sh) that simply calls the directory-level bash scripts (i.e. 0-prep-data.sh, 0-run-analysis.sh, 0-run-figures.sh, etc.) is a powerful tool to rerun every script in your project. See the included example bash scripts for more details.

• Running Bash Scripts in Background: Running a long bash script is not trivial. Normally you would run a bash script by opening a terminal and typing something like ./run-project.sh. But what if you leave your computer, log out of your server, or close the terminal? Normally, the bash script will exit and fail to complete. To run it in background, type ./run-project.sh &; disown. You can see the job running (and CPU utilization) with the command top or ps -v and check your memory with free -h.

Alternatively, to keep code running in the background even when an SSH connection is broken, you can use tmux. In terminal or gitbash follow the steps below. This site has useful tips on using tmux.

```
# create a new tmux session called session_name
tmux new -ssession_name

# run your job of interest
R CMD BATCH myjob.R &

# check that it is running
ps -v

# to exit the tmux session (Mac)
ctrl + b
d

# to reopen the tmux session to kill the job or
# start another job
tmux attach -tsession_name
```

- Deleting Previously Computed Results: One helpful lesson we've learned is that your bash scripts should remove previous results (computed and saved by scripts run at a previous time) so that you never mix results from one run with a previous run. This can happen when an R script errors out before saving its result, and can be difficult to catch because your previously saved result exists (leading you to believe everything ran correctly).
- Ensuring Things Ran Correctly: You should check the .Rout files generated by the R scripts run by your bash scripts for errors once things are run. A utility file is include in this repository, called runFileSaveLogs, and is used by the example bash scripts to... run files and save the generated logs. It is an awesome utility and one I definitely recommend using. Before using runFileSaveLogs, it is necessary to put the file in the home working directory. For help and documentation, you can use the command ./runFileSaveLogs -h. See example code and example usage for runFileSaveLogs below.

10.6.1 Example code for runfileSaveLogs

```
#!/usr/bin/env python3
# Type "./runFileSaveLogs -h" for help
import os
import sys
```

```
import argparse
import getpass
import datetime
import shutil
import glob
import pathlib
# Setting working directory to this script's current directory
os.chdir(os.path.dirname(os.path.abspath(__file__)))
# Setting up argument parser
parser = argparse.ArgumentParser(description='Runs the argument R script(s) - in parallel if spec
# Function ensuring that the file is valid
def is_valid_file(parser, arg):
    if not os.path.exists(arg):
        parser.error("The file %s does not exist!" % arg)
    else:
        return arg
# Function ensuring that the directory is valid
def is_valid_directory(parser, arg):
    if not os.path.isdir(arg):
        parser.error("The specified path (%s) is not a directory!" % arg)
    else:
        return arg
# Additional arguments that can be added when running runFileSaveLogs
parser.add_argument('-p', '--parallel', action='store_true', help="Runs the argument R scripts in
parser.add_argument("-i", "--identifier", help="Adds an identifier to the directory name where the
parser.add_argument('filenames', nargs='+', type=lambda x: is_valid_file(parser, x))
args = parser.parse_args()
args_dict = vars(args)
print(args_dict)
# Run given R Scripts
for filename in args_dict["filenames"]:
  system_call = "R CMD BATCH" + " " + filename
  if args dict["parallel"]:
    system_call = "nohup" + " " + system_call + " &"
  os.system(system_call)
```

```
# Create the directory (and any parents) of the log files
currentUser = getpass.getuser()
currentTime = datetime.datetime.now().strftime("%Y-%m-%d %H:%M:%S")
logDirPrefix = "/home/kaiserData/logs/" # Change to the directory where the logs shoul
logDir = logDirPrefix + currentTime + "-" + currentUser

# If specified, adds the identifier to the filename of the log
if args.identifier is not None:
    logDir += "-" + args.identifier

logDir += "/"

pathlib.Path(logDir).mkdir(parents=True, exist_ok=True)

# Find and move all logs to this new directory
currentLogPaths = glob.glob('./*.Rout')

for currentLogPath in currentLogPaths:
    filename = currentLogPath.split("/")[-1]
    shutil.move(currentLogPath, logDir + filename)
```

10.6.2 Example usage for runfileSaveLogs

This example bash script runs files and generates logs for five scripts in the kaiserflu/3-figures folder. Note that the -i flag is used as an identifier to add figures to the filename of each log.

```
#!/bin/bash

# Copy utility run script into this folder for concision in call
cp ~/kaiserflu/runFileSaveLogs ~/kaiserflu/3-figures/

# Run folder scripts and produce output
cd ~/kaiserflu/3-figures/
./runFileSaveLogs -i "figures" \
fig-mean-season-age.R \
fig-monthly-rate.R \
fig-point-estimates-combined.R \
fig-point-estimates.R \
fig-weekly-rate.R

# Remove copied utility run script
rm runFileSaveLogs
```

Reproducible Environments

by Anna Nguyen

11.1 Package Version Control with renv

11.1.1 Introduction

Replicable code should produce the same results, regardless of when or where it's run. However, our analyses often leverage open-source R packages that are developed by other teams. These packages continue to be developed after research projects are completed, which may include changes to analysis functions that could impact how code runs for both other team members and external replicators.

For example, suppose we had used a function that took in one argument, such that our code contained example_function(arg_a = "a"). A few months after we publish our code, the package developers update the function to take in another mandatory argument arg_b. If someone runs our code, but has the most recent version of the package, they'll receive an error message that the argument arg_b is missing and will not be able to full reproduce our results.

To ensure that the right functions are used in replication efforts, it is important for us to keep track of package versions used in each project.

renv can be to promote reproducible environments within R projects. renv creates individual package libraries for each project instead of having all projects, which may use different versions of the same package, share the same package library. However, for projects that use many packages, this process can be memory intensive and increase the time needed for a new users to start running code.

In this lab manual chapter, we provide a quick tutorial for integrating renv

into research workflows. For more detailed instructions, please refer to the renv package vignette.

11.1.2 Implementing renv in projects

Ideally, renv should be initiated at the start of projects and updated continuously when new packages are introduced in the codebase. However, this process can be initated at any point in a project

To add renv to your workflow, follow these steps:

- 1. Install the renv package by running install.packages("renv")
- 2. Create an RProject file and ensure that your working directory is set to the correct folder
- 3. In the R console, run renv::init() to intialize renv in your R Project
- 4. This will create the following files: renv.lock, .Rprofile, renv/settings.json and renv/activate.R. Commit and push these files to GitHub so that they're accessible to other users.
- 5. As you write code, update the project's R library by running renv::snapshot() in the R console
- 6. Add renv::restore() to the head of your config file, to make sure that all users that run your code are on the same package versions.

11.1.3 Using projects with renv

If you're starting to work on an ongoing project that already has renv set up, follow these steps to ensure that you're using the same project versions.

- 1. Install the renv package by running install.packages("renv")
- 2. Pull the most updated version of the project from GitHub
- 3. Open the project's RProject file
- 4. Run renv::restore(). In our lab's projects, this is often already found at the top of the config file, so you can just run scripts as is.
- 5. This will pull up a list of the project's packages that need to be updated for you to be consistent with the project. The console will ask if you want to proceed with updating these packages type "Y" to continue.
- 6. Wait for the correct versions of each package to install/update. This may take some time, depending on how many packages the project uses.
- 7. Your R environment should now be using the same package versions as specified in the renv lock file. You should now be able to replicate the code.
- 8. If you make edits to the code and introduce new/updated packages, see the section above for instructions on how to make updates.

Code Publication

by Nolan Pokpongkiat

12.1 Checklist overview

- 1. Fill out file headers
- 2. Clean up comments
- 3. Document functions
- 4. Remove deprecated filepaths
- 5. Ensure project runs via bash
- 6. Complete the README
- 7. Clean up feature branches
- 8. Create Github release

12.2 Fill out file headers

Every file in a project should have a header that allows it to be interpreted on its own. It should include the name of the project and a short description for what this file (among the many in your project) does specifically. See template here.

12.3 Clean up comments

Make sure comments in the code are for code documentation purposes only. Do not leave comments to self in the final script files.

12.4 Document functions

Every function you write must include a header to document its purpose, inputs, and outputs. See template for the function documentation here.

12.5 Remove deprecated filepaths

All file paths should be defined in 0-config.R, and should be set relative to the project working directory. All absolute file paths from your local computer should be removed, and replaced with a relative path. If a third party were to re-run this analysis, if they need to download data from a separate source and change a filepath in the 0-config.R to match, make sure to specify in the README which line of 0-config.R needs to be substituted.

12.6 Ensure project runs via bash

The project should be configured to be entirely reproducible by running a master bash script, run-project.sh, which should live at the top directory. This bash script can call other bash scripts in subfolders, if necessary. Bash scripts should use the runFileSaveLogs utility script, which is a wrapper around the Rscript command, allowing you to specify where .Rout log files are moved after the R scripts are run.

See usage and documentation here.

12.7 Complete the README

A README.md should live at the top directory of the project. This usually includes a Project Overview and a Directory Structure, along with the names of the contributors and the Creative Commons License. See below for a template:

Overview

To date, coronavirus testing in the US has been extremely limited. Confirmed COVID-19 case counts underestimate the total number of infections in the population. We estimated the total COVID-19 infections – both symptomatic and asymptomatic – in the US in March 2020. We used a semi-Bayesian approach to correct for bias due to incomplete testing and imperfect test performance.

Directory structure

- 0-config.R: configuration file that sets data directories, sources base functions, and loads required libraries
- 0-base-functions: folder containing scripts with functions used in the analysis

- 0-base-functions.R: R script containing general functions used across the analysis
- 0-bias-corr-functions.R: R script containing functions used in bias correction
- O-bias-corr-functions-undertesting.R: R script containing functions used in bias correction to estimate the percentage of underestimation due to incomplete testing vs. imperfect test accuracy
- 0-prior-functions.R: R script containing functions to generate priors
- 1-data: folder containing data processing scripts NOTE: some scripts are deprecated
- 2-analysis: folder containing analysis scripts. To rerun all scripts in this subdirectory, run the bash script 0-run-analysis.sh.
 - 1-obtain-priors-state.R: obtain priors for each state
 - 2-est-expected-cases-state.R: estimate expected cases in each state
 - 3-est-expected-cases-state-perf-testing.R: estimate expected cases in each state, estimate the percentage of underestimation due to incomplete testing vs. imperfect test accuracy
 - 4-obtain-testing-protocols.R: find testing protocols for each state.
 - 5-summarize-results.R: summarize results; obtain results for in text numerical results.
- 3-figure-table-scripts: folder containing figure scripts. To rerun all scripts in this subdirectory, run the bash script 0-run-figs.sh.
 - 1-fig-testing.R: creates plot of testing patterns by state over time
 - 2-fig-cases-usa-state-bar.R: creates bar plot of confirmed vs. estimated infections by state
 - 3a-fig-map-usa-state.R: creates map of confirmed vs. estimated infections by state
 - 3b-fig-map-usa-state-shiny.R: creates map of confirmed vs. estimated infections by state with search functionality by state
 - 4-fig-priors.R: creates figure with priors for US as a whole

- 5-fig-density-usa. R: creates figure of distribution of estimated cases in the ${\rm US}$
- 6-table-data-quality.R: creates table of data quality grading from COVID Tracking Project
- 7-fig-testpos.R: creates figure of the probability of testing positive among those tested by state
- $-\,$ 8-fig-percent-undertesting-state. R: creates figure of the percentage of under estimation due to incomplete testing
- 4-figures: folder containing figure files.
- 5-results: folder containing analysis results objects.
- 6-sensitivity: folder containing scripts to run the sensitivity analyses

Contributors: Jade Benjamin-Chung, Sean L. Wu, Anna Nguyen, Stephanie Djajadi, Nolan N. Pokpongkiat, Anmol Seth, Andrew Mertens

Wu SL, Mertens A, Crider YS, Nguyen A, Pokpongkiat NN, Djajadi S, et al. Substantial underestimation of SARS-CoV-2 infection in the United States due to incomplete testing and imperfect test accuracy. medRxiv. 2020; 2020.05.12.20091744. doi:10.1101/2020.05.12.20091744

When possible, also include a description of the RDS results that are generated, detailing what data sources were used, where the script lives that creates it, and what information the RDS results hold.

12.8 Clean up feature branches

In the remote repository on Github, all feature branches aside from master should be merged in and deleted. All outstanding PRs should be closed.

12.9 Create Github release

Once all of these items are verified, create a tag to make a Github release, which will tag the repository, creating a marker at this specific point in time.

Detailed instructions here.

Data Publication

Adapted from Fanice Nyatigo and Ben Arnold's chapter in the Proctor-UCSF Lab Manual

13.1 Overview

Warning! NEVER push a dataset into the public domain (e.g., GitHub, OSF) without first checking with Jade to ensure that it is appropriately de-identified and we have approval from the sponsor and/or human subjects review board to do so. For example, we will need to re-code participant IDs (even if they contain no identifying information) before making data public to completely break the link between IDs and identifiable information stored on our servers.

If you are releasing data into the public domain, then consider making available at minimum a .csv file and a codebook of the same name (note: you should have a codebook for internal data as well). We often also make available .rds files as well. For example, your mystudy/data/public directory could include three files for a single dataset, two with the actual data in .rds and .csv formats, and a third that describes their contents:

analysis_data_public.csv
analysis_data_public.rds
analysis_data_public_codebook.txt

In general, datasets are usually too big to save on GitHub, but occasionally they are small. Here is an example of where we actually pushed the data directly to GitHub: https://github.com/ben-arnold/enterics-seroepi/tree/master/data .

If the data are bigger, then maintaining them under version control in your git repository can be unweildy. Instead, we recommend using another stable repository that has version control, such as the Open Science Framework (osf.io). For example, all of the data from the WASH Benefits trials (led by investigators at Berkeley, icddr,b, IPA-Kenya and others) are all stored through data components nested within in OSF projects: https://osf.io/tprw2/. Another good option is Dryad (datadryad.org) or the (Stanford Digital Repository)[https://sdr.stanford.edu/].

We recommend cross-linking public files in GitHub (scripts/notebooks only) and OSF/Dryad/Stanford Digital Repository.

Below are the main steps to making data public, after finalizing the analysis datasets and scripts:

- 1. Remove Protected Health Information (PHI)
- 2. Create public IDs or join already created public IDs to the data
- 3. Create an OSF repository and/or Dryad/Stanford Digital Repository
- 4. Edit analysis scripts to run using the public datasets and test (optional)
- 5. Create a public github page for analysis scripts and link to OSF and/or Dryad/Zenodo
- 6. Go live

13.2 Removing PHI

Once the data is finalized for analysis, the first step is to strip it of Protected Health Information (PHI), or any other data that could be used to link back to specific participants, such as names, birth dates, or GPS coordinates at the village/neighborhood level or below. PHI includes, but is not limited to:

13.2.1 Personal information

These are identifiers that directly point to specific individuals, such as:

- Names, addresses, photographs, date of birth
- A combination of age, sex, and geographic location (below population 20,000) is considered identifiable

13.2.2 Dates

Any specific dates (e.g., study visit dates, birth dates, treatment dates) are usually problematic.

- If a dataset requires high resolution temporal information, coarsen visit or measurement dates to be two variables: year and week of the year (1-52).
- If a dataset requires age, provide that information without a birth date (typically month resolution is sufficient)

Caution! If making changes to the format of dates or ages, make sure your analysis code runs on these modified versions of the data (step 3)!

13.2.3 Geographic information

Do not include GPS coordinates (longitude, latitude) except in special circumstances where they have been obfuscated/shifted. Reach out to Jade before doing this because it can be complicated.

Do not include place names or codes (e.g., US Zip Codes) if the place contains <20,000 people. For villages or neighborhoods, code them with uninformative IDs. For sub-districts or districts, names are fine.

If an analysis requires GPS locations (e.g., to make a map), then typically we include a disclaimer in the article's data availability statement that explains we cannot make GPS locations public to protect participant confidentiality. As a middle ground, we typically make our *code* public that runs on the geo-located data for transparency, even if independent researchers can't actually run that code (although please be careful to ensure the code itself does not in any way include geographic identifiers).

For more examples of what constitutes PHI, please refer to this link: https://cphs.berkeley.edu/hipaa/hipaa18.html

13.3 Create public IDs

13.3.1 Rationale

The Stanford IRB requires that public datasets not include the original study IDs to identify participants or other units in the study (such as village IDs). The reason is that those IDs are linked in our private datasets to PHI. By creating a new set of public IDs, the public dataset is one step further removed from the potential to link to PHI.

13.3.2 A single set of public IDs for each study

For each study, it is ideal to create a single set of public IDs whenever possible. We could create a new set of public IDs for every public dataset, but the downside is that independent researchers could no longer link data that might be related. By creating a single set of public IDs associated with each internal study ID, public files retain the link.

Maintaining a single set of public IDs requires a shared "bridge" dataset, that includes a row for each study ID and has the associated public ID. For studies

with multiple levels of ID, we would typically have separate bridge datasets for each type of ID (e.g., cluster ID, participant ID, etc.)

Create a public ID that can be used to uniquely identify participants and that can internally be linked to the original study IDs. We recommend creating a subdirectory in the study's shared data directory to store the public IDs. The shared location enables multiple projects to use the same IDs. Create the IDs using a script that reads in the study IDs, creates a unique (uninformative) public ID for the study IDs, and then saves the bridge dataset. The script should be saved in the same directory as the public ID files.

Caution! Note that small differences may arise if the new public IDs do not necessarily order participants in the same way as the internal IDs. The small differences are all in estimates that rely on resampling, such as Bootstrap CIs, permutation P-values, and TMLE, as the resampling process may lead to slightly different re-samples. The key here, to ensure the results are consistent irrespective of the dataset used, is simply to not assign public IDs randomly. Use rank() on the internal ID instead of row_number() to ensure that the order is always the same.

13.3.3 Example scripts

We have created a self-contained and reproducible example that you can run and replicate when making data public for your projects. It contains the following files and folders:

- data/final/- folder containing the projects final data in both csv and rds formats
- 2. code/DEMO_generate_public_IDs.R- creates randomly generated public IDs that can be matched to the trial's assigned patient IDs.
- 3. data/make_public/DEMO_internal_to_publicID.csv- the output from step #2, a bridge dataset with two variables- the new public ID and the patient's assigned ID.
- 4. code/DEMO_create_public_datasets.R- joins the public IDs to the trial's full dataset, and strips it of the assigned patient ID.
- 5. data/public/- folder containing the output from step #3- de-identified public dataset, in csv and rds formats, with uniquely identifying public IDs that cannot be easily linked back to the patient's ID.

The example workflow is accessible via GitHub: https://github.com/proctor-ucsf/dcc-handbook/tree/master/templates/making-data-public

13.4 Create a data repository

First, ensure that you create a codebook and metadata file for each public dataset See the DCC guide on Documenting datasets. Use the same name as the datasets, but with "-codebook.txt" / "-codebook.html" / "-codebook.csv" at the end (depending on the file format for the codebook). One nice option is the R codebook package, which also generates JSON output that is machine-readable.

13.4.1 Steps for creating an Open Science Framework (OSF) repository:

- 1. Create a new OSF project per these instructions: https://help.osf.io/article/252-create-a-project
- Create a data component and upload the datasets in .csv and .rds format along with the codebooks. The primary format for public dissemination is .csv but we make the .rds files available too as auxiliary files for convenience.
- 3. Create a notebook component and upload the final .html files (which will not be on github... but see optional item below)
- 4. On the OSF landing Wiki, provide some context. Here is a recent example: https://osf.io/954bt/
- 5. Create a Digital Object Identifier (DOI) for the repository. A DOI is a unique identifier that provides a persistent link to content, such as a dataset in this case. Learn more about DOIs
- Optional: Complete the software checklist and system requirement guide for the analysis to guide others. Include it on the GitHub README for the project: https://github.com/proctor-ucsf/mordor-antibody

13.5 Edit and test analysis scripts

Make minor changes to the analysis scripts so that they run on public data. If using version control in GitHub, the most straight-forward way is to create a branch from the main git branch that reads in the public files, and then renames the new public ID variable, e.g., "id_public" to the internally recognized ID variable name, e.g. "recordID", when reading in the public data. Re-run all the analysis scripts to ensure that they still work with the public version of the dataset.

13.6 Create a public GitHub page for public scripts

At minimum, we should include all of the scripts required to run the analyses. **IMPORTANT**: ensure you have taken a snapshot and saved your computing

environment using the renv package (renv).

See examples:

- ACTION https://github.com/proctor-ucsf/ACTION-public
- NAITRE https://github.com/proctor-ucsf/NAITRE-primary

Caution! Read through the scripts carefully to ensure there is no PHI in the code itself

Once a public GitHub page exists, you can create a new component on an OSF project (step 3, above) and link it to the public version of the GitHub repo.

13.7 Go live

On GitHub, it is useful to create an official "release" version to freeze the repository, where you can have "associated files" with each version. Include the .html notebook output as additional files — since they aren't tracked in GitHub, it does provide a way of freezing / saving the HTML output for us and others. OSF examples of a few Proctor trials:

- ACTION https://osf.io/ca3pe/
- NAITRE https://osf.io/ujeyb/
- MORDOR Niger antibody study https://osf.io/dgsq3/

Further reading on end-to-end data management: How to Store and Manage Your Data - PLOS

Slurm and cluster computing

by Anna Nguyen, Jade Benjamin-Chung, and Gabby Barratt Heitmann

When you need to run a script that requires a large amount of RAM, large files, or that uses parallelization, you can use Sherlock, Stanford's computing cluster. Sherlock uses Slurm, an open source, scalable cluster management and job scheduling system for computing clusters. Jade can email Sherlock managers to get you an account. Please refer to the Sherlock user guide to learn about the system and how to use it. Below, we include a few tips specific to how we use Sherlock in our lab.

14.1 Getting started

To access Sherlock, in terminal, log in using the following syntax and replace "USERNAME" with your Stanford alias. You will be prompted to enter your Stanford password (the same one you use for your email and other accounts) and to complete two-factor authentication.

ssh USERNAME@login.sherlock.stanford.edu

Once you log in, you can view the contents of your home directory in command line by entering cd \$HOME. You can create subfolders within this directory using the mkdir command. For example, you could make a "code" subdirectory and clone a Github repository there using the following code:

cd \$HOME
mkdir code
git clone https://github.com/jadebc/covid19-infections.git

14.1.1 One-Time System Set-Up

To keep the install packages consistent across different nodes, you will need to explicitly set the pathway to your R library directory.

Open your ~/.Renviron file (vi ~/.Renviron) and append the following line:

Note: Once you open the file using vi [file_name], you must press i (on Mac OS) or Insert (on Windows) to make edits. After you finish, hit Esc to exit editing mode and type :wq to save and close the file.

```
R_LIBS=~/R/x86_64-pc-linux-gnu-library/4.0.2
```

Alternatively, run an R script with the following code on Sherlock:

```
r_environ_file_path = file.path(Sys.getenv("HOME"), ".Renviron")
if (!file.exists(r_environ_file_path)) file.create(r_environ_file_path)

cat("\nR_LIBS=~/R/x86_64-pc-linux-gnu-library/4.0.2",
    file = r_environ_file_path, sep = "\n", append = TRUE)
```

To load packages that run off of C++, you'll need to set the correct compiler options in your R environment.

Open the Makevars file in Sherlock (vi ~/.R/Makevars) and append the following lines

```
CXX14FLAGS=-03 -march=native -mtune=native -fPIC CXX14=g++
```

Alternatively, create an R script with the following code, and run it on Sherlock:

14.2 Moving files to Sherlock

The \$HOME directory is a good place to store code and small test files (quota: 15 GB per user). Save large files to the \$SCRATCH directory (quota: 100 TB per user). You can read more about storage options on Sherlock here. On the \$SCRATCH directory, files that are not modified after 90 days are automatically deleted. For this reason, it's best to create a bash script that records the file

transfer process for a given project. See example code below:

```
# note: the following steps should be done from your local
# (not after ssh-ing into sherlock)

# securely transfer folders from Box to sherlock home directory
# note: the -r option is for folders and is not needed for files
scp -r "Box/malaria-project/folder-1/" USERNAME@login.sherlock.stanford.edu:/home/users/USERNAME@login.sherlock.stanford.edu:/scratch/users/USERNAME@login.sherlock.stanford.edu:/scratch/users/USERNAME@login.sherlock.stanford.edu:/scratch/users/USERNAME@login.sherlock.stanford.edu:/scratch/group/jadeb@login-r "Box/malaria-project/folder-3/" USERNAME@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/jadeb@login.sherlock.stanford.edu:/scratch/group/j
```

14.3 Installing packages on Sherlock

When you begin working on Sherlock, you will most likely encounter problems with installing packages. To install packages, login to Sherlock on the command line and open a development node using the command sdev. Do not attempt to do this in the RStudio Server (see next section), as you will have to re-do it for every new session you open.

```
ssh USERNAME@login.sherlock.stanford.edu
sdev
```

There is a package installation file explicitly written for Sherlock that you should run before testing any code and sourcing the configuration file. You should only have to install packages once. Sherlock requires that you specify the repository where the package is downloaded from. You may also need to add an additional argument to install.packages to prevent the packages from locking after installation:

In order for some R packages to work on Sherlock, it is necessary to load specific software modules before running R. These must be loaded in Sherlock each time you want to use the package in R. For example, for spatial and random effects analyses, you may need the modules/packages below. These modules must also be loaded on the command line prior to opening R in order for package installation to work.

```
module --force purge # remove any previously loaded modules, including math and devel module load math module load math gmp/6.1.2
```

```
module load devel
module load gcc/10
module load system
module load json-glib/1.4.4
module load curl/7.81.0
module load physics
module load physics udunits geos
module load physics gdal/2.2.1 # for R/4.0.2
module load physics proj/4.9.3 # for R/4.0.2
module load R/4.0.2
```

R # Open R in the Shell window to install individual packages or test code
Rscript install-packages-sherlock.R # Alternatively, run the entire package installati

Figuring out the issues with some packages will require some trial and error. If you are still encountering problems installing a package, you may have to install other dependencies manually by reading through the error messages. If you try to install a dependency from CRAN and it isn't working, it may be a module. You can search for it using the module spider command:

```
module spider DEPENDENCY NAME
```

However, you can also reach out to the Sherlock team for help. You can email them at srcc-support@stanford.edu. They also hold office hours.

14.4 Testing your code

Both of the following ways to test code on Sherlock are recommended for making small changes, such as editing file paths and making sure the packages and source files load. You should write and test the functionality of your script locally, only testing on Sherlock once major bugs are out.

14.4.1 The command line

There are two main ways to explore and test code on Sherlock. The first way is best for users who are comfortable working on the command line and editing code in base R. Even if you are not comfortable yet, this is probably the better way because these commands will transfer between Sherlock and other cluster computers using Slurm.

Typically, you will want to initially test your scripts by initiating a development node using the command sdev. This will allocate a small amount of computing resources for 1 hour. You can access R via command line using the following code.

```
# open development node
sdev

# Load all the modules required by the packages you are using
module load MODULE NAME

# Load R (default version)*
module load R

# initiate R in command line
R
```

*Note: for collaboration purposes, it's best for everyone to work with one version of R. Check what version is being used for the project you are working on. Some packages only work with some versions of R, so it's best to keep it consistent.

14.4.2 The Sherlock OnDemand Dashboard

The second way to test and edit code is to use the Sherlock OnDemand Dashboard, accessed by typing login.sherlock.stanford.edu into a web browser. You will be prompted to authenticate the way you would for any Stanford website. This is the best way to edit code for people who are not comfortable accessing & editing in base R in a Shell application.

You can test your code via the Rstudio server on Sherlock. To access this, login to the Dashboard, then click on Interactive Apps in the menu bar and choose R Studio Server. Similar to the sdev node, you have to set various parameters for your session. Choose a version of R and set the time – max. 2 hours. You can play with the other configurations, but this is likely unnecessary, as you should not need huge computing power to test small amounts of code. Keep in mind the more computing power you request, the lower priority your request becomes. You will then wait for the resources to become available, and you will be able to click "Launch" when they are (if you don't mess with the CPU or GPU, this is usually less than 2 minutes). The screen that opens will look very similar to the RStudio on your local.

Do NOT use the RStudio Server's Terminal to install packages, set your R environment, and do everything else needed to configure Sherlock because you will likely need to re-do it for every session/project. It's best to use the Dashboard/RStudio Server if you are more comfortable testing & editing in RStudio rather than through base R in a Shell application.

14.4.3 Filepaths & configuration on Sherlock

In most cases, you will want to test that the file paths work correctly on Sherlock. You will likely need to add code to the configuration file in the project repository that specifies Sherlock-specific file paths. Here is an example:

```
# set sherlock-specific file paths
if(Sys.getenv("LMOD_SYSHOST")=="sherlock"){
    sherlock_path = pasteO(Sys.getenv("HOME"), "/malaria-project/")
    data_path = pasteO(sherlock_path, "data/")
    results_path = pasteO(sherlock_path, "results/")
}
```

14.5 Storage & group storage access

14.5.1 Individual storage

There are multiple places to store your files on Sherlock. Each user has their own \$HOME directory as well as a \$SCRATCH directory. These are directories that can be accessed via the command line once you've logged in to Sherlock:

```
cd $HOME
cd /home/users/USERNAME # Alternatively, use the full path
cd $SCRATCH
cd /scratch/users/USERNAME # Full path
```

You can also navigate to these using the File Explorer on Sherlock OnDemand.

\$HOME has a volume quota of 15 GB. \$SCRATCH has a volume quota of 100 TB, but files here get deleted 90 days after their last modification. Thus, use \$SCRACTH for test files, exploratory analyses, and temporary storage. Use \$HOME for long-term storage of important files and more finalized analyses.

You can read more about storage options on Sherlock here.

14.5.2 Group storage

The lab also has a \$GROUP_HOME and a \$GROUP_SCRATCH to store files for collaborative use. \$GROUP_HOME has a volume quota of 1 TB and infinite retention time, whereas \$GROUP_SCRATCH has a volume quota of 100 TB and the same 90-day retention limit. You can access these via the command line or navigate to them using the File Explorer:

```
cd $GROUP_HOME
cd /home/groups/jadebc

cd $GROUP_SCRATCH
cd /scratch/groups/jadebc
```

However, saving files to group storage can be tricky. You can try using the scp

command in the section "Moving files to Sherlock" to see if you have permission to add files to group directories. Read the next section to ensure any directories you create have the right permissions.

14.5.3 Folder permissions

Generally, when we put folders in \$GROUP_HOME or \$GROUP_SCRATCH, it is so that we can collaborate on an analysis within the research group, so multiple people need to be able to access the folders. If you create a new folder in \$GROUP_HOME or \$GROUP_SCRATCH, please check the folder's permissions to ensure that other group members are able to access its contents. To check the permissions of a folder, navigate to the level above it, and enter 1s -1. You will see output like this:

drwxrwxrwx 2 jadebc jadebc 2204 Jun 17 13:12 myfolder

Please review this website to learn how to interpret the code on the left side of this output. The website also tells you how to change folder permissions. In order to ensure that all users and group members are able to access a folder's contents, you can use the following command:

chmod ugo+rwx FOLDER_NAME

14.6 Running big jobs

Once your test scripts run successfully, you can submit an sbatch script for larger jobs. These are text files with a .sh suffix. Use a text editor like Sublime to create such a script. Documentation on sbatch options is available here. Here is an example of an sbatch script with the following options:

- job-name=run_inc: Job name that will show up in the Sherlock system
- begin=now: Requests to start the job as soon as the requested resources are available
- dependency=singleton: Jobs can begin after all previously launched jobs with the same name and user have ended.
- mail-type=ALL: Receive all types of email notification (e.g., when job starts, fails, ends)
- cpus-per-task=16: Request 16 processors per task. The default is one processor per task.
- mem=64G: Request 64 GB memory per node.
- output=00-run_inc_log.out: Create a log file called 00-run_inc_log.out that contains information about the Slurm session
- time=47:59:00: Set maximum run time to 47 hours and 59 minutes. If you don't include this option, Sherlock will automatically exit scripts after 2 hours of run time.

The file analysis.out will contain the log file for the R script analysis.R.

```
#!/bin/bash
#SBATCH --job-name=run_inc
#SBATCH --begin=now
#SBATCH --dependency=singleton
#SBATCH --mail-type=ALL
\#SBATCH --cpus-per-task=16
#SBATCH --mem=64G
#SBATCH --mem=64G
#SBATCH --output=00-run_inc_log.out
#SBATCH --time=47:59:00
cd $HOME/malaria-code-repo/2-analysis/
module purge
# load R version 4.0.2 (required for certain packages)
module load R/4.0.2
# load gcc, a C++ compiler (required for certain packages)
module load gcc/10
# load software required for spatial analyses in R
module load physics gdal
module load physics proj
R CMD BATCH --no-save analysis.R analysis.out
```

To submit this job, save the code in the chunk above in a script called myjob.sh and then enter the following command into terminal:

```
sbatch myjob.sh
```

To check on the status of your job, enter the following code into terminal:

```
squeue -u $USERNAME
```

Checklists

by Jade Benjamin-Chung

15.1 Pre-analysis plan checklist

- Brief background on the study (a condensed version of the introduction section of the paper)
- Hypotheses / objectives
- Study design
- Description of data
- Definition of outcomes
- Definition of interventions / exposures
- Definition of covariates
- Statistical power calculation
- Statistical model description
- Covariate selection / screening
- Standard error estimation method
- Missing data analysis
- Assessment of effect modification / subgroup analyses
- Sensitivity analyses
- Negative control analyses

15.2 Code checklist

- Does the script run without errors?
- Is code self-contained within repo and/or associated Box folder?
- Is all commented out code / remarks removed?
- Does the header accurately describe the process completed in the script?
- Is the script pushed to its github repository?

- Does the code adhere to the coding style guide?
- Are all warnings ignorable? Should any warnings be intentionally suppressed or addressed?

15.3 Manuscript checklist

This is adapted in part from this article.

- Have you completed the relevant reporting checklist, if applicable? (Collection of checklists)
- Are the study results within the manuscript replicable (i.e., if you rerun
 the code in the study's repository, the tables and figures will be exactly
 replicated?)
- Is a target journal selected?
- Is the title declarative, in other words, does it state the object/findings rather than suggest them?
- Is the word count of the manuscript close to the target journal's allowance?
- Does the manuscript adhere to the formatting guide of the target journal?
- Does the manuscript use a consistent voice (passive or active usually active is preferred ... pun intended)?
- Is each figure and table (including supplementary material) referenced in the main text?
- Is there a caption for each figure and table (including supplementary material)?
- Are tables/figures and supplementary material numbered in accordance with their appearance in the main text?
- Does the text use past tense if it is reporting research findings or future tense if it is a study protocol?
- Does the text avoid subjective wording (e.g., "interesting", "dramatic")?
- Does the text use minimal abbreviations, and are all abbreviations defined at first use?
- Does the text avoid directionless words? (e.g., instead of writing, 'Precipitation influences disease risk', write, 'Precipitation was associated with increased disease risk').
- Does the text avoid making causal claims that are not supported by the study design? Be careful about the words "effect", "increase", and "decrease", which are often interpreted as causal.
- Does the text avoid describing results with the word "significant", which can easily be confused with statistical significance? (see references on this topic here)
- Have you drafted author contributions? Do they follow the CRediT Taxonomy for author contributions?

15.4 Figure checklist

- Are the x-axis and y-axis labeled?
- If the figure includes panels, is each panel labeled?
- Are there sufficient numerical / text labels and breaks on the x-axis and y-axis?
- Is the font size appropriate (i.e., large enough to read, not so large that it distracts from the data presented in the figure?)
- Are the colors used colorblind friendly? See a colorblind-friendly palette here, a neat palette generator with colorblind options here, and an article on why this matters here
- Are colors/shapes/line types defined in a legend?
- Are the legends and other labels easy to understand with minimal abbreviations?
- If there is overplotting, is transparency used to show overlapping data?
- Are 95% confidence intervals or other measures of precision shown, if applicable?

Resources

by Jade Benjamin-Chung and Kunal Mishra

16.1 Resources for R

- dplyr and tidyr cheat sheet
- ggplot cheat sheet
- data table cheat sheet
- RMarkdown cheat sheet
- Hadley Wickham's R Style Guide
- Jade's R-for-epi course
- Tidy Eval in 5 Minutes (video)
- Tidy Evaluation (e-book)
- Data Frame Columns as Arguments to Dplyr Functions (blog)
- Standard Evaluation for *_join (stackoverflow)
- Programming with dplyr (package vignette)

16.2 Resources for Git & Github

- Data Camp introduction to Git
- Introduction to Github

16.3 Scientific figures

• Ten Simple Rules for Better Figures

16.4 Writing

- Tips on how to write a great science paper
- ICMJE Definition of authorship
- Nature article on elements of style for scientific writing
- The Pathway to Publishing: A Guide to Quantitative Writing in the Health Sciences
- Secret, actionable writing tips

16.5 Presentations

- How to tell a compelling story in scientific presentations
- How to give a killer narratively-driven scientific talk
- How to make a better poster
- How to make an even better poster

16.6 Professional advice

• Professional advice, especially for your first job

16.7 Funding

• Building Your Funding Train

16.8 Ethics and global health research

- Global Code of Conduct For Research in Resource-Poor Settings
- Who is a global health expert? Advice for aspiring global health experts
- Transforming Global Health Partnerships