

# Preparing Data and Code for Publication

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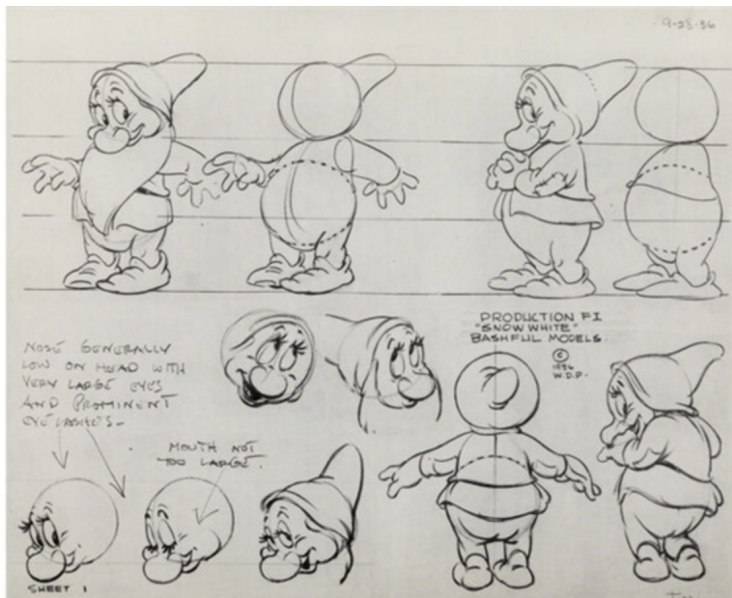
# Barriers to reproducible papers

In theory, some of the barriers to making published papers computationally reproducible are:

- ▶ Necessary to know what to include and how to share it
- ▶ Data are very large
- ▶ Data cannot ethically or legally be shared (e.g. private health data)
- ▶ Necessary to know how to share important information about the environment in which the code was run
- ▶ Must address randomness introduced by random number generation

We will cover these topics in this session.

# Barriers to reproducible papers



# Barriers to reproducible papers

In practice, though, some of the barriers keeping people from making published papers computationally reproducible are actually:

- ▶ I don't want to share the code / data
  - ▶ The code's too messy
  - ▶ Someone might scoop my work
  - ▶ Someone might find a bug
- ▶ The code's available, but very hard to understand
  - ▶ I'll put the code up, but it's not worth taking the time to clean it first
  - ▶ Subconsciously creating a barrier to prevent easy reproduction

The other sessions of the workshop have focused on approaches that address these barriers.

# What to include with a computationally reproducible paper?

Remember, to be computationally reproducible, the reader must be able to start from the data that were collected and arrive at the same results, including tables and figures.

- ▶ All data used in analysis in the paper
- ▶ All code to get from these data to the results shown in the paper
- ▶ Any environmental information (e.g., package versions) that are necessary for the code to generate the results

It's also helpful to include:

- ▶ Adequate documentation for the user to recreate the results from the data using the code and environmental information
- ▶ Guidance on how the code can be reused (license)

## Including data for the paper

Ideally, you will include all the data that were used to generate the paper's results.

However, sometimes there are challenges with including some or all of the data. These include:

- ▶ Data cannot be legally or ethically shared
- ▶ Data are very large

## Sensitive or protected data

If your research includes human health data or other types of sensitive or protected data, you may not be able to publish that data.

As a result, you will not be able to make your paper fully computationally reproducible.

However, if you consider reproducibility as a spectrum, there are steps you can take to make the paper *more* computationally reproducible, even if you cannot share all the elements required to be fully reproducible.

## Sensitive or protected data

If you cannot include the data with other reproducibility materials, consider the following steps to make the paper as reproducible as possible:

- ▶ Include mock dataset (same format, different numbers) to use to test and demonstrate the function of the code
- ▶ Describe the data that you were not able to include, so that readers can understand how the code would work with the data
- ▶ Use `.gitignore` to include the data in a git repo on a local computer (or a secure server you're working on) but not push it to remote versions of that repo, like one on GitHub
- ▶ When working on a server for security reasons, consider having RStudio Server installed, as this provides a friendlier interface for working with git version control on the server (avoids having to do much from the terminal)



# Sensitive or protected data

In the next lab, we'll explore a paper that has taken steps to be computationally reproducible, even those it cannot share its data.

## AIR POLLUTION

# Differential Mortality Risks Associated With PM<sub>2.5</sub> Components

## A Multi-Country, Multi-City Study

Masselot, Pierre<sup>a</sup>; Sera, Francesco<sup>a,b</sup>; Schneider, Rochelle<sup>a,c,d</sup>; Kan, Haidong<sup>e</sup>; Lavigne, Éric<sup>f,g</sup>; Stafoggia, Massimo<sup>h</sup>; Tobias, Aurelio<sup>i,j</sup>; Chen, Hong<sup>k</sup>; Burnett, Richard T.<sup>k</sup>; Schwartz, Joel<sup>l</sup>; Zanobetti, Antonella<sup>l</sup>; Bell, Michelle L.<sup>m</sup>; Chen, Bing-Yu<sup>n</sup>; Guo, Yue-Liang Leon<sup>n</sup>; Ragettli, Martina S.<sup>o</sup>; Vicedo-Cabrera, Ana Maria<sup>p,q</sup>; Åström, Christofer<sup>r</sup>; Forsberg, Bertil<sup>r</sup>; Íñiguez, Carmen<sup>s,t</sup>; Garland, Rebecca M.<sup>u,v,w</sup>; Scovronick, Noah<sup>x</sup>; Madureira, Joana<sup>y,z</sup>; Nunes, Baltazar<sup>aa,bb</sup>; De la Cruz Valencia, César<sup>cc</sup>; Hurtado Diaz, Magali<sup>cc</sup>; Honda, Yasushi<sup>dd,ee</sup>; Hashizume, Masahiro<sup>ff</sup>; Ng, Chris Fook Cheng<sup>g</sup>; Samoli, Evangelia<sup>gg</sup>; Katsouyanni, Klea<sup>gg,hh</sup>; Schneider, Alexandra<sup>ii</sup>; Breitner, Susanne<sup>ii,jj</sup>; Ryti, Niilo R.I.<sup>kk,ll</sup>; Jaakkola, Jouni J.K.<sup>kk,ll,mm</sup>; Maasikmets, Marek<sup>nn</sup>; Orru, Hans<sup>oo</sup>; Guo, Yuming<sup>pp</sup>; Valdés Ortega, Nicolás<sup>qq</sup>; Matus Correa, Patricia<sup>rr</sup>; Tong, Shilu<sup>rr,ss,tt,uu</sup>; Gasparrini, Antonio<sup>a,c,vv</sup>

Author Information ☺

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# Sensitive or protected data

In the documentation of the GitHub repository that the authors use to share the code for the paper, they describe why they cannot include the health data:

## Data and Results

Data are not available currently due to restricted data sharing agreement between the collaborators of this study. Therefore, the code is not fully reproducible.

Data are normally included in a subfolder *Data*. It should contain:

- Mortality and pollution data, stored in a list of city-specific `data.frames`. Also contains a descriptive `data.frame` with one line for each city.
- PM2.5 components, stored in one csv files per year of data. Each csv file contains one line per city.
- City-specific characteristics, stored as a `data.frame` with one line per city.

## .gitignore file

When you track a directory with git version control, you will have a file added to the directory called “.gitignore”.



## .gitignore file

This is a plain text file. You can edit it to specify the files or groups of files that you want `git` to ignore as it tracks changes to that directory.

If you are sharing the `git` repo through GitHub, you can avoid posting certain files online by listing them in this “.gitignore” file.

## .gitignore file

If you look through the repository for the sample paper for the lab, you'll see that they listed all data in the ".gitignore" file. This allows them to have the data on their local computer but not share it publicly with the rest of the repo.

```
# Session Data files
```

```
.RData
```

```
**/*.RData
```

```
# RStudio files
```

```
.Rproj.user/
```

```
# Other
```

```
Data/
```

## Extremely large data

Sometimes, the paper will include results based on datasets that are very large.

These data sizes can exceed the limits for some platforms that you otherwise might use to share the reproducibility materials (e.g., GitHub, the journal's website, the author's university website).

Repositories built for research data curation might be better suited for storing very large datasets.

# Research data repositories

One example is the ImmPort data repository, which is sponsored by US agencies including the National Institute of Allergy and Infectious Diseases.

 **Register** to join us for ImmPort's upcoming webinar on **VIGET: A web portal for study of vaccine-induced host responses based on Reactome pathways and ImmPort data** this July 27, 2023 at 12:00 PM PST/3:00 PM EST [here!](#) 



ImmPort is funded by the NIH, NIAID and DAIT in support of the NIH mission to share data with the public. Data shared through ImmPort has been provided by NIH-funded programs, other research organizations and individual scientists ensuring these discoveries will be the foundation of future research.

Data uploading or sharing questions? Please contact [ImmPort\\_Helpdesk@import.org](mailto:ImmPort_Helpdesk@import.org).



# Extremely large data

Some things to keep in mind about these repositories include:

- ▶ Some repositories might have APIs—data can be downloaded programatically (from the code script)
- ▶ Some repositories allow options to toggle private versus public
- ▶ Some repositories have suggested or required data models
- ▶ Some repositories include platforms to work interactively with the data

dkNET has a curated list of repositories for research data at <https://dknet.org/rin/suggested-data-repositories>



## Data to include

It can be useful to save intermediate versions of the data, as the code moves from raw data to the final figures, tables, and other results. Intermediate data can include:

- ▶ Processed data (e.g., if raw data are from flow cytometry, the results after gating and counting the data)
- ▶ Data points that are plotted in figures (i.e., data at the point immediately before it is graphed)

Note that this is in addition to the raw data.

For these intermediate data sets, it's helpful if you save them in plain text formats (e.g., “.csv” or “.txt” file).

# Data to include

There's a nice discussion of why to include all intermediate results in an article available through PLoS Computational Biology.

OPEN ACCESS Freely available online



## Editorial

# Ten Simple Rules for Reproducible Computational Research

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# Sharing code and environment information

Usually, you will not have any problems with the code and environmental information being sensitive or extremely large, as with the research data.

However, there are some other things you should consider as you aim to share code to improve the computational reproducibility of a paper.

- ▶ The code will not work correctly if you use absolute rather than relative pathnames for files.
- ▶ The code might not work correctly if it is run on software with a different version.
- ▶ The code will not, unless you take appropriate steps, recreate the same results if some of the steps in the code use random number generation.

# Absolute versus relative pathnames

When you want to tell R about a file, you can either give it the file's full address (from the root directory of your computer) or you can give it directions from the working directory. The first is an **absolute** filepath and the second is a **relative** filepath.

```
read_csv("/Users/ganders/my_proj/data/my_data.csv")  
read_csv("data/my_data.csv")
```

Which will be robust when someone else tries to run the code on their own computer?

## Versions of software

When you run R code, your computer not only runs the code that you wrote, but also code within your installation of base R as well as code from packages that you have installed.

Your code essentially is built on top of these other pieces of code.

At an even deeper level, your computer is also using code from its operating system to execute your R code script.

## Versions of software

All of these pieces of software are evolving. When you install a new version of any of these pieces of software, it will change the environment in which your R code runs.

Similarly, if someone else tries to run your code, it may fail if they have a different version of one or more of these pieces of software.

## Versions of software

There is a gradient in how quickly different pieces of software evolve (in terms of updates that affect the execution of R code). Code for your operating system and base R tend to evolve more slowly (in terms of things that affect R code), while package extensions to R tend to change more quickly.

Some R package projects are in stages of significant evolution. Two types of R packages which I've repeatedly seen introduce reproducibility issues based on the package version are the tidyverse suite of packages and the Bioconductor collection of packages.

## Versions used in original analysis

There are a few approaches you can take to address this issue. Your aim is to provide the user with enough information that they can recreate the environment you had when you applied the code to the data to generate the paper's results.

- ▶ Provide an in-depth description of the versions of software used when running the paper's analysis
- ▶ Help the user recreate the original environment
- ▶ Save and share the full environment



## Providing session information when running code

The simplest way to provide environment information is to share the versions of all software that was used when the paper's analysis was conducted.

Most open-source software will archive older versions. A user can obtain an older version of the software from these archives and install it on R. Here's an example of how to find old sources on CRAN:

Package source: [dplyr 1.1.2.tar.gz](https://cran.r-project.org/web/packages/dplyr/dplyr_1.1.2.tar.gz)

Windows binaries: r-devel: [dplyr 1.1.2.zip](https://cran.r-project.org/web/packages/dplyr/dplyr_1.1.2.zip), r-release: [dplyr 1.1.2.zip](https://cran.r-project.org/web/packages/dplyr/dplyr_1.1.2.zip), r-oldrel: [dplyr 1.1.2.zip](https://cran.r-project.org/web/packages/dplyr/dplyr_1.1.2.zip)

macOS binaries: r-release (arm64): [dplyr 1.1.2.tgz](https://cran.r-project.org/web/packages/dplyr/dplyr_1.1.2.tgz), r-oldrel (arm64): [dplyr 1.1.2.tgz](https://cran.r-project.org/web/packages/dplyr/dplyr_1.1.2.tgz), r-releas

Old sources: [dplyr archive](https://cran.r-project.org/web/packages/dplyr/dplyr_archive)

This approach may not work for proprietary software (e.g., SAS, MATLAB), if they do not make prior software versions available.

# Providing session information when running code

R has some functions that will print information about the software in its working environment, including the names and versions of all loaded packages.

These functions include `sessionInfo` from base R and `session_info` from devtools.

attached base packages:

```
[1] stats      graphics  grDevices  utils      datasets  methods    base
```

other attached packages:

```
[1] purrr_1.0.1  forcats_1.0.0
```

loaded via a namespace (and not attached):

```
[1] vctrs_0.6.3      cli_3.6.1        knitr_1.43        rlang_1.1.1       xfun_0.39
[6] stringi_1.7.12   generics_0.1.3   glue_1.6.2        janitor_2.2.0     htmltools_0.5.5
[11] hms_1.1.3         fansi_1.0.4      rmarkdown_2.23    snakecase_0.11.0  evaluate_0.21
[16] tibble_3.2.1     tzdb_0.4.0       fastmap_1.1.1     yaml_2.3.7        lifecycle_1.0.3
[21] stringr_1.5.0    compiler_4.3.0   timechange_0.2.0  pkgconfig_2.0.3   rstudioapi_0.15.0
[26] digest_0.6.33    R6_2.5.1         tidyselect_1.2.0  readr_2.1.4       utf8_1.2.3
[31] pillar_1.9.0     magrittr_2.0.3   tools_4.3.0       lubridate_1.9.2
```

## Providing session information from running code

You can include a call to `sessionInfo` or `session_info` at the end of an RMarkdown document.

This will print out all the information for the environment in which the RMarkdown file was rendered, including:

- ▶ The version of base R
- ▶ The platform (this provides information about the operating system and its version)
- ▶ Versions of other packages of routines (e.g., LAPACK for FORTRAN)
- ▶ Attached and loaded packages, as well as the version of each

## Recreating the original environment

When you record the session information, it still leaves a lot of work on a later user to find and install all the old versions of packages.

To alleviate this, there are some R packages that automate part of the process. These help the user recreate the environment that code ran in originally. In particular, they can help when a user wants to recreate the environments for several different projects on one computer, with different software versions for each project.

# Recreating the original environment

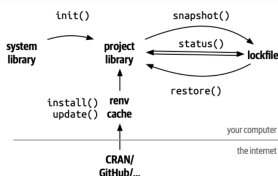
The `renv` package is one of these packages that helps automating the process of recreating an environment. It has extensive help documentation online:

## Introduction to `renv`

Source: [vignettes/renv.Rmd](#)

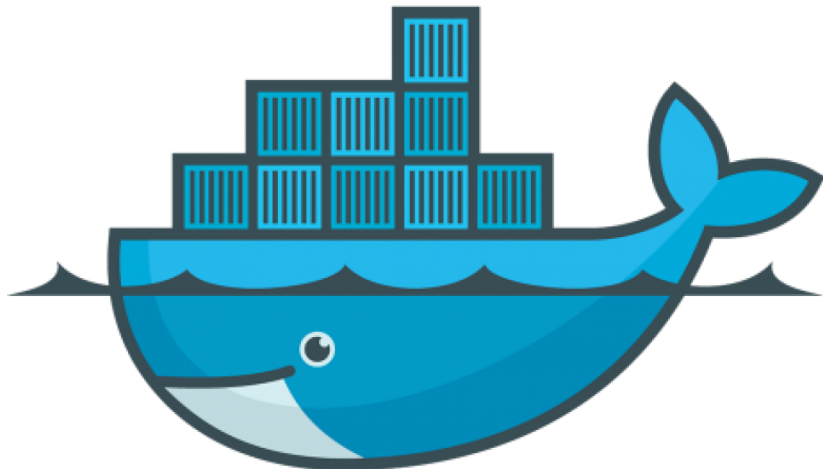


The `renv` package helps you create reproducible environments for your R projects. This vignette introduces you to the basic nouns and verbs of `renv`, like the user and project libraries, and key functions like `renv::init()`, `renv::snapshot()` and `renv::restore()`. You'll also learn about some of the infrastructure that makes `renv` tick, some problems that `renv` doesn't help with, and how to uninstall it if you no longer want to use it.



## Saving and sharing the environment

A number of researchers take the approach of saving and sharing the environment in which the code originally ran. One approach is to use a container (e.g., a Docker container).



# Container

A container includes all files and directory organization. Also includes the software needed to run code. It does not include all the code for the operating system, but it does provide information to help recreate that part of the environment.

This set-up allows the user to rerun the analysis *in its original environment* by running it within the container.

# Container

## Downsides:

- ▶ File size of container is often large
- ▶ Higher threshold at present for both creating and using containers with R code versus scripts paired with `renv`
- ▶ Can be somewhat of a black box, in terms of dissecting what's in the container
- ▶ Can be hard to adapt parts for new tasks (often relies on code that might be out of date)



## Future-proof your code

You can also take some steps to try to avoid or delay problems that are created as the packages that the code depends on evolves.

One is to try to avoid using superseded or deprecated functions in your code.

These are functions where an improved version exists, with plans that the new version will become the default.

A function that is **superseded** will be maintained, but won't be a key part of the evolving package (in particular, it won't receive any new updates, only enough changes to still work).

A function that is **deprecated** will eventually be removed from the package, and a replacement is already available and preferred.

# Future-proof your code

You can often find information about deprecation in the helpfiles for a file.

`spread {tidyr}`

R Documentation

## Spread a key-value pair across multiple columns

### Description

lifecycle **superseded**

For `count ( )`: if `FALSE` will include counts for empty groups (i.e. for levels of factors that don't exist in the data).

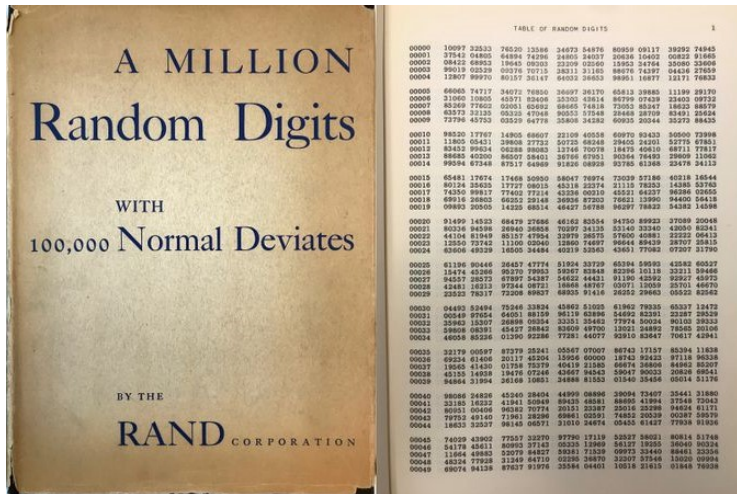
`.drop`

lifecycle **deprecated**

For `add_count ( )`: deprecated since it can't actually affect the output.

# Reproducing randomness

Many statistical methods require randomization, implemented through the generation of random numbers.



# Reproducing randomness

Your code might be using random number generation if you:

- ▶ are sampling
- ▶ are using Monte Carlo methods / simulations
- ▶ are doing Bayesian statistics

# Reproducing randomness

There are ways to generate truly random numbers:



## Reproducing randomness

However, computers typically use a pseudorandom number generator.

For R's random number generators, you can force the same random numbers each time you run a piece of code by setting something called a “seed” before any function calls that involve random number generation.

## Reproducing randomness

If you don't set a seed, you will get different results when you run code that involves random number generation, because of the randomness involved.

```
sample(1:5)
```

```
## [1] 1 4 5 3 2
```

```
sample(1:5)
```

```
## [1] 4 5 1 2 3
```

## Reproducing randomness

If you set the same seed each time before you run that code, on the other hand, you will get the same “random” results each time you generate random numbers:

```
set.seed(100)  
sample(1:5)
```

```
## [1] 2 3 5 4 1
```

```
set.seed(100)  
sample(1:5)
```

```
## [1] 2 3 5 4 1
```