Tools for Reproducible Research

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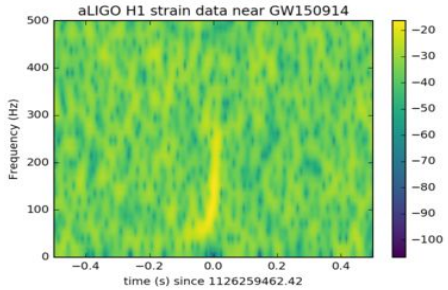
LIGO experiment

Jupyter Notebooks analyzing the data:

```
                                                    noverlap=NOVL, cma
at])
plt.xlabel('time (s) since '+str(tevent))
plt.ylabel('Frequency (Hz)')
plt.colorbar()
plt.axis([-0.5, 0.5, 0, 500])
plt.title('aLIGO L1 strain data near GW150914')
plt.savefig('GW150914_L1_spectrogram_whitened.png')
```



https://losc.ligo.org/s/events/GW150914/GW150914_tutorial.html

Is the experiment reproducible?

Quora

Ask or Search Quora

Ask Question

Detection of Gravitational Waves (February 2016) +2

Gravitational waves discovery - is LIGO experiment reproducible or is it just a lucky timing that it caught a signal?

It took so many years for LIGO to detect the waves - is it because the instrumentation improved a lot recently? Will this enable us to detect these waves every day or will it require signals from massive black hole collisions?

general relativity - Why didn't LIGO wait for a second observation of a ...

physics.stackexchange.com/...**didnt-ligo-wait-for-a-second**.../246611 Stack Exchange

Apr 1, 2016 - My whole life I have been taught that the very hallmark of scientific **experiment** are reproducible results. So **why didn't LIGO wait for a second** ...

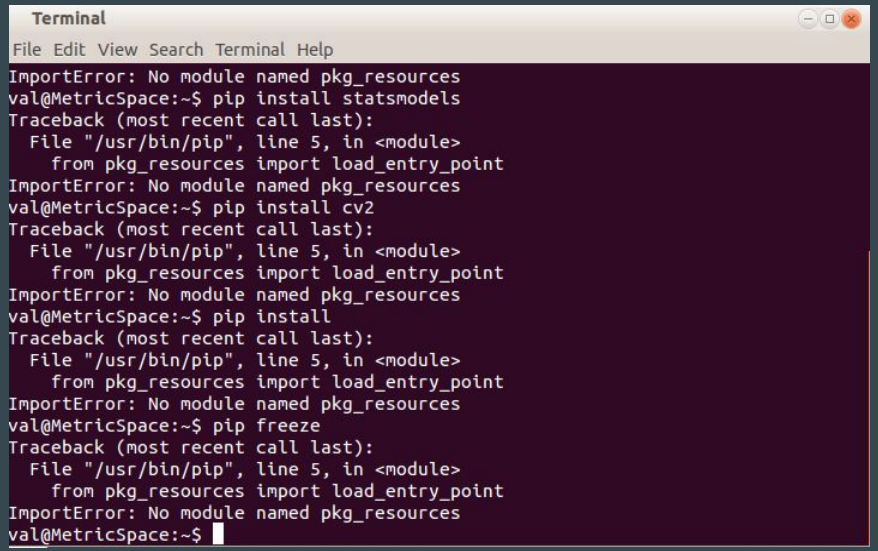
Second Gravitational Wave Detected!

Reproducibility vs. Replicability

Two main notions:

- Results of an experiment are regenerated using the same data and methods.
- Results of an experiment are regenerated using new data or alternative methods.

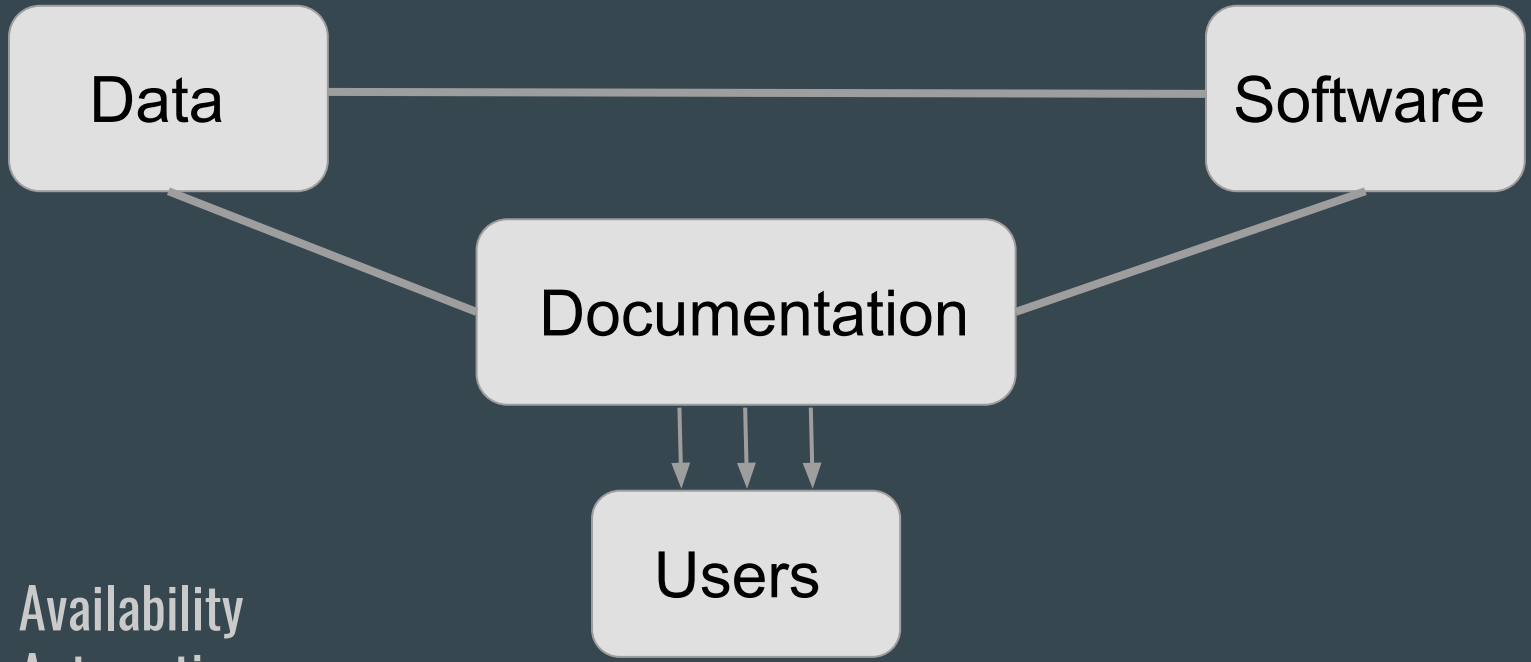
It is hard...



It is not about reproducible or not reproducible.

It is about more reproducible.

Improving Reproducibility



- Availability
- Automation
- Sustainability

Project Templates

- Python Module Template: Shablona
- R Project Structure: https://nicercode.github.io/blog/2013-04-05-projects/
- Data Science Project Structure: Cookiecutter

```
.
├── AUTHORS.md
├── LICENSE
├── README.md
├── bin                <- Your compiled model code can be stored here (not tracked by git)
├── config             <- Configuration files, e.g., for doxygen or for your model if needed
├── data
│   ├── external       <- Data from third party sources.
│   ├── interim        <- Intermediate data that has been transformed.
│   ├── processed      <- The final, canonical data sets for modeling.
│   └── raw            <- The original, immutable data dump.
├── docs               <- Documentation, e.g., doxygen or scientific papers (not tracked by git)
├── notebooks          <- Ipython or R notebooks
├── reports            <- For a manuscript source, e.g., LaTeX, Markdown, etc., or any project reports
│   └── figures        <- Figures for the manuscript or reports
└── src                <- Source code for this project
    ├── data           <- scripts and programs to process data
    ├── external       <- Any external source code, e.g., pull other git projects, or external libraries
    ├── models         <- Source code for your own model
    ├── tools          <- Any helper scripts go here
    └── visualization  <- Scripts for visualisation of your results, e.g., matplotlib, ggplot2 related.
```

Choose a license for your code

Code without a license is protected by the author's copyright law.

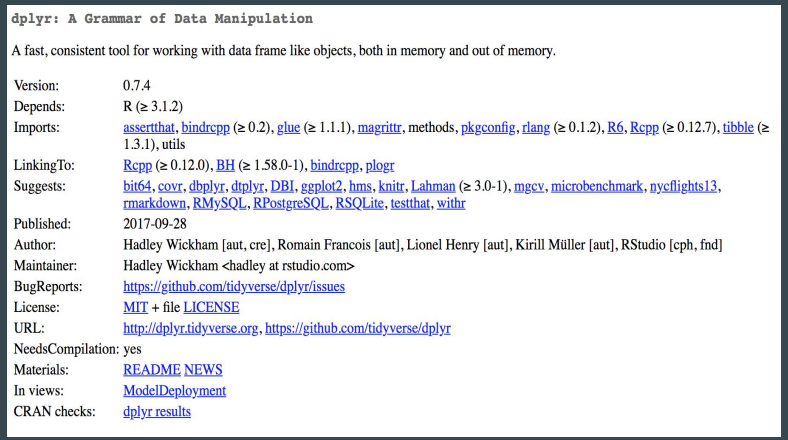
Choose a license website: http://choosealicense.com/

- Permissible licenses: MIT, BDS
- Copyleft licenses: GPL

Documentation

Python - Sphinx, Read the Docs

R - Vignettes



dplyr: A Grammar of Data Manipulation

A fast, consistent tool for working with data frame like objects, both in memory and out of memory.

Version:	0.7.4
Depends:	R (≥ 3.1.2)
Imports:	assertthat, bindrcpp (≥ 0.2), glue (≥ 1.1.1), magrittr, methods, pkgconfig, rlang (≥ 0.1.2), R6, Rcpp (≥ 0.12.7), tibble (≥ 1.3.1), utils
LinkingTo:	Rcpp (≥ 0.12.0), BH (≥ 1.58.0-1), bindrcpp, plogr
Suggests:	bit64, covr, dbplyr, dtplyr, DBI, ggplot2, hms, knitr, Lahman (≥ 3.0-1), mgcv, microbenchmark, nycflights13, rmarkdown, RMySQL, RPostgreSQL, RSQLite, testthat, withr
Published:	2017-09-28
Author:	Hadley Wickham [aut, cre], Romain Francois [aut], Lionel Henry [aut], Kirill Müller [aut], RStudio [cph, fnd]
Maintainer:	Hadley Wickham <hadley at rstudio.com>
BugReports:	https://github.com/tidyverse/dplyr/issues
License:	MIT + file LICENSE
URL:	http://dplyr.tidyverse.org, https://github.com/tidyverse/dplyr
NeedsCompilation:	yes
Materials:	README NEWS
In views:	ModelDeployment
CRAN checks:	dplyr results

- Journal of Open Source Software
- Journal of Statistical Software

Literate Programming

Combining documentation and code in a single program.

“Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do.”

R Reporting and sharing: Knitr, RPubs
Notebooks - Jupyter, R Notebooks, Zeppelin, Sage, Beaker
Notebook Environments: Binder, CoCalc, Colaboratory

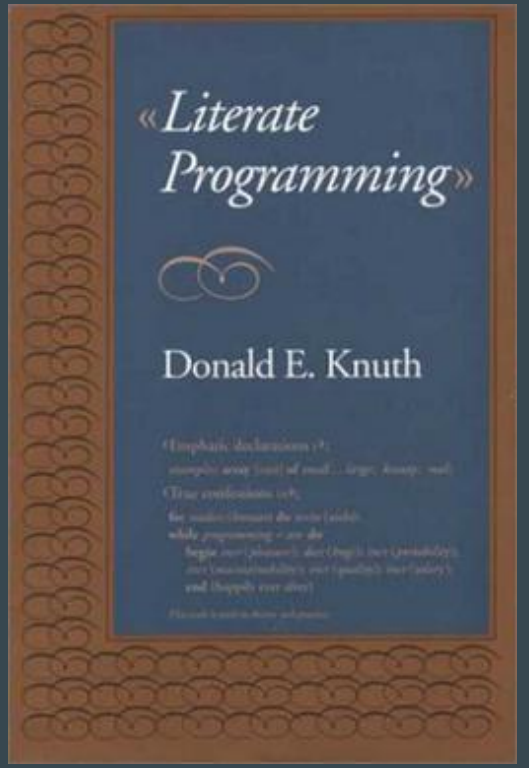
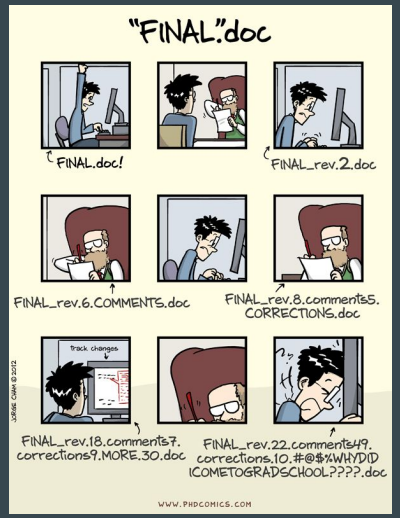


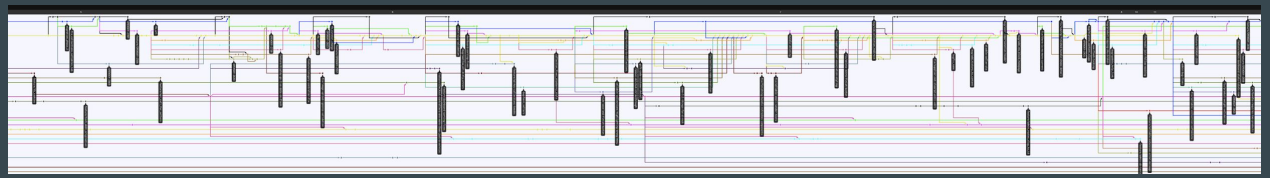
Image by Wikipedia

Virtualization

- Virtual Environments (Conda) - package dependencies
- Docker Containers - Linux environment, works on all OS, scriptable
- Vagrant - virtual machine manager, can run both Docker containers and full VMs
- Virtual Machines - VirtualBox, VMWare
- Cloud Images - AWS AMIs

Versioning

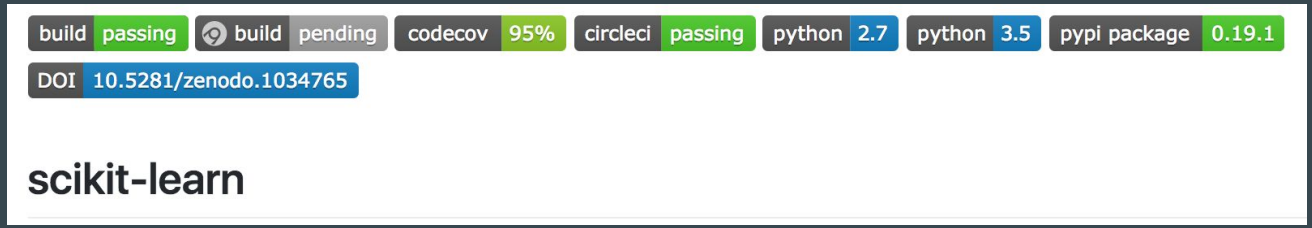




http://justinhileman.info/article/changing-history/opensky-branches.png

- Version control for code: git & Github
- Version control for data: https://quiltdata.com/

Testing



We are already writing tests, need to save them.

- Locally
  - Python - nose, pytest
  - R - testthat

- Remotely - Continuous Integration
  - Travis, CircleCI, AppVeyor

Start by testing the environment.

Data Repositories

zenodo	figshare	DRYAD
Up to 50GB free Not-for-profit - EU funded	100GB free per manuscript Institutional plans For-profit	Publishing Fee - $120 Excess fees after 20GB Associated with articles Not-for-profit

- Cloud Storage: free to upload, fees to download
- Datasets receive Digital Object Identifier (DOI)
- Nature Journal Scientific Data: https://www.nature.com/sdata/

Get Feedback

eScience Office Hours: http://escience.washington.edu/office-hours/

Reproducibility Mailing List: escience_reproducibility

References

Reproducibility vs Replicability: or is it the other way around: http://languagelog.ldc.upenn.edu/nll/?p=21956

Chris Drummond's Interpretation: https://core.ac.uk/download/files/21/107703.pdf

Talk Link: https://github.com/valentina-s/presentations/blob/master/ReproducibleResearchTools.pdf