Toward Reproducible Data Science

Tips and tricks of making data science projects more reproducible.

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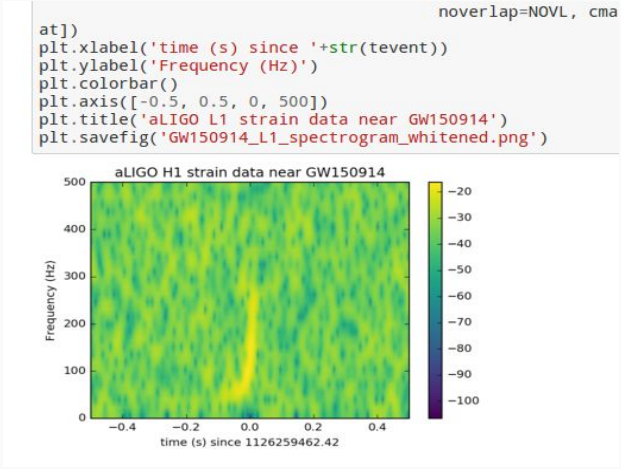
Reliable data science studies?

Many more retractions!

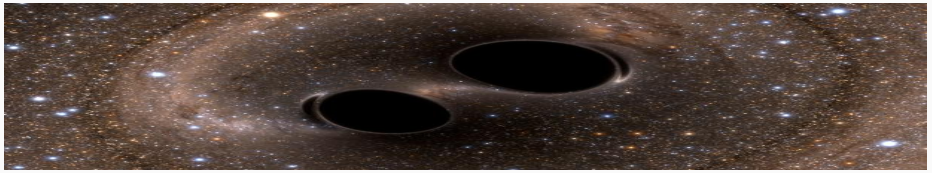
LIGO experiment

Jupyter Notebooks analyzing the data:

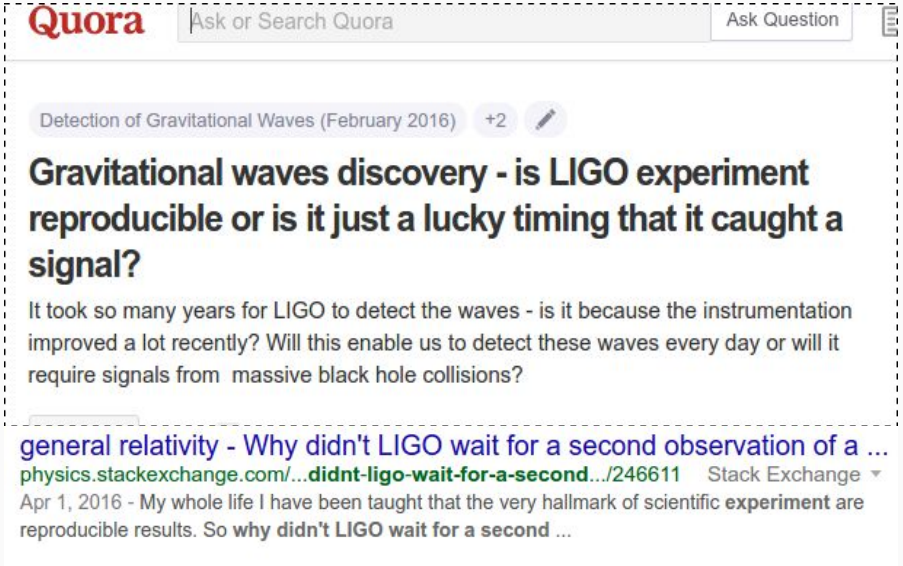
```
                                                noverlap=NOVL, cma
at])
plt.xlabel('time (s) since '+str(tevent))
plt.ylabel('Frequency (Hz)')
plt.colorbar()
plt.axis([-0.5, 0.5, 0, 500])
plt.title('aLIGO L1 strain data near GW150914')
plt.savefig('GW150914_L1_spectrogram_whitened.png')
```



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



Is the experiment reproducible?



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.

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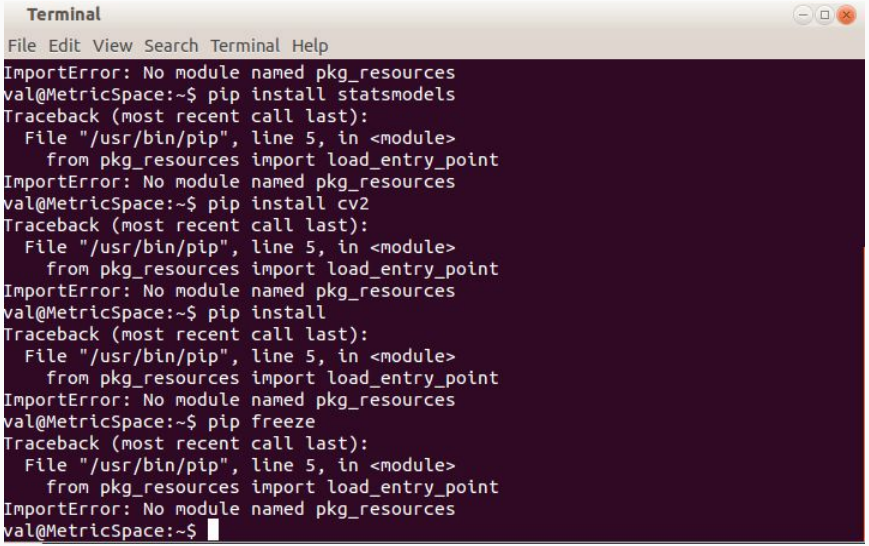
Reproducibility vs. Replicability: A Brief History of a Confused Terminology

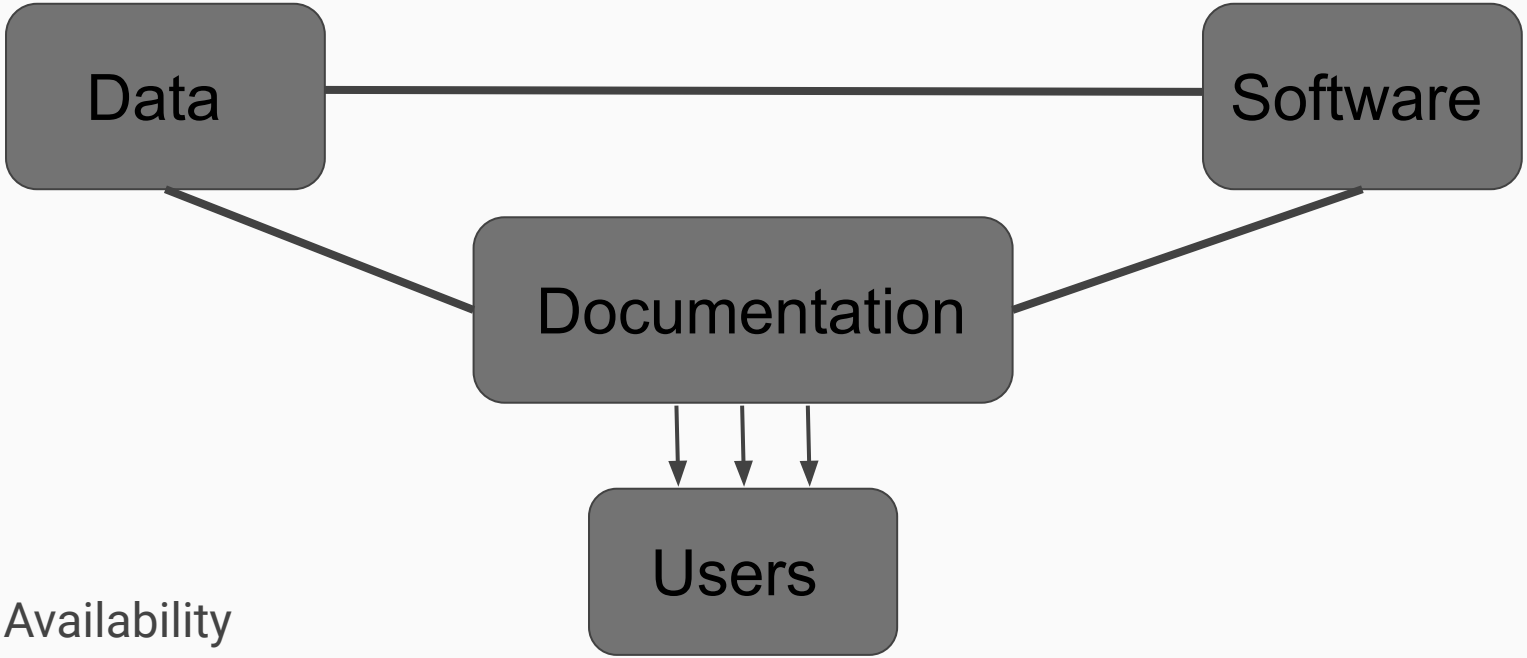
It is hard...



It is not about reproducible or not reproducible.

It is about more reproducible.

Improving Reproducibility



- Availability
- Automation
- Sustainability

Tips for more reproducible data science.

So far you have learnt:

- Some programming/data analysis
- Code style and documentation
- Version control and collaborative programming

What we will discuss today:

- Project Organization
- Modular Programming
- Literate Programming
- Virtualization
- Testing
- Software Licensing
- Data Sharing

Project Repository Organization

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

Start simple:

```
.
+-- data
|   +-- raw
|   +-- processed
|
+-- src
|   +-- PythonModules
|   +-- tests
|
+-- notebooks
|   +-- exploratory
|   +-- expositionary
|
+-- references
|   +-- papers
|   +-- tutorials
|
+-- results
+-- README.md
+-- LICENSE.txt
```

Expand as needed:

```
.
├── 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.
```

Pick and adjust for your project!

Software License Selection

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

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

I need to work in a community.

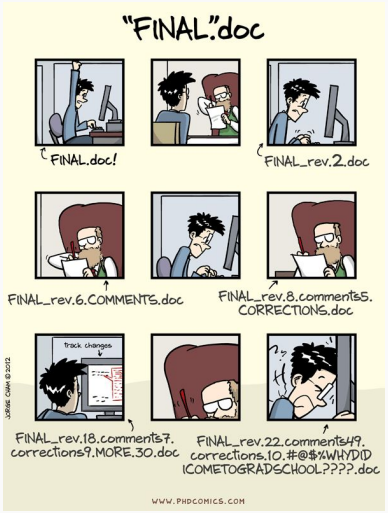
I want it simple and permissive.

I care about sharing improvements.

- **Permissible licenses**: MIT, BDS, Apache
  - With/without attribution, with/without explicit modification explanation
- **Copyleft licenses**: GPL
  - Forces all derivatives to have the same license
  - Viral licensing: for example GPL code may be hard to integrate with MIT code.
- **Creative Commons** (good for documents or educational materials)
  - with/without attribution, with/without derivatives, with/without commercial use
  - https://chooser-beta.creativecommons.org/

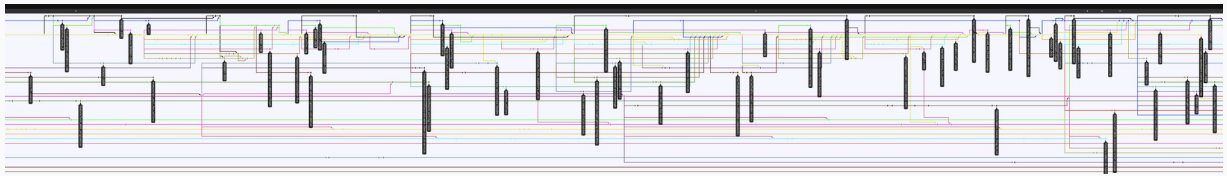
Code in a private repository can also have a license/sharing&use agreement.

Version Control Workflow



- Version control for code: git & Github
  - Software Carpentry Tutorials: https://swcarpentry.github.io/git-novice/
  - Atlassian Tutorials: https://www.atlassian.com/git/tutorials/what-is-version-control
  - Cheetsheets: https://services.github.com/on-demand/downloads/github-git-cheat-sheet.pdf
- Version control for data:
  - Git Large File Storage
  - Quilt: https://quiltdata.com/
  - Data Version Control: https://dvc.org/ (for Machine Learning Projects)

Decide on a strategy with your team!

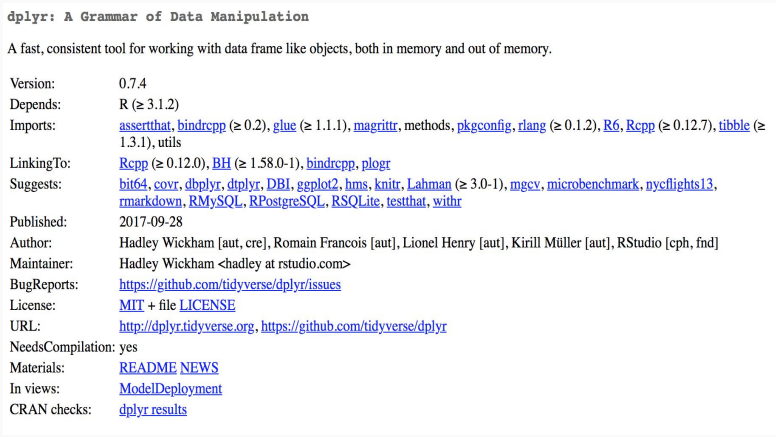


http://justinhileman.info/article/changing-history/opensky-branches.png

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, CoCalc
Notebook Environments: Binder, Colaboratory, Kaggle, VSCode Notebooks, AWS Sagemaker Notebooks

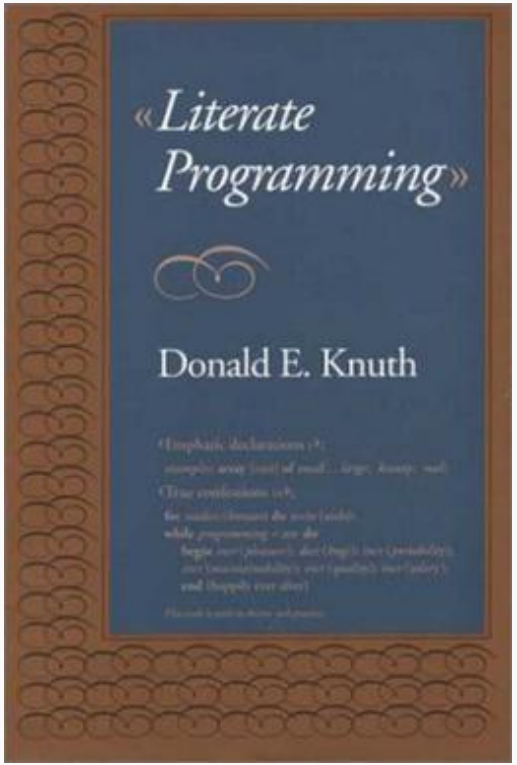


Image by Wikipedia

Free Notebook Environments

Colaboratory Notebooks (Google)

- 13GB RAM
- 107 GB disk
- GPU support
- Notebooks and data on Google Drive
- Integration with Github
- Simultaneous Editing
- Python only so far

Cons:

- not real filesystem
- Github integration funky
- Can get blocklisted from GPU support
- Need to pip install packages

Kaggle Kernels (Google)

- 30GB RAM
- 20GB disk
- GPU support
- Upload/Edit/Download Notebooks
- Kaggle Datasets: public and private(20GB)
- Version Control Support
- R and Python

Cons:

- no Github integration
- Specialized dataset loading

Binder

- 2GB RAM
- Works with Github Repos
- Python, R, Julia
- Good for demos

Cons:

- Ephemeral workspace
- Limits the number of simultaneous users

Jupyter Lite

- Runs in browser
- Great for interactive widgets

Cons:

- might not run out-of-box

Domain specific: Planetary Computer, Google Earth Engine
Non-free: Colab Pro, VS Code & Azure, AWS Sagemaker for ML

Combining Notebooks

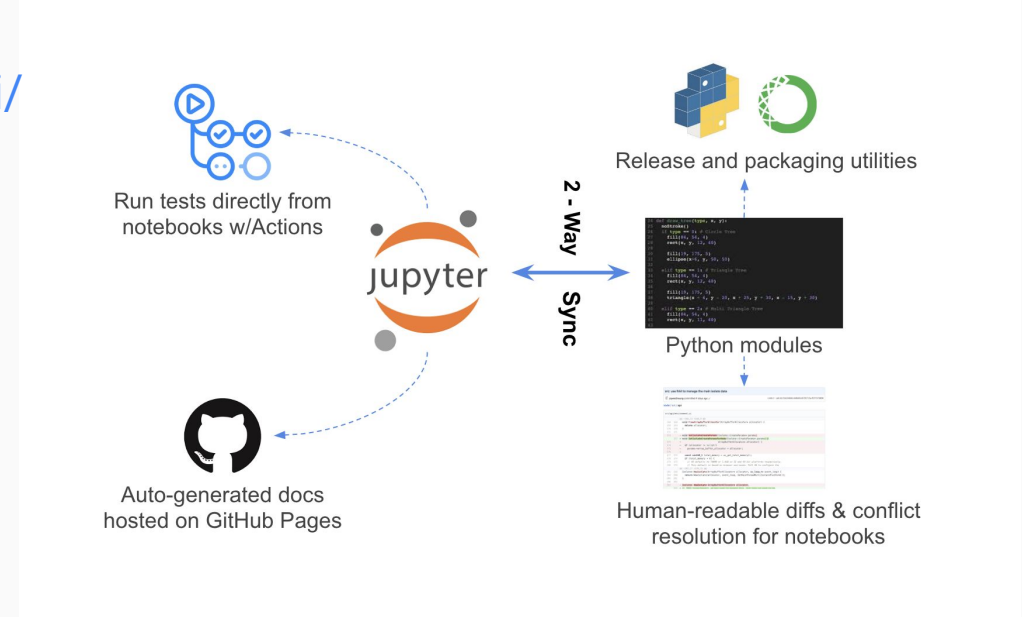
- Binder (mybinder.org)
  - Binds and demos notebooks on a github repo
    - xarray example
    - Your notebook example
- Jupyterbook (https://jupyterbook.org/intro.html)
  - Combines notebooks into a static website
- Papermill (https://papermill.readthedocs.io/en/latest/)
  - Executes notebooks, parameterizes notebooks, generates reports

From Notebooks to Modules

Modular Programming:

- convert commands -> functions -> modules/libraries
- convert notebooks/scripts -> modules/libraries

[nbdev](https://nbdev.fast.ai/)
https://nbdev.fast.ai/



Virtualization

Virtual Environment
(conda, pyenv, renv)

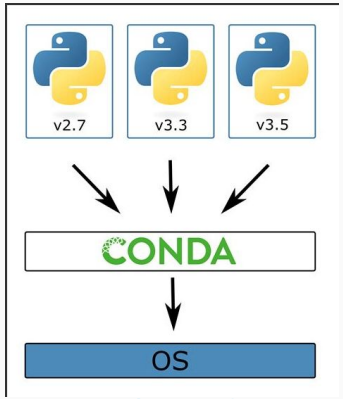


Image Source

Virtual Container
(Docker)

Virtual Machine
(Virtual Box, Vmware)

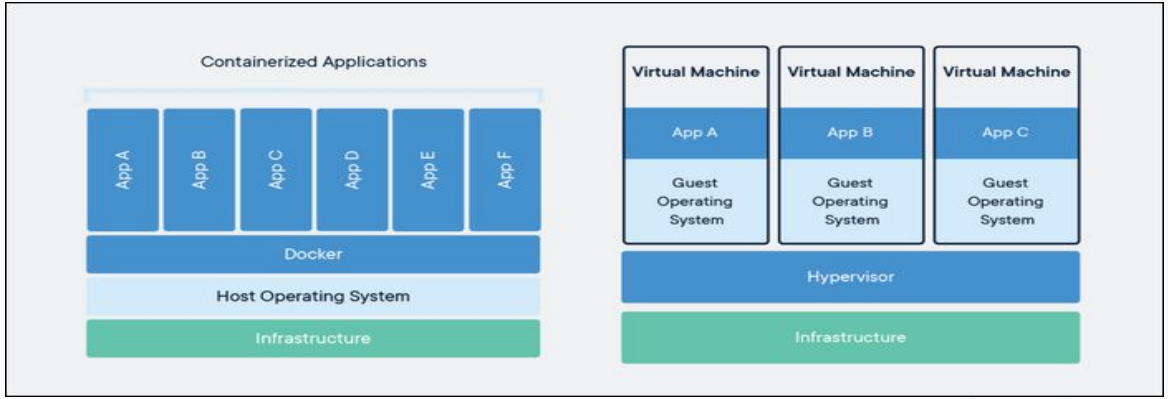


Image Source

Lighter, less isolated

heavier, more isolated

Virtualization - Virtual Environments

- Virtual Environments - handle package and distribution dependencies
  - Conda supports both for Python and R
  - Make your virtual environment now!
  - Store your dependencies in a `requirements.txt` file (or .yml file)
  - Document each installation while doing it not later!

Python

```
> conda create -n py38 python=3.8 jupyter numpy
> conda activate py38
> jupyter notebook
  #Do something, install extra packages
> conda deactivate
```

Setting up different envs showing up in jupyter: tutorial

Virtual Environments - handle package and distribution dependencies

Deeper under the hood:

- Conda has its own version of language distributions
- Each library is a .whl wheel file which is precompiled for your OS
- Many packages included in anaconda, extra packages in community channels
  - https://conda-forge.org/
  - Contribute your own!
- Conda vs pip
  - Pipy is another package manager
  - Avoid mixing them if possible
- Other options:
  - pyenv

Virtualization - Virtual Containers

- Docker Containers - Linux environment, works on all OS
  - Dockerfile: scriptable setup (complex example, simple example)
  - DockerHub: ready-to-go images
    - E.g. postgres database
    - E.g. rocker images
  - Resolve installation mess
  - Deploy, Scale -> Kubernetes

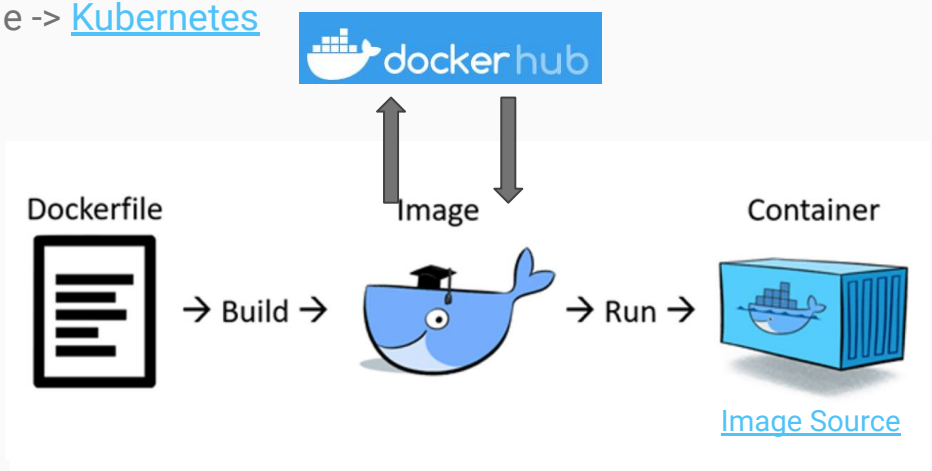


Image Source

https://carpentries-incubator.github.io/docker-introduction/

Virtualization - Other

- Vagrant - virtual machine manager, can run both Docker containers and full VMs
- Virtual Machines - VirtualBox, VMWare
- On Windows: Subsystem for Linux
- Cloud Images - AWS AMIs
- Cloud Container Services
- Terraform: abstract the cloud provider (infrastructure as code)
- ....

Testing

We are already writing tests, need to save them.

Types of testing: unit, integration, system, regression

- Locally
  - Python - nose, pytest, tox

- Remotely - Continuous Integration
  - Github Actions, CircleCI, AppVeyor

Start by testing the environment.

Digital Object Identifiers

README.md

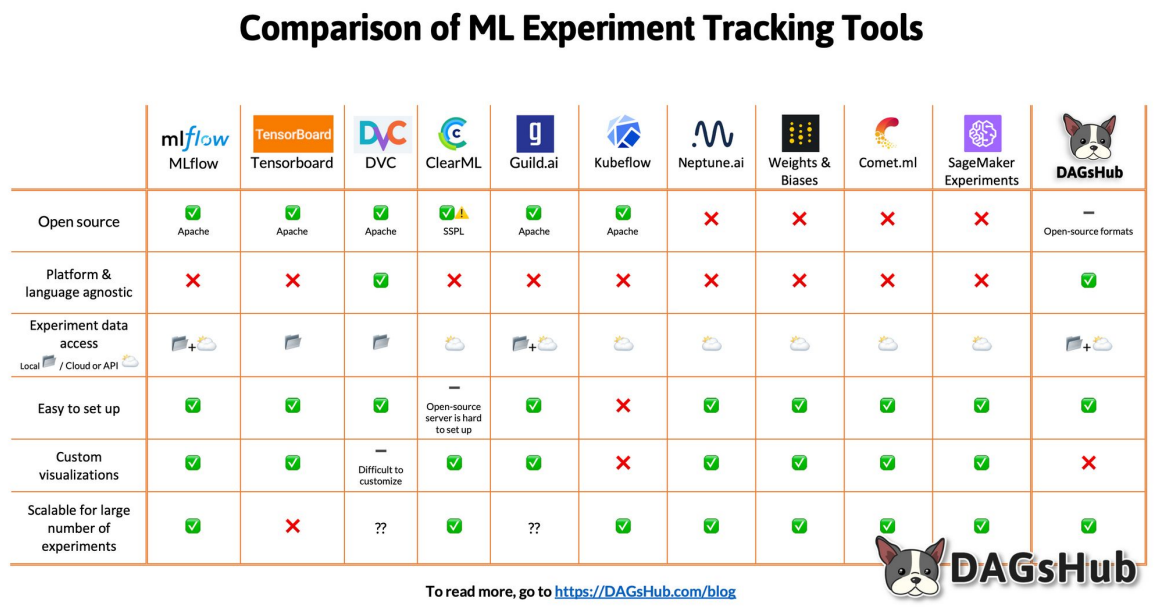
- Articles :
  - Arxiv, preprint server
  - journals create it for you
    - read instructions about journal access
- Slides, Posters:
  - F1000 Research
- Software:
  - For any github repository using Zenodo
  - Register releases
- Datasets:
  - Persistent repositories provide DOI

Machine Learning Reproducibility

Field	Paper	Number of papers reviewed	Number of papers with pitfalls	[L1.1] No test set	[L1.2] Pre-proc. on train-test	[L1.3] Feature sel. on train-test	[L1.4] Duplicates	[L2] Illegitimate features	[L3.1] Temporal leakage	[L3.2] Non-ind. b/w train-test	[L3.3] Sampling bias	Comput. reproducibility issues	Data quality issues	Metric choice issues	Standard dataset used?
Medicine	Bouwmeester et al. (2012)	71	27	○								○			
Neuroimaging	Whelan & Garavan (2014)	–	14	○		○									
Autism Diagnostics	Bone et al. (2015)	–	3				○				○	○	○	○	
Bioinformatics	Blagus & Lusa (2015)	–	6		○										
Nutrition Research	Ivanescu et al. (2016)	–	4	○								○	○		
Software Eng.	Tu et al. (2018)	58	11					○			○	○		○	
Toxicology	Alves et al. (2019)	–	1				○				○	○			
Satellite Imaging	Nalepa et al. (2019)	17	17						○			○		○	
Tractography	Poulin et al. (2019)	4	2	○							○	○	○	○	
Clinical Epidem.	Christodoulou et al. (2019)	71	48			○						○			
Brain-computer Int.	Nakanishi et al. (2020)	–	1	○										○	
Histopathology	Oner et al. (2020)	–	1						○						
Neuropsychiatry	Poldrack et al. (2020)	100	53	○	○							○	○		
Medicine	Vandewiele et al. (2021)	24	21			○				○	○	○	○		○
Radiology	Roberts et al. (2021)	62	62	○			○				○	○			○
IT Operations	Lyu et al. (2021)	9	3					○							○
Medicine	Filho et al. (2021)	–	1						○						
Neuropsychiatry	Shim et al. (2021)	–	1			○					○				
Genomics	Barnett et al. (2022)	41	23			○						○			
Computer Security	Arp et al. (2022)	30	30	○	○	○		○		○	○	○	○		

Kapoor S. and Narayan A.,Leakage and the Reproducibility Crisis in ML-based Science

Experiment Tracking



Comparison of ML Experiment Tracking Tools

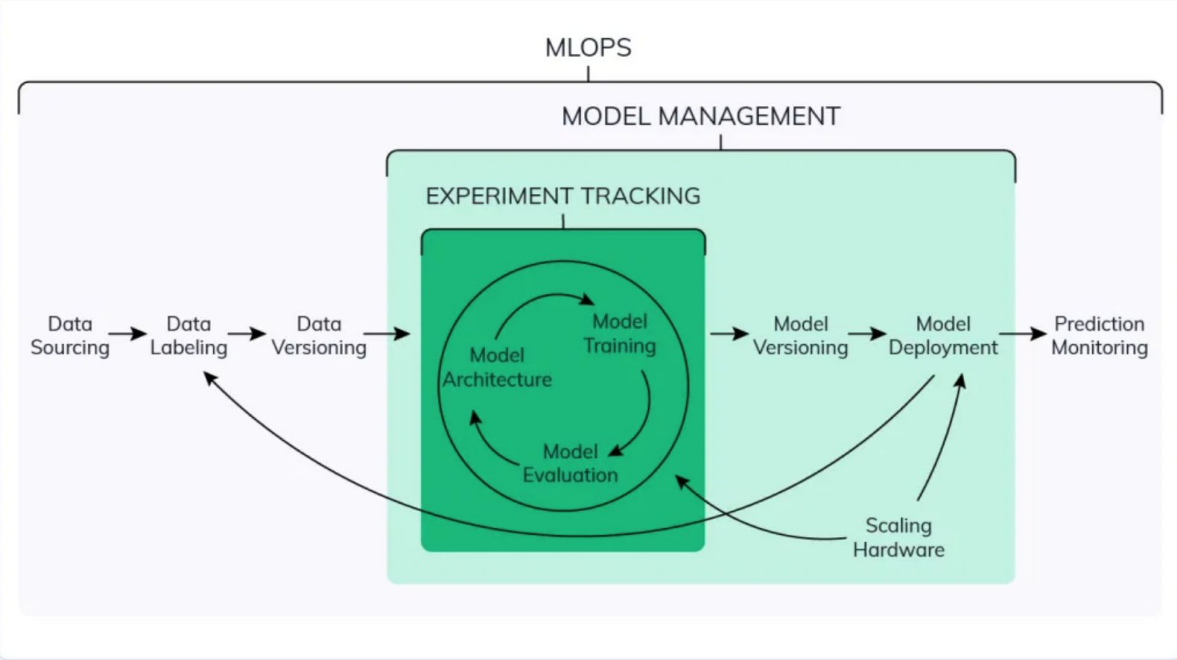
	MLflow	Tensorboard	DVC	ClearML	Guild.ai	Kubeflow	Neptune.ai	Weights & Biases	Comet.ml	SageMaker Experiments	DAGsHub
Open source	✅ Apache	✅ Apache	✅ Apache	✅⚠ SSPL	✅ Apache	✅ Apache	❌	❌	❌	❌	– Open-source formats
Platform & language agnostic	❌	❌	✅	❌	❌	❌	❌	❌	❌	❌	✅
Experiment data access (Local / Cloud or API)	+				+						+
Easy to set up	✅	✅	✅	– Open-source server is hard to set up	✅	❌	✅	✅	✅	✅	✅
Custom visualizations	✅	✅	– Difficult to customize	✅	✅	❌	✅	✅	✅	✅	❌
Scalable for large number of experiments	✅	❌	??	✅	??	✅	✅	✅	✅	✅	✅

To read more, go to https://DAGsHub.com/blog

DAGsHub

- Explosion of ML experiment tracking tools

Experiment Tracking



Source: [neptune.ai]

- Explosion of ML experiment tracking tools
- Some tools can be used for general experiment tracking (non ML analysis)

Data Repositories

zenodo	DRYAD	figshare	IEEE DataPort
Up to 50GB free Not-for-profit - EU funded (contact if more)	Publishing Fee - $120 Excess fees after 50GB Associated with articles Not-for-profit	20GB free per manuscript Institutional plans For-profit	Up to 2TB Subscription Based Free Promo Codes

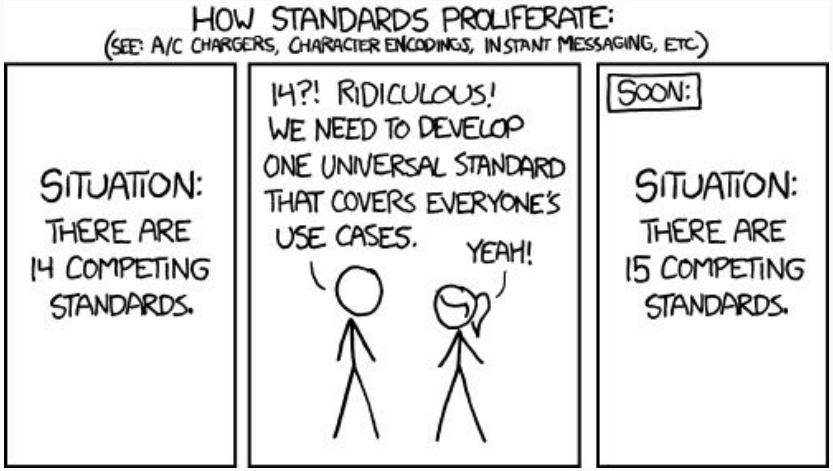
- Datasets receive Digital Object Identifier (DOI)
- Cloud Storage: free to upload, fees for storage, higher fees to download
  - Some public datasets can be stored for free: https://registry.opendata.aws/
- Nature Journal Scientific Data: https://www.nature.com/sdata/

Data and Metadata

'FAIR Guiding Principles for scientific data management and stewardship', Wilkinson et.al, Nature Scientific Data, 2016

The CARE Principles for Indigenous Data Governance

Standardization



- Try using standard formats whenever possible!
- If format does not fit your case discuss with the community! ISO, NIST
- Often standards are more permissive than data formats!
- Interoperability
- Persistency

Standardization: examples

Example 1: you have pulled some environmental data for a regions and you want to organize it so that it is easy for other researchers to analyse it

- Store it in excel sheets
- Store it in csv files
- Check how the data for other states is stored and store it the same format
- Check out if there are standards for this type of data (e.g. Climate and Forecast Conventions)

Example 2: you want to save a Deep Learning model so you can apply to future data:

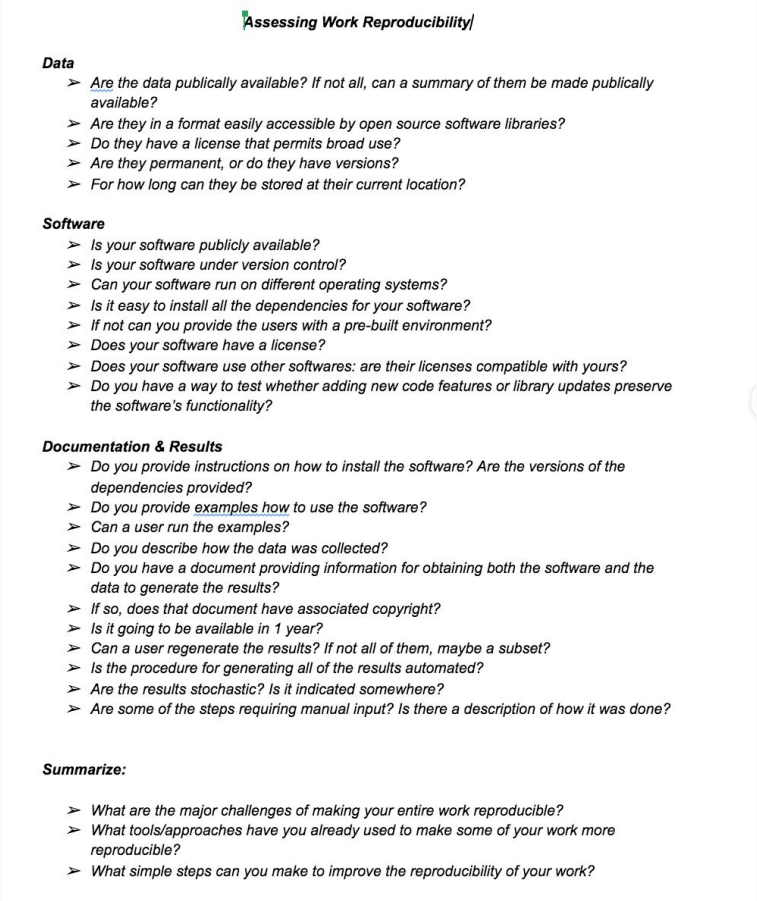
- Python pickle file (Python specific, sometimes version dependent)
- HDF format (Python and domain independent, local database: but fields are not standardized)
- Tensorflow HDF (libraries come and go)
- ONNX (Open Neural Network Exchange) format (library/language independent, stores the ‘math’, i.e. the computational graph operations, hardware)

Beyond exact reproducibility

- Design your study
- Register Hypothesis
- Create a Baseline
- Test simple scenarios first
- Test different methods
- Understand your errors:
  - Precision Recall Curves:
    - Baseline changes for different class distributions
  - Cross-validation with dependence in time series and groups
    - https://scikit-learn.org/stable/modules/cross_validation.html
  - Multiple Testing Problem
    - The more hypotheses we are testing, the more likely one of them will be falsely true

What about your projects?

Reproducibility Checklist:



Assessing Work Reproducibility

Data

- *Are the data publically available? If not all, can a summary of them be made publically available?*
- *Are they in a format easily accessible by open source software libraries?*
- *Do they have a license that permits broad use?*
- *Are they permanent, or do they have versions?*
- *For how long can they be stored at their current location?*

Software

- *Is your software publicly available?*
- *Is your software under version control?*
- *Can your software run on different operating systems?*
- *Is it easy to install all the dependencies for your software?*
- *If not can you provide the users with a pre-built environment?*
- *Does your software have a license?*
- *Does your software use other softwares: are their licenses compatible with yours?*
- *Do you have a way to test whether adding new code features or library updates preserve the software's functionality?*

Documentation & Results

- *Do you provide instructions on how to install the software? Are the versions of the dependencies provided?*
- *Do you provide examples how to use the software?*
- *Can a user run the examples?*
- *Do you describe how the data was collected?*
- *Do you have a document providing information for obtaining both the software and the data to generate the results?*
- *If so, does that document have associated copyright?*
- *Is it going to be available in 1 year?*
- *Can a user regenerate the results? If not all of them, maybe a subset?*
- *Is the procedure for generating all of the results automated?*
- *Are the results stochastic? Is it indicated somewhere?*
- *Are some of the steps requiring manual input? Is there a description of how it was done?*

Summarize:

- *What are the major challenges of making your entire work reproducible?*
- *What tools/approaches have you already used to make some of your work more reproducible?*
- *What simple steps can you make to improve the reproducibility of your work?*

Built upon:
Assessing Reproducibility

Survey

Survey

Thanks!