

DATA MANAGEMENT WITH DATALAD

AN INTRODUCTION

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Institute of Neuroscience and Medicine, Brain & Behavior (INM-7)
Research Center Jülich

Slides: <https://github.com/datalad-handbook/course/>

WHAT IS (RESEARCH) DATA MANAGEMENT?

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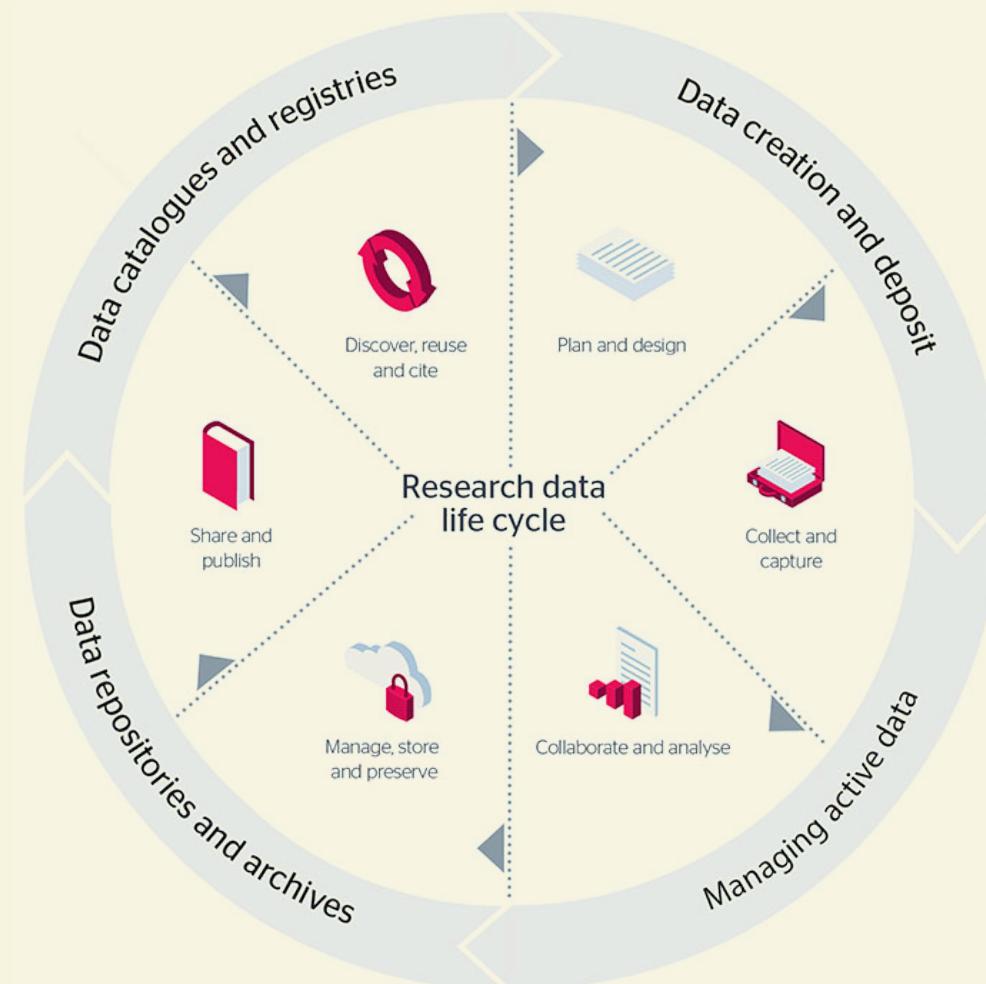
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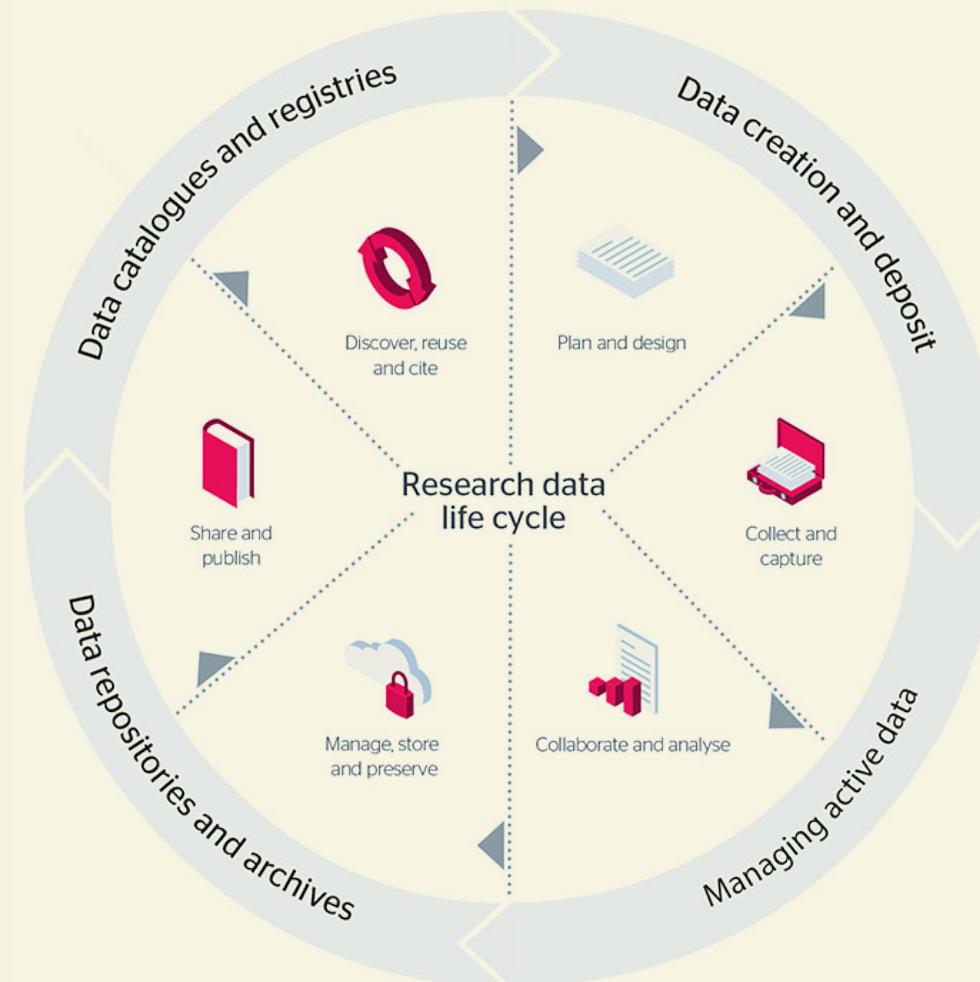
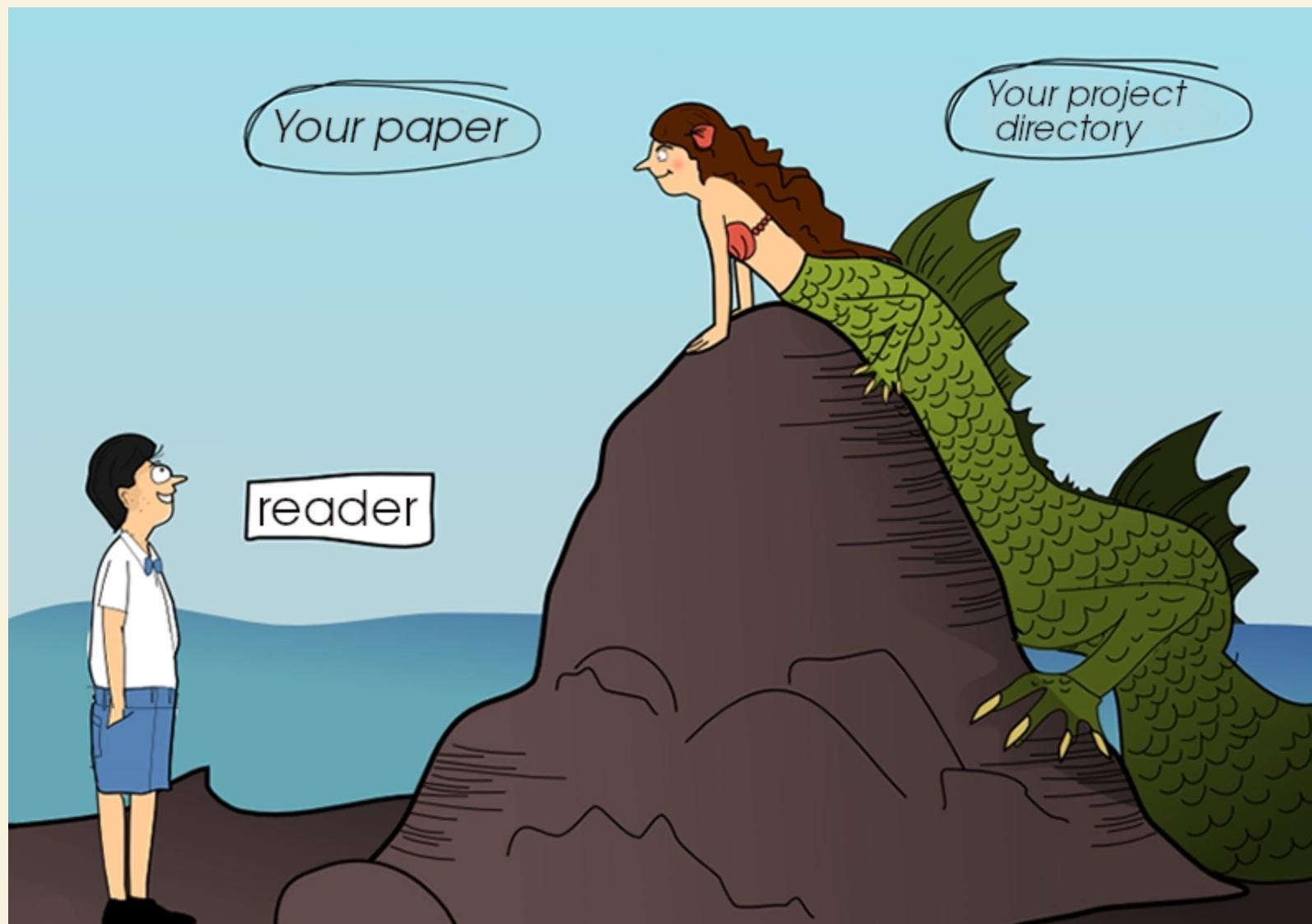


Image credit: JISC; CC-BY-SA-ND

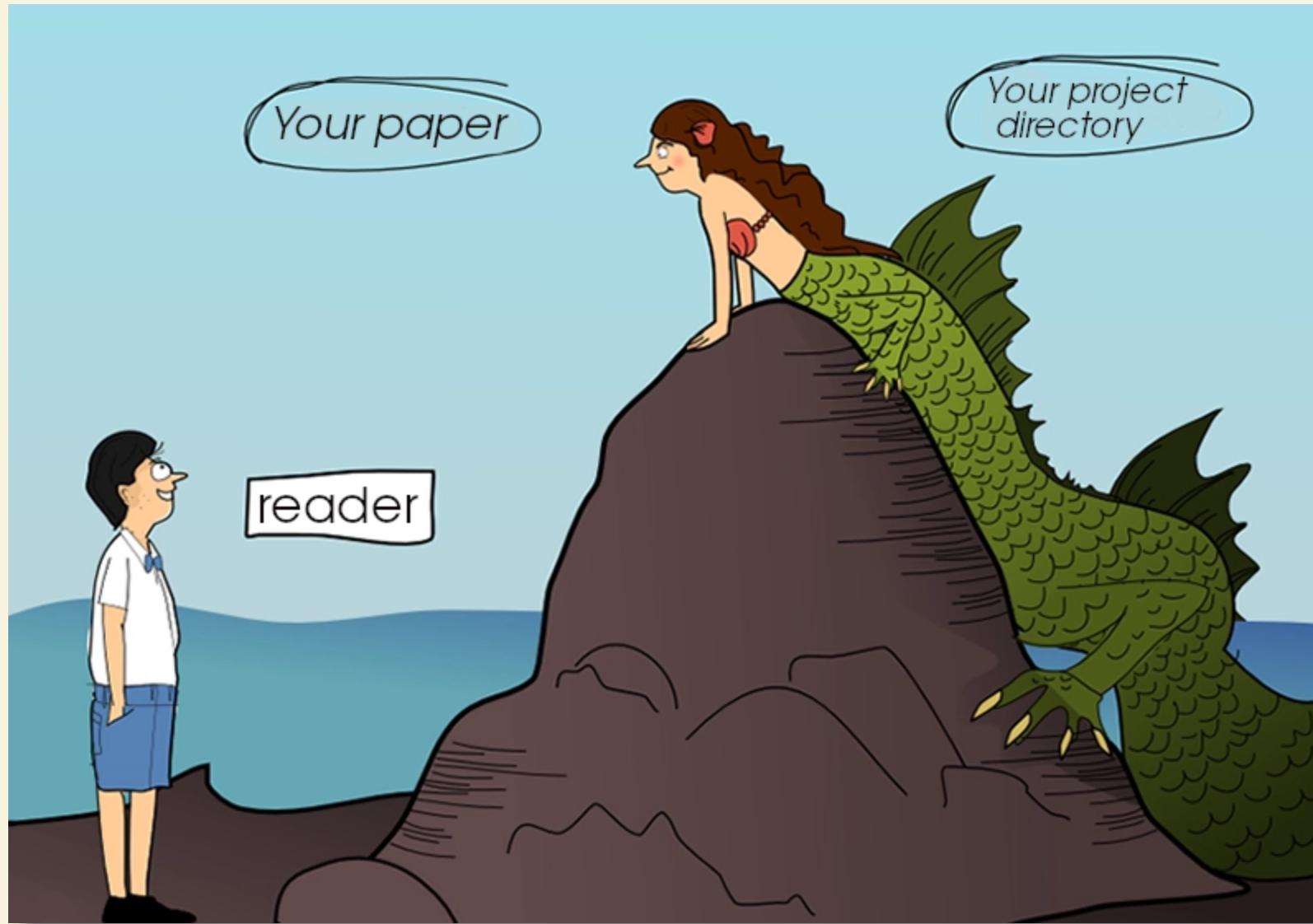
- Research data management is a key component for reproducibility, efficiency, and impact/reach of data analysis projects

WHY DATA MANAGEMENT?



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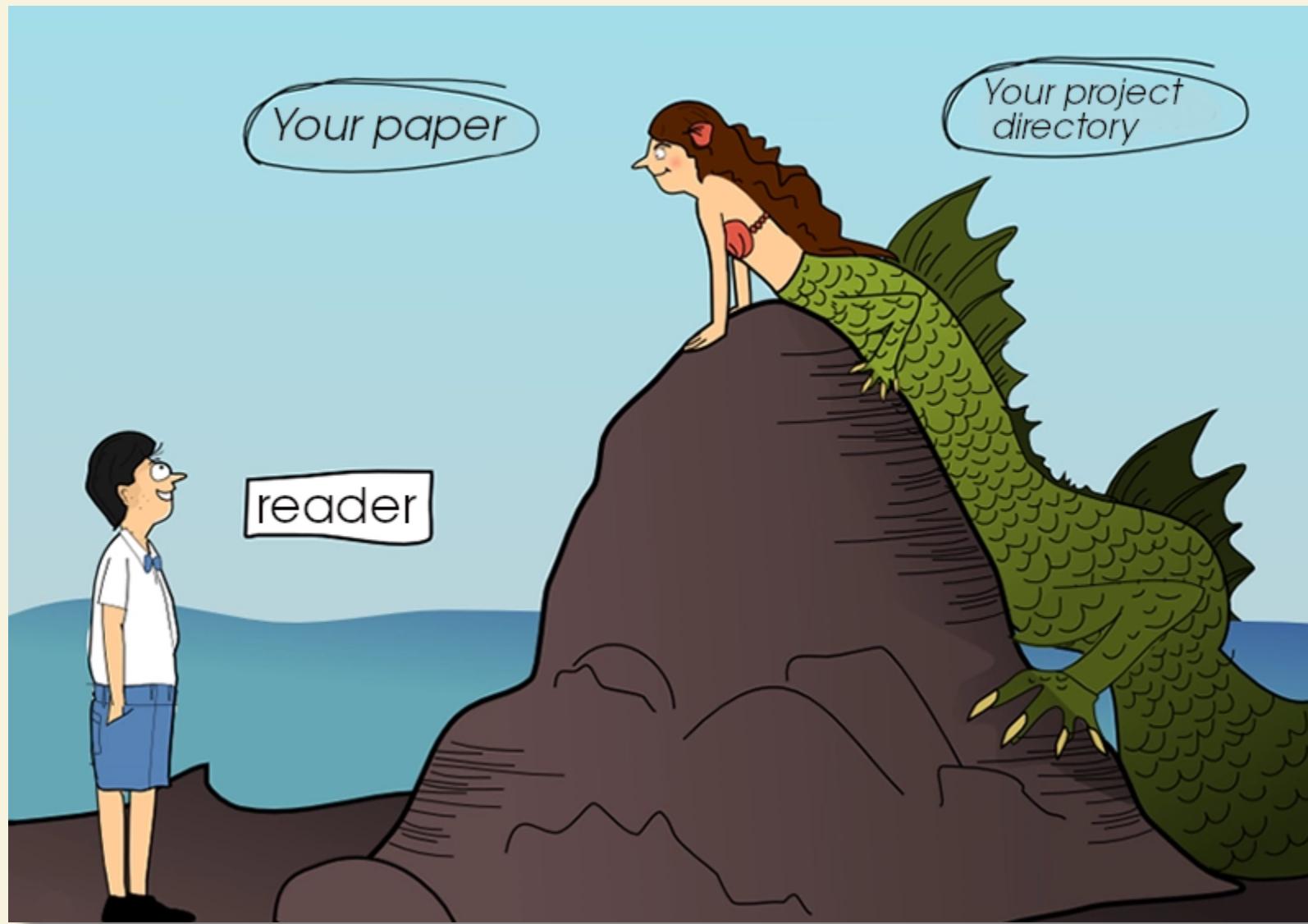
Image credit: adapted from <https://dribbble.com/shots/3090048-Front-end-vs-Back-end>



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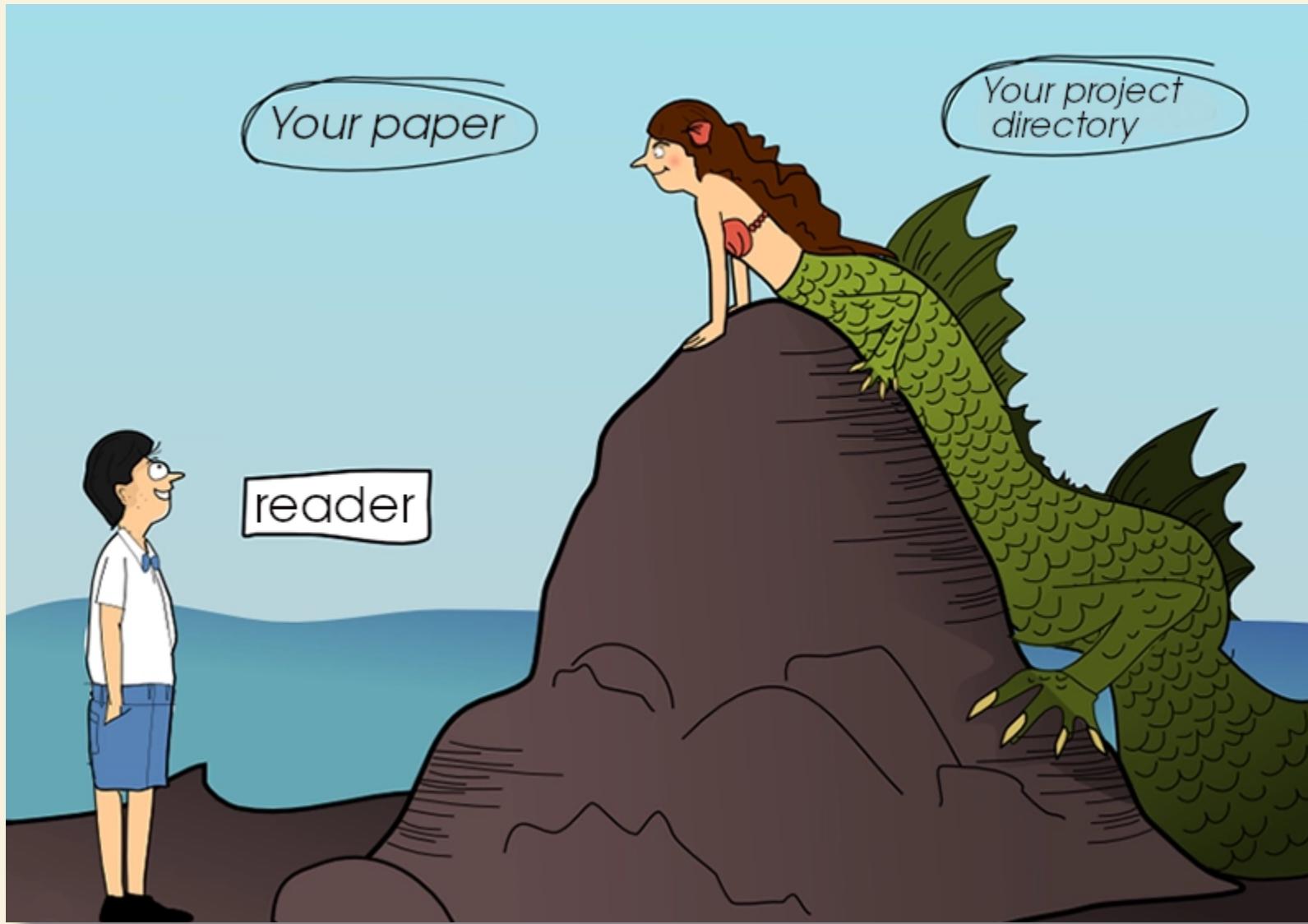
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THE MOST INTERESTING DATASETS OF OUR FIELD REQUIRE IT!



Image credit: https://infostory.files.wordpress.com/2013/03/big_data_cartoon.jpeg

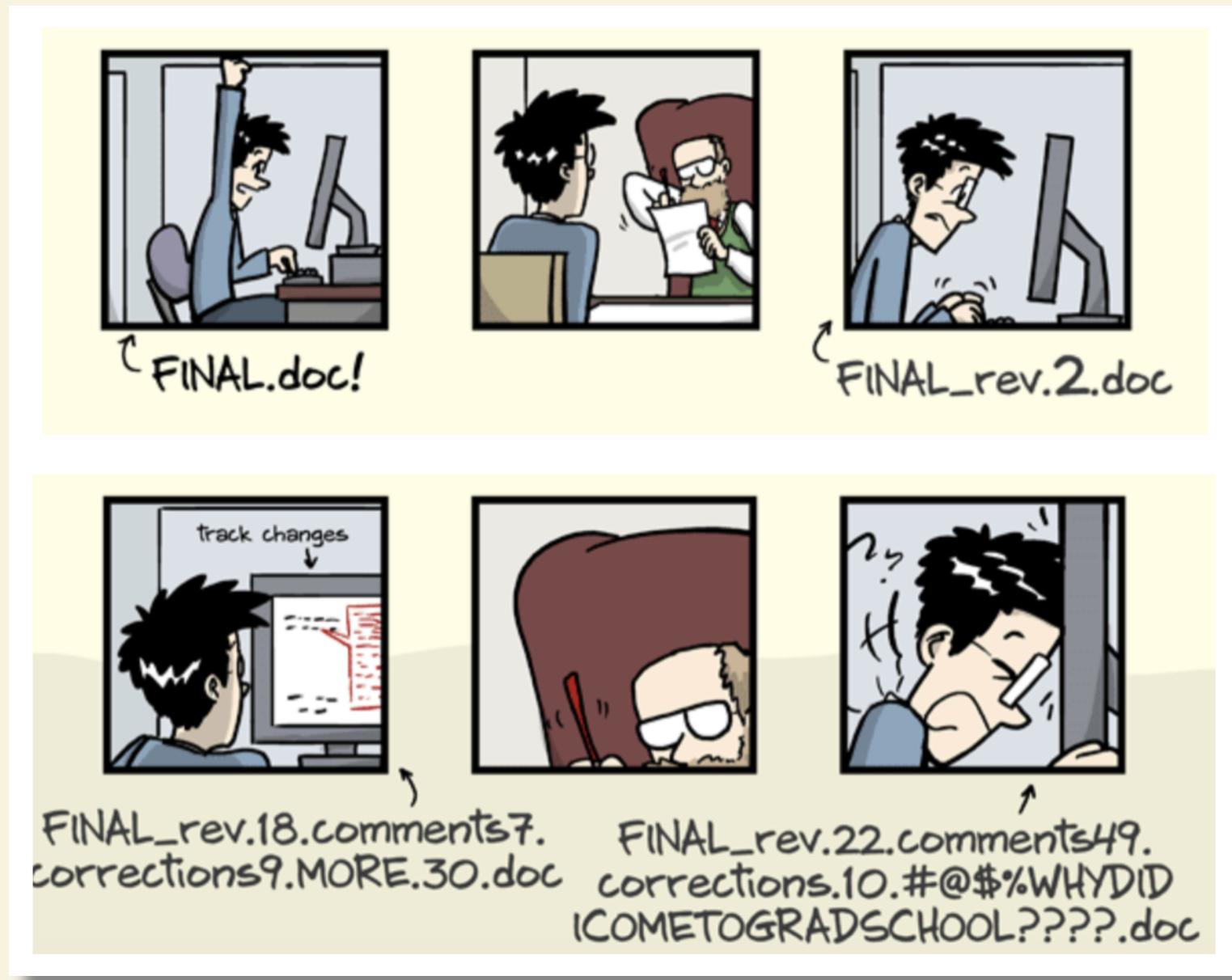
- Exciting datasets (UKBiobank, HCP, ...) are orders of magnitudes larger than previous public datasets, and neither the computational infrastructure nor analysis workflows scale to these dataset sizes.

HOW IS (RESEARCH) DATA MANAGEMENT POSSIBLE?

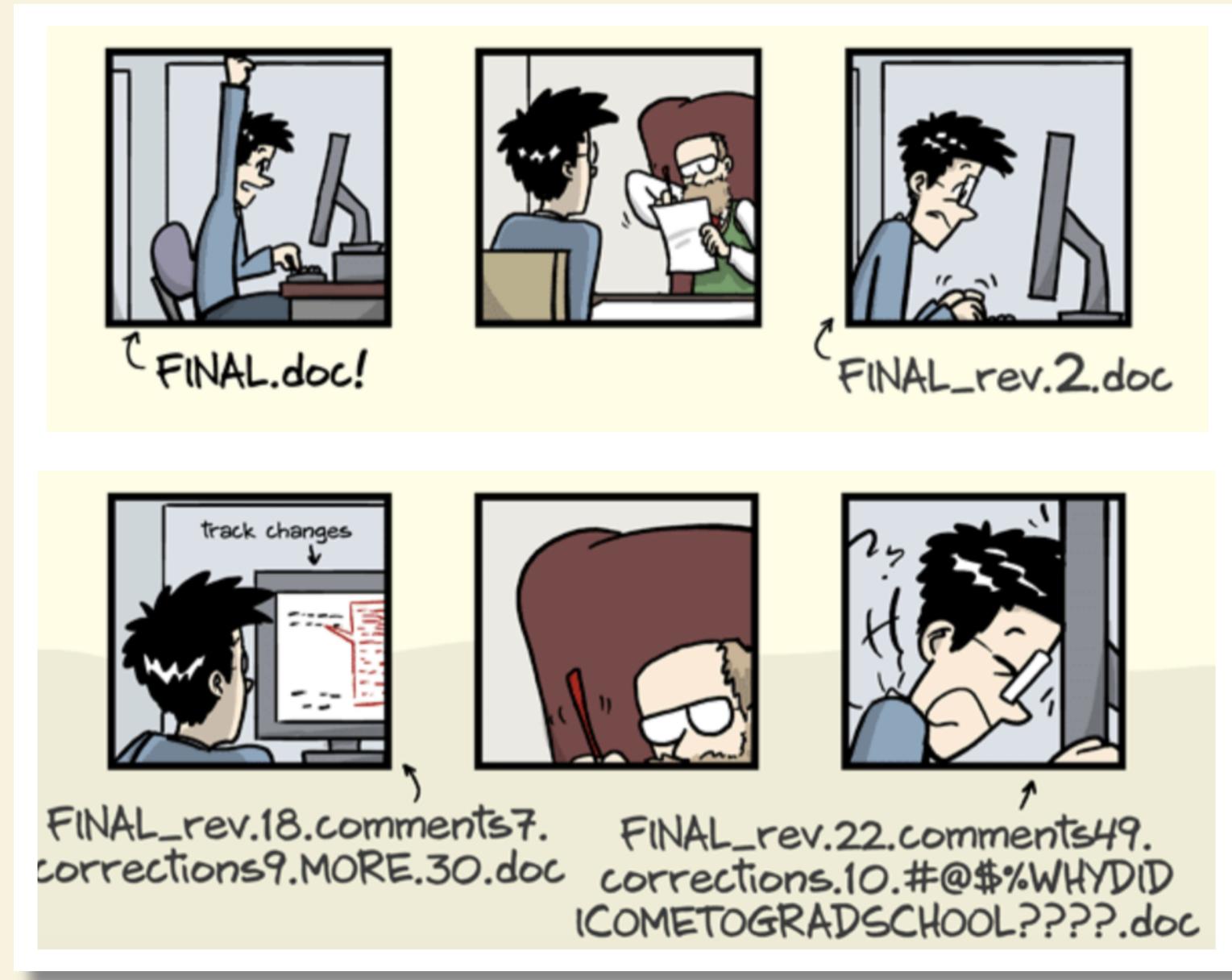
There are tools and concepts that can help:

- **Version control** your data
- **Document everything**, ideally automatically (Provenance capture)

WHY VERSION CONTROL?

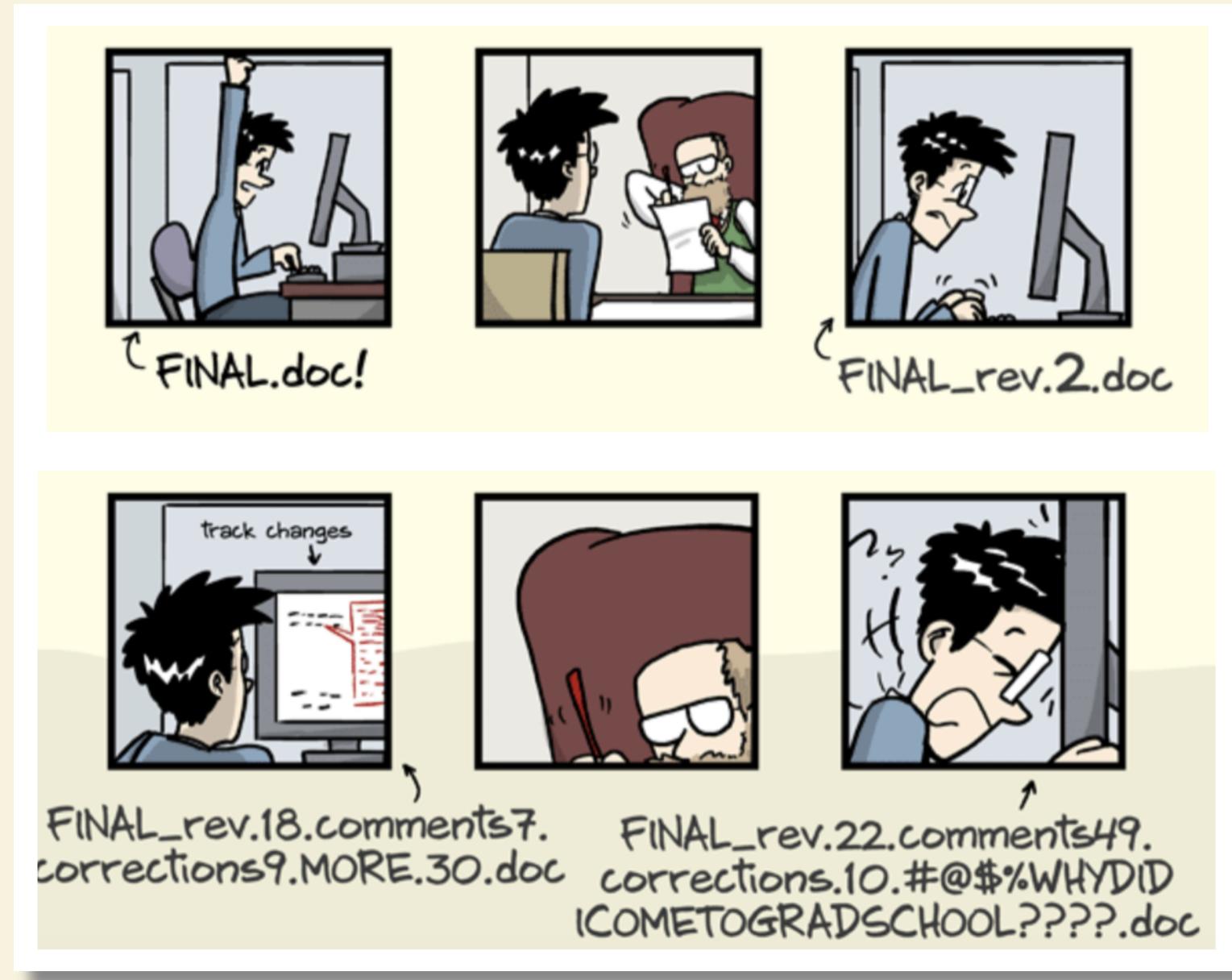


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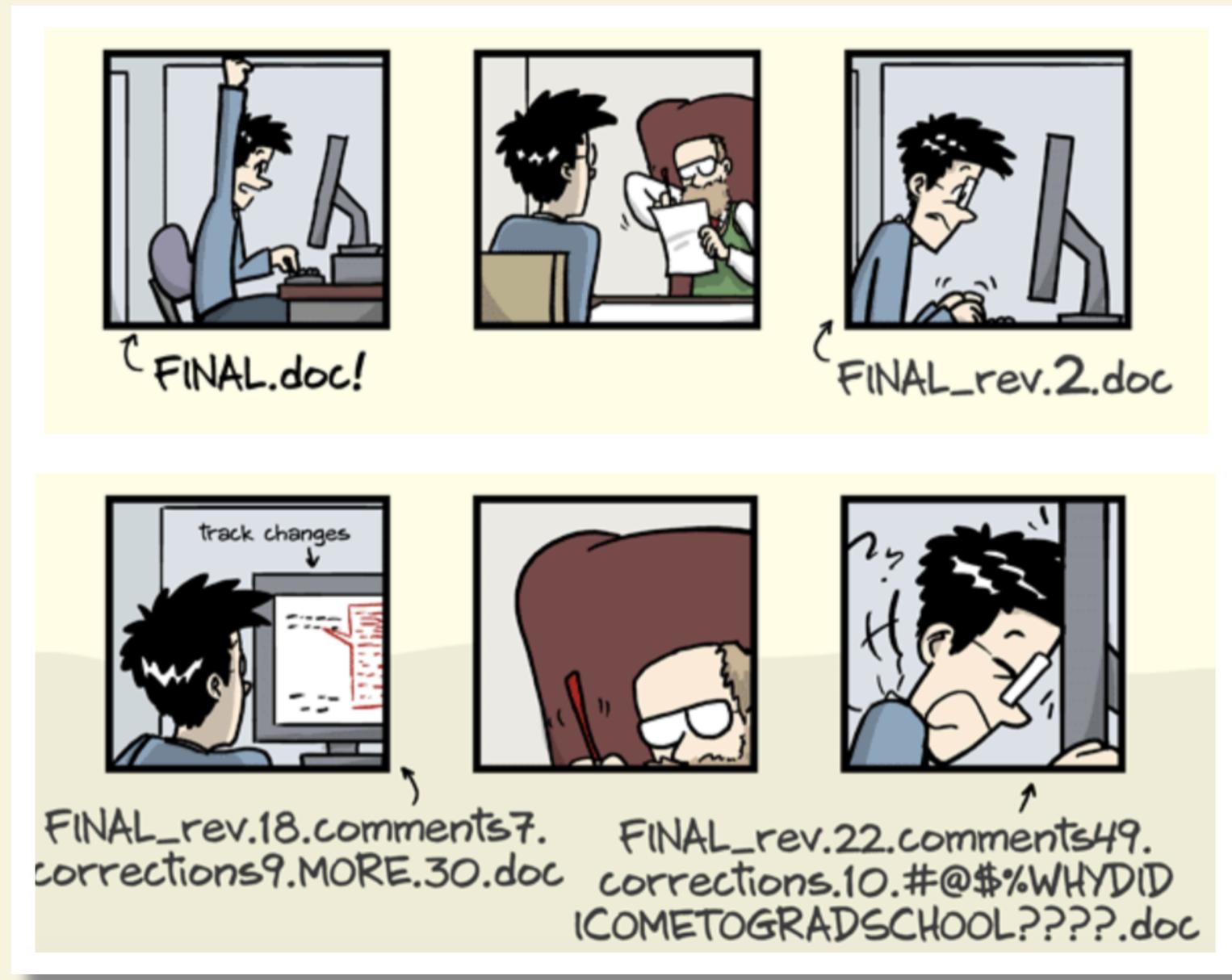
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WHY VERSION CONTROL?



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- keep track of changes

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- Mostly done for code, but data changes as well!

WHY PROVENANCE CAPTURE?

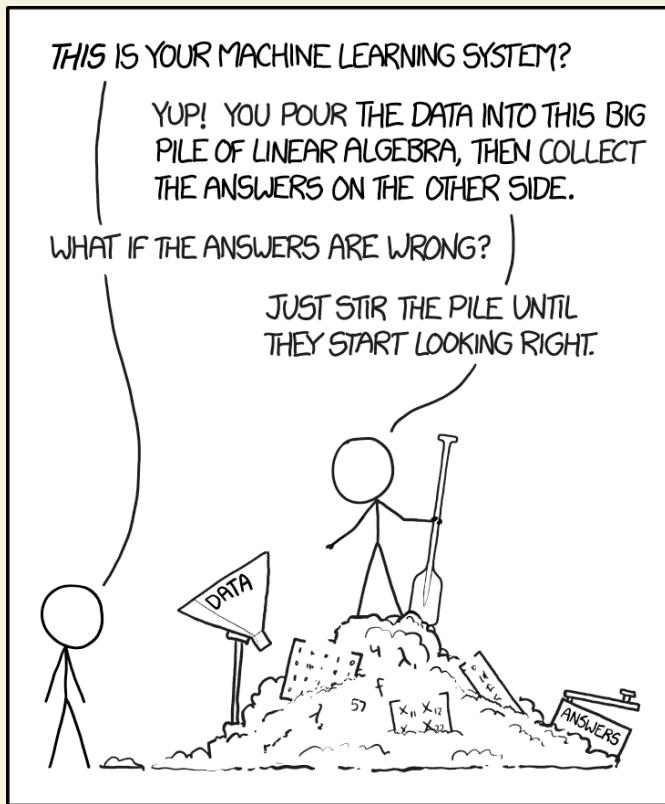


Image credit: <https://xkcd.com/1838/>

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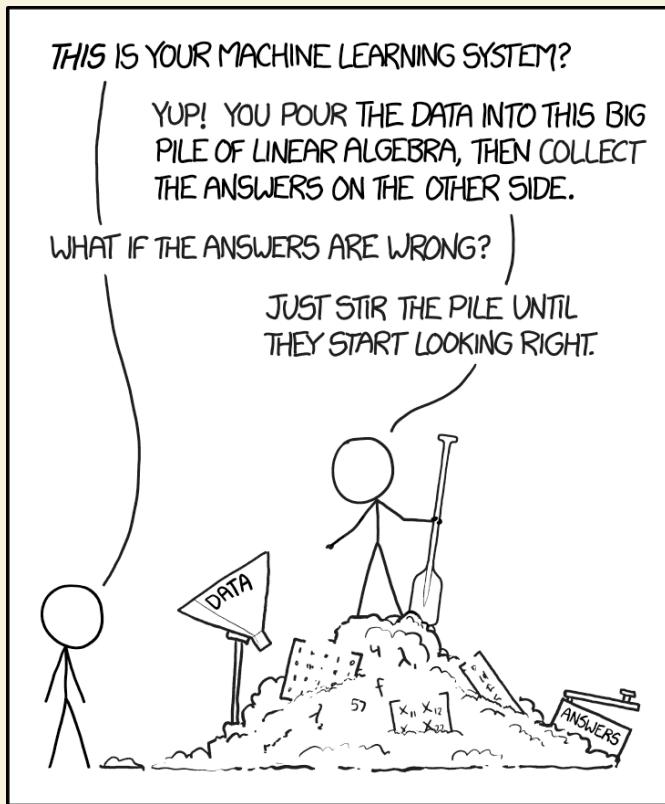


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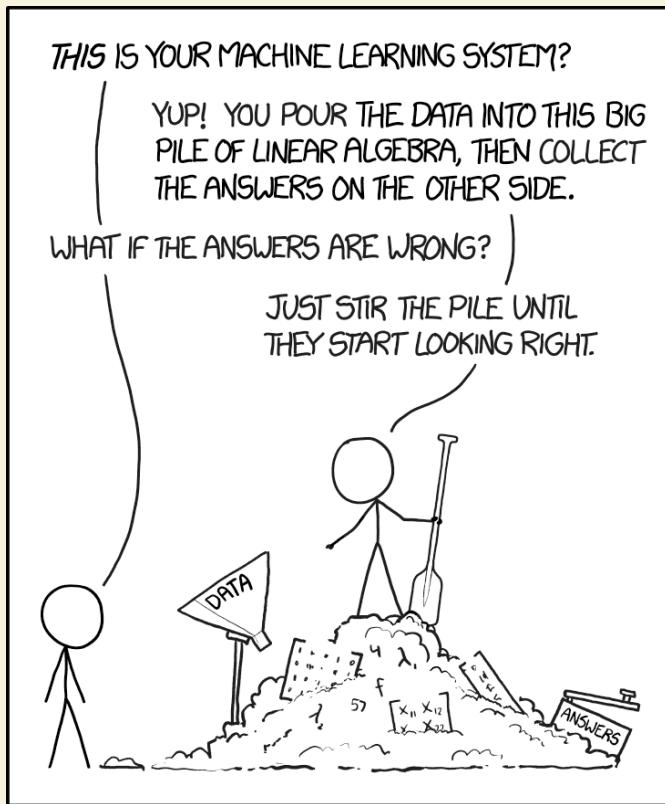


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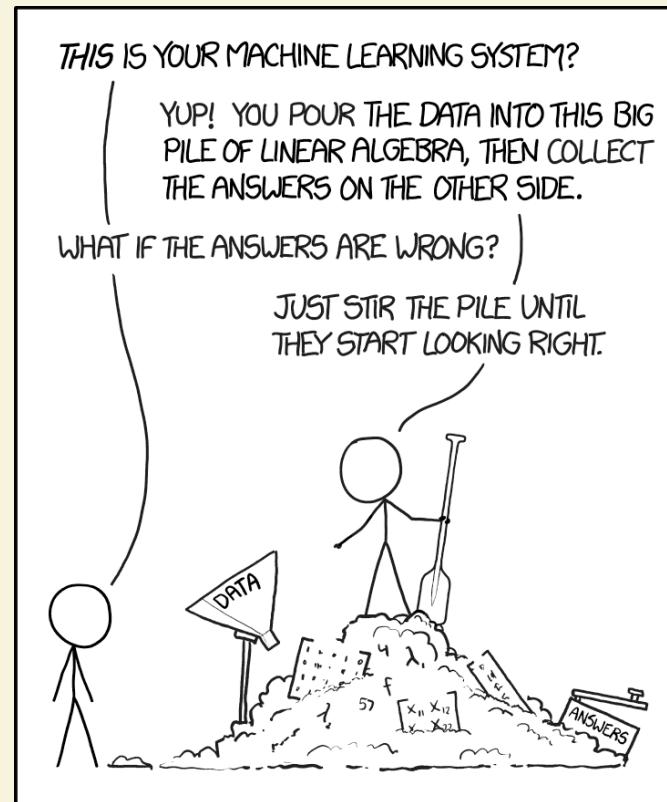


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 - Which (version of which) data was used, and where does this input data come from?
 - Which scripts with which parameters created which results, and how?
 - What is the software (libraries, environment) used for a computation and its dependencies to data or code?

DATALAD CAN HELP WITH DATA MANAGEMENT



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What is it?

Why should I use it?

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What is it?

Why should I use it?

How can I use it?



DataLad is a data management multitool.



Let's see it in action

REPRODUCIBLE PAPER - A MAGIC TRICK?

If curious, you can read up all the details and a step-by-step instruction [here](#).

Data Lad IN BRIEF

- A command-line tool, available for all major operating systems (Linux, macOS/OSX, Windows)
- Build on top of **Git** and **Git-annex**
- **Allows...**
 - ... version-controlling arbitrarily large content,
 - ... easily sharing and obtaining data (note: no data hosting!),
 - ... (computationally) reproducible data analysis,
 - ... and *much* more
- Completely domain-agnostic

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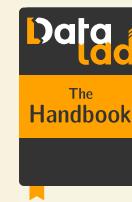
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☞ For more: Read the DataLad Handbook



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 - Datasets can be nested: *linked subdirectories*

EXPERIENCE A DATALAD DATASET

Code to follow along:

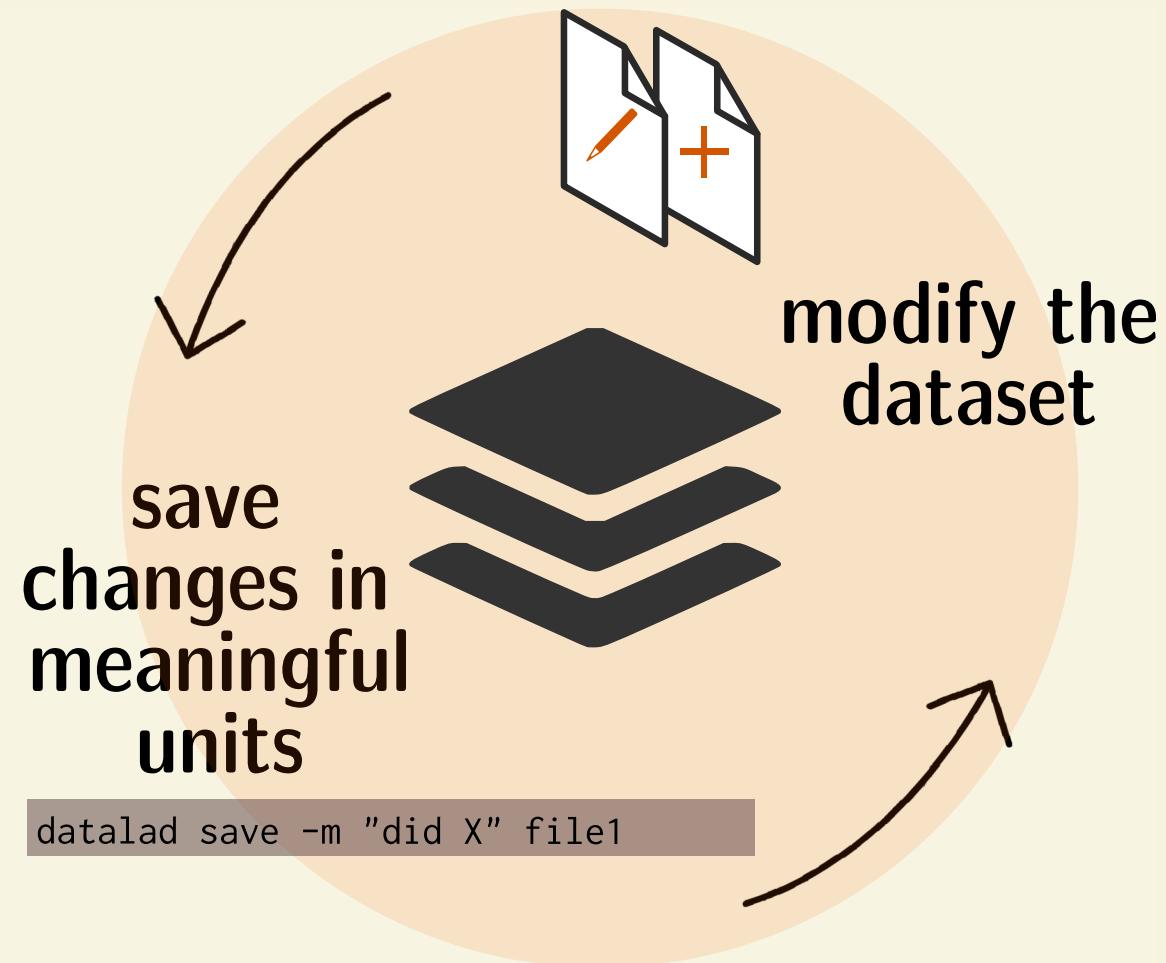
http://handbook.datalad.org/en/latest/code_from_chapters/01_dataset_basics_code.html

LOCAL VERSION CONTROL

Procedurally, version control is easy with DataLad!

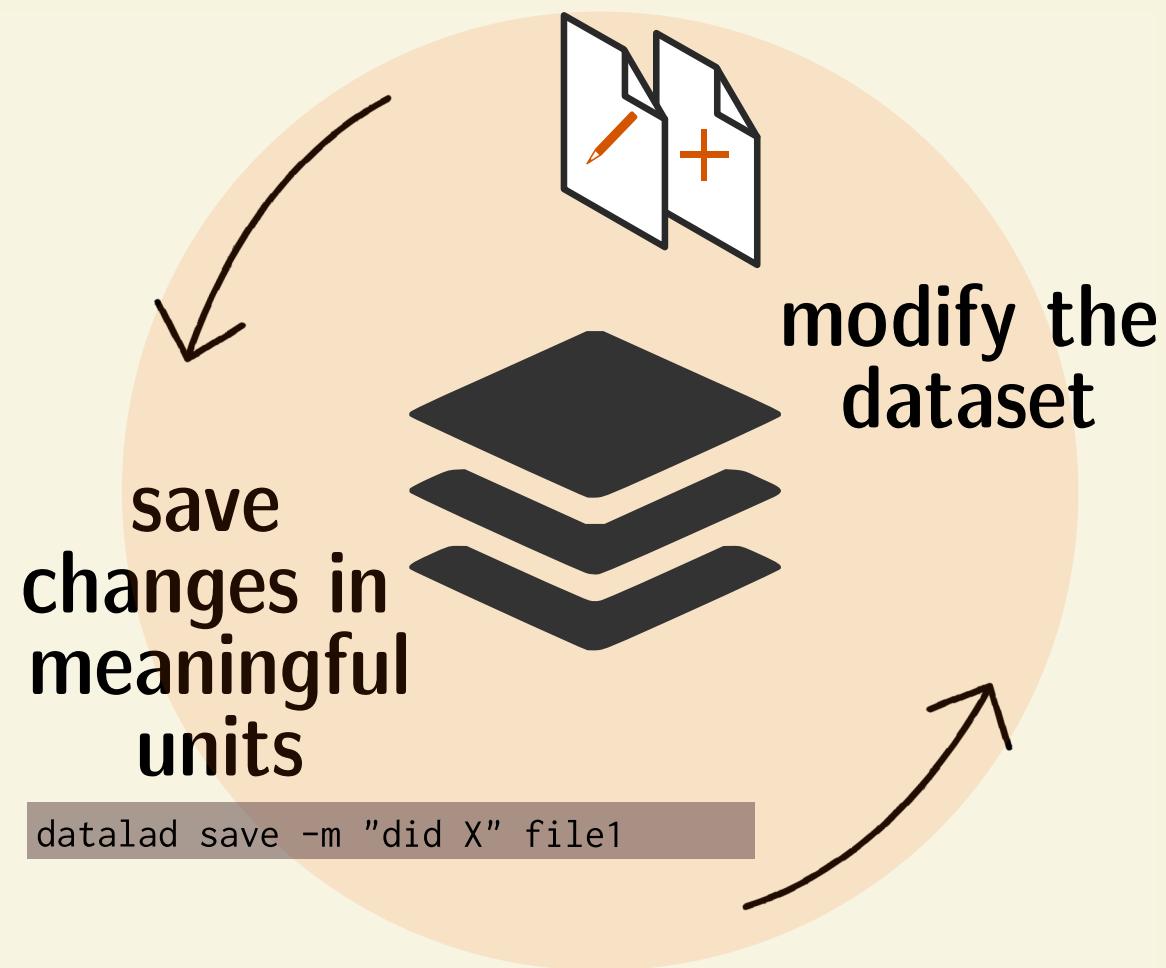
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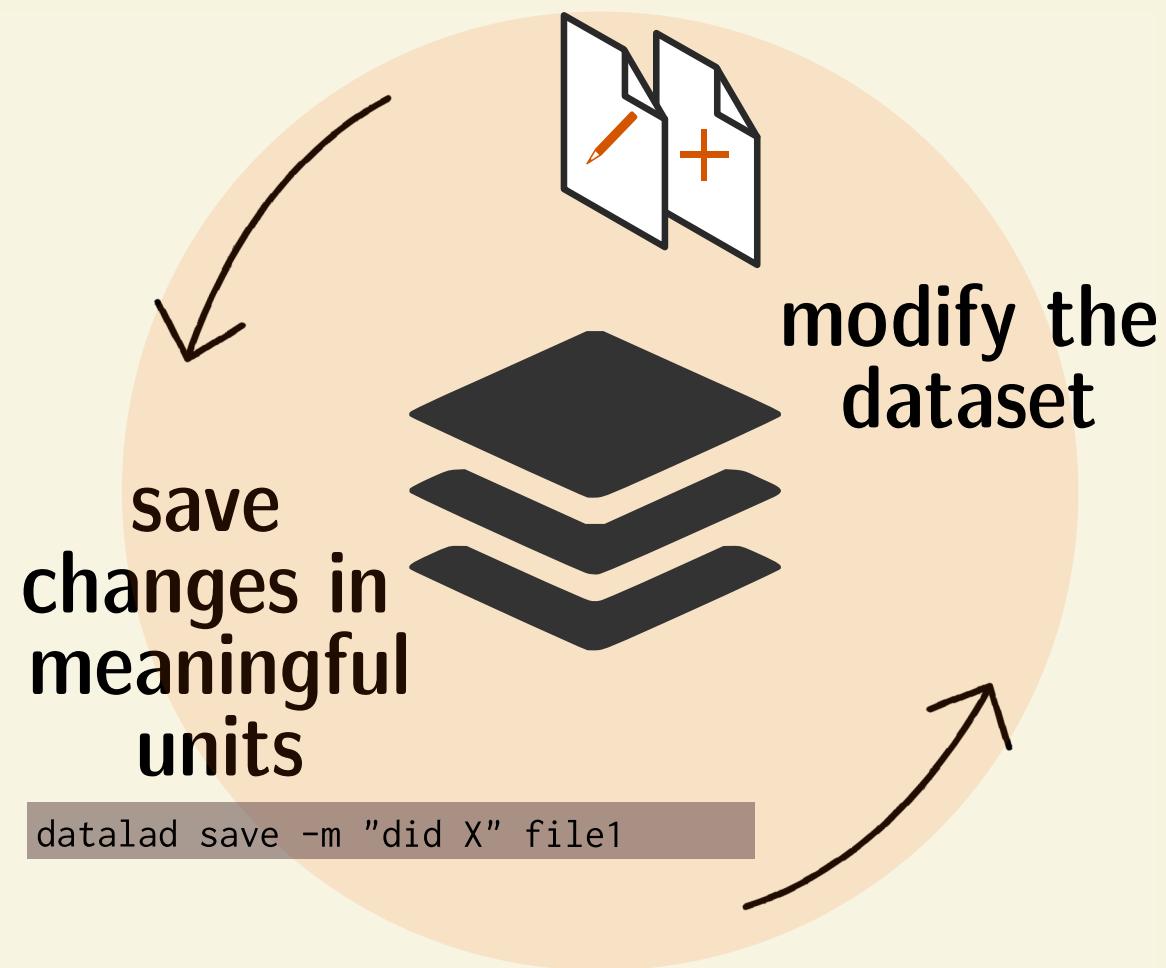
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Advice:

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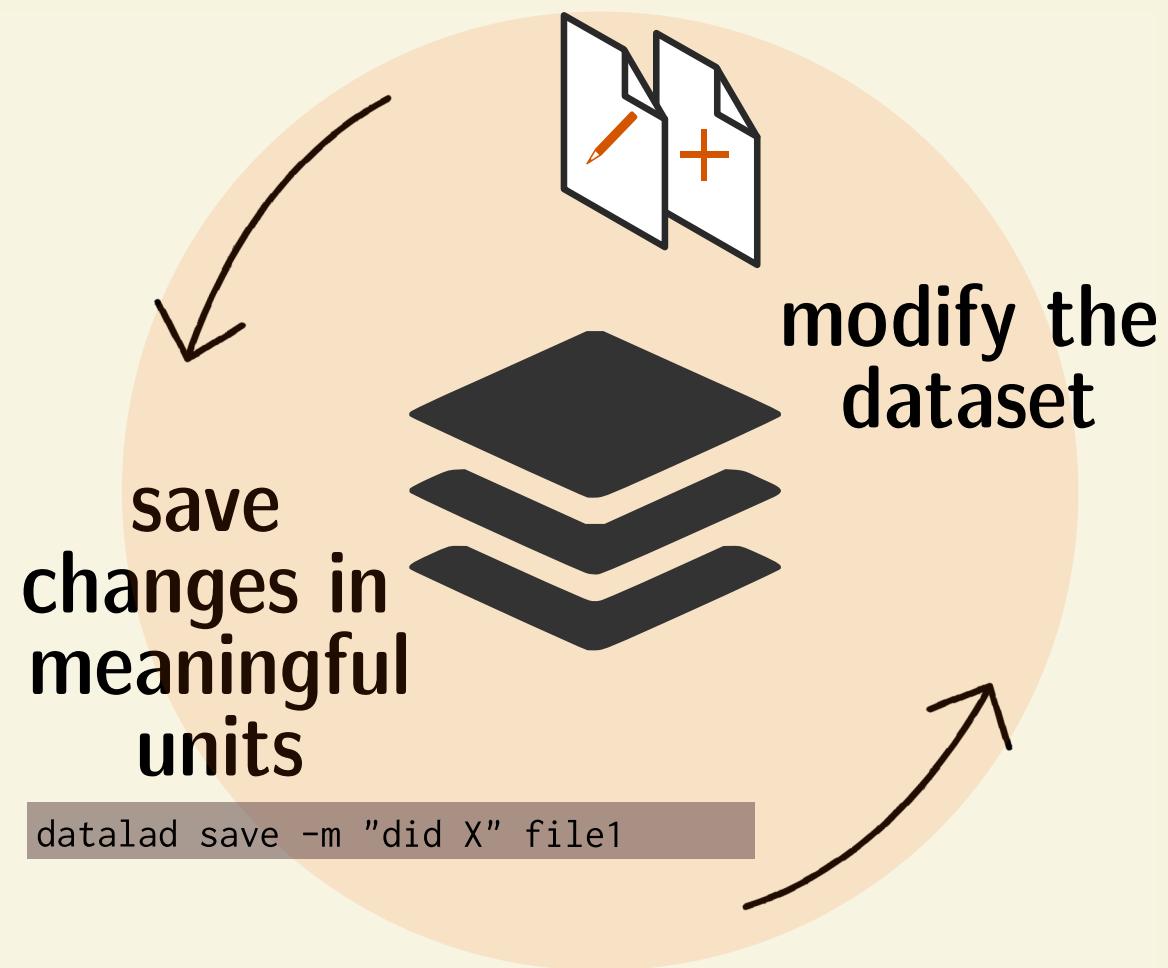


- Save *meaningful* units of change

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- Advice:**
- Save *meaningful* units of change
 - Attach helpful commit messages

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A clean dataset status is good practice.

FROM HERE

"FINAL".doc



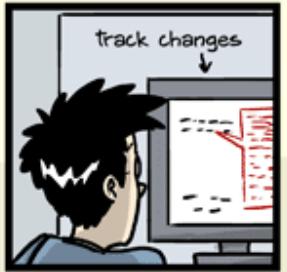
FINAL.doc!

FINAL_rev.2.doc



FINAL_rev.6.COMMENTS.doc

FINAL_rev.8.comments5.
CORRECTIONS.doc

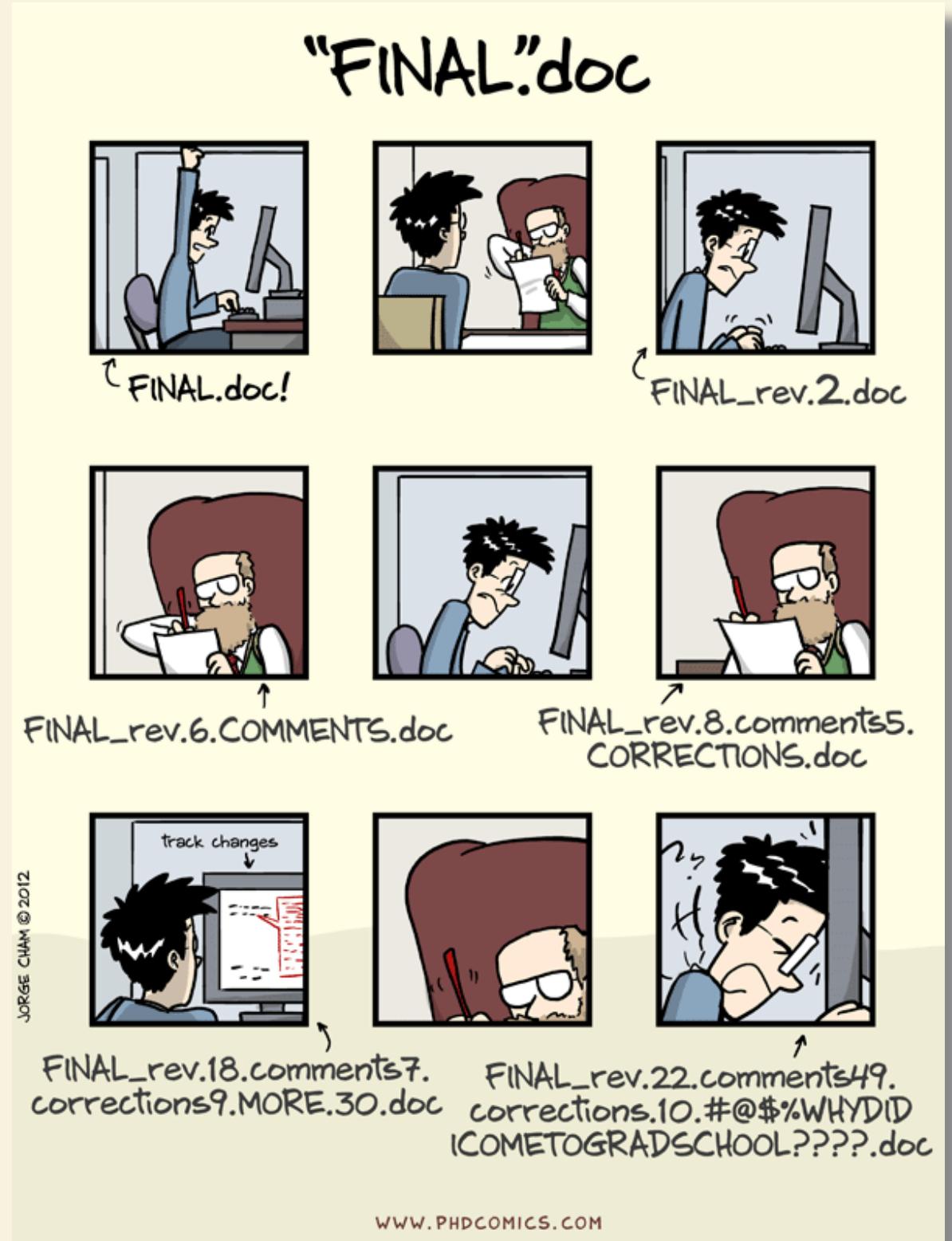


JORGE CHAM © 2012

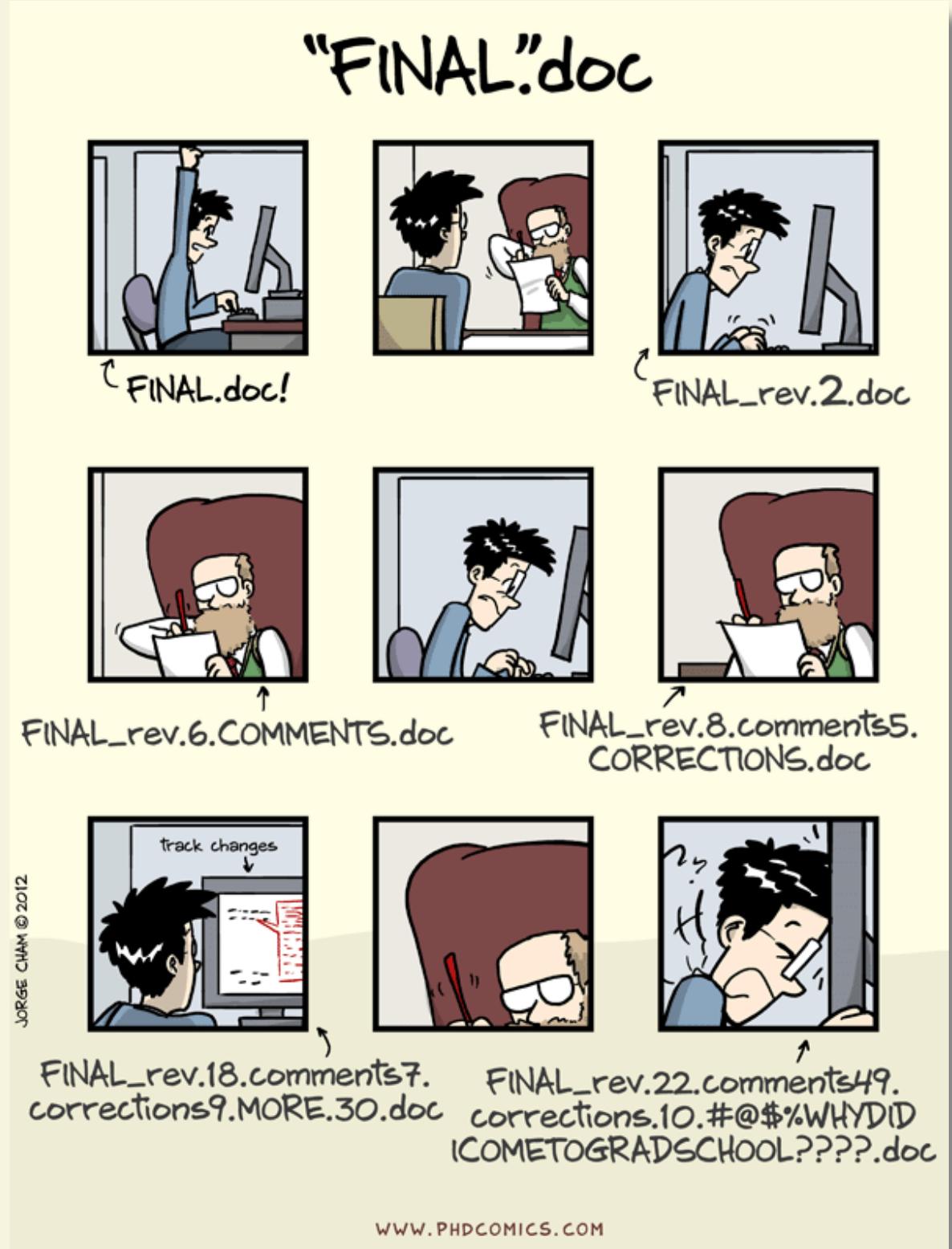
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corrections9.MORE.30.doc

FINAL_rev.22.comments49.
corrections.10.#@\$%WHYDID
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FROM HERE TO THIS:



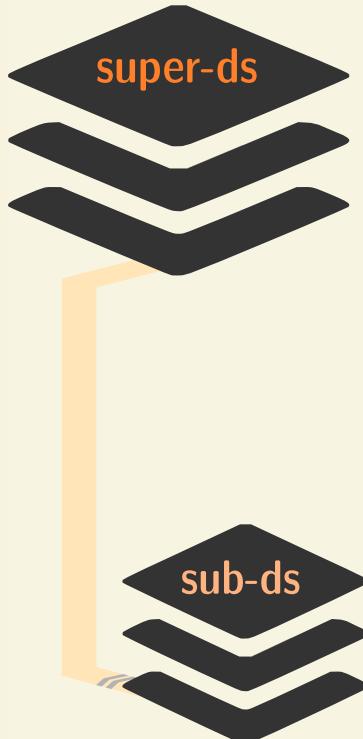
FROM HERE TO THIS:



BUT: Version control is only one aspect of data management

CONSUMING DATASETS

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DataLad-101/

books/

byte-of-python.pdf

progit.pdf

TLCL.pdf

recordings/

longnow/

Long_Now__Conv[...]/

...

Long_Now__Seminars[...]/

2003_12_13[...]

2003_11_15[...]

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notes.txt

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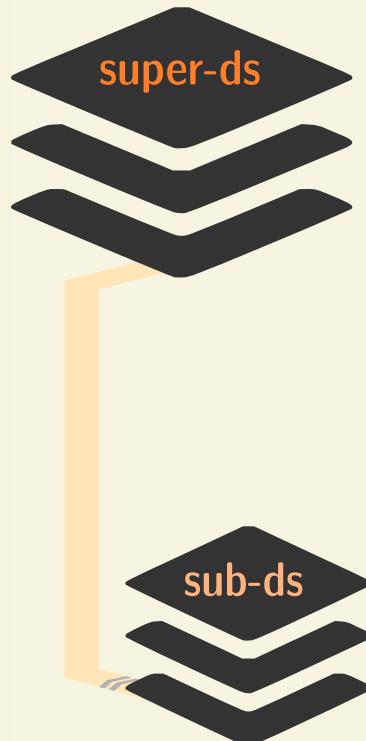
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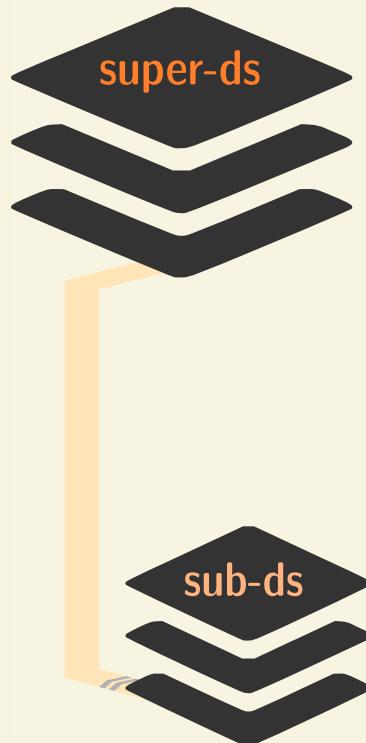
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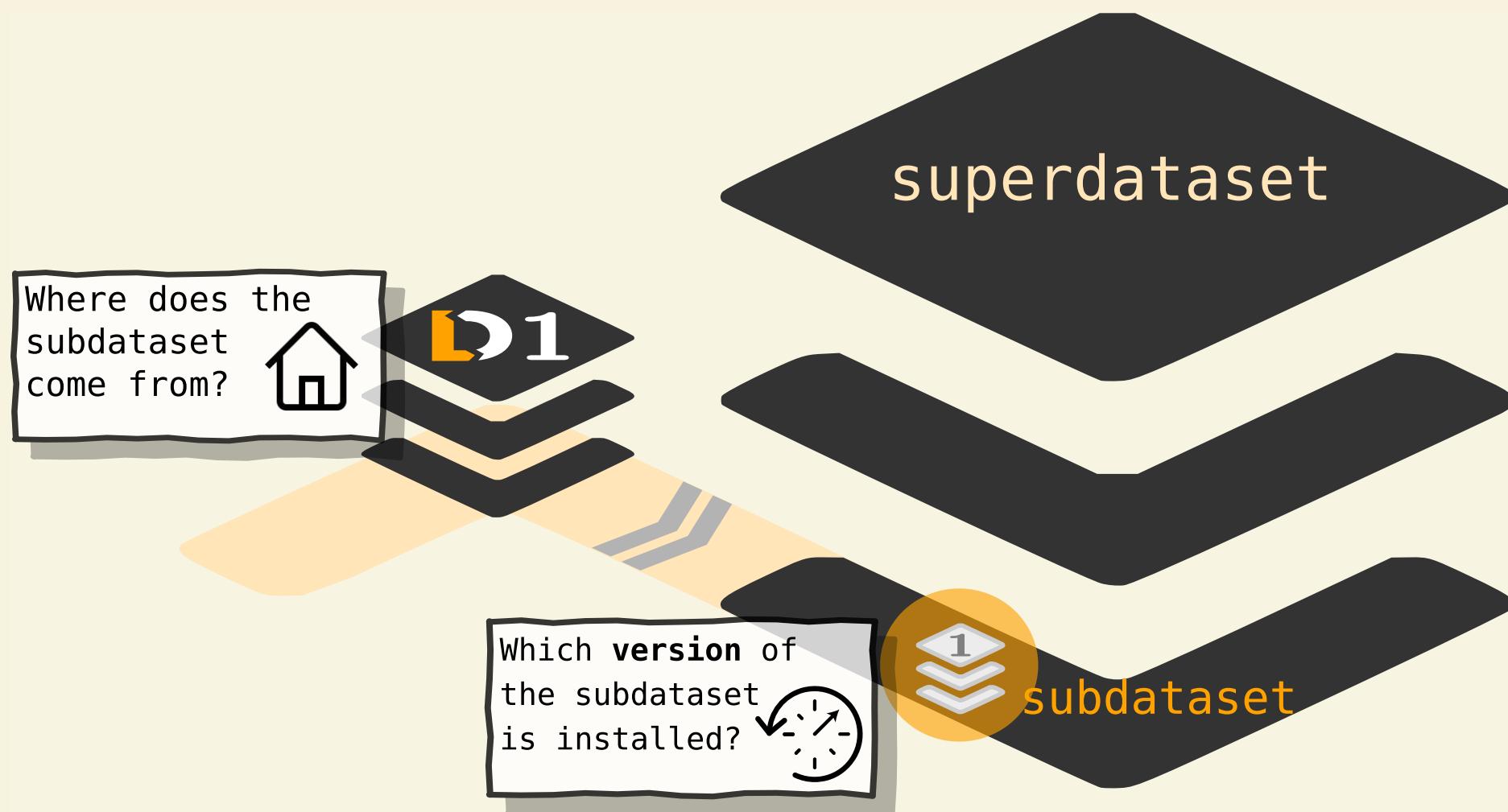
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DATASET NESTING



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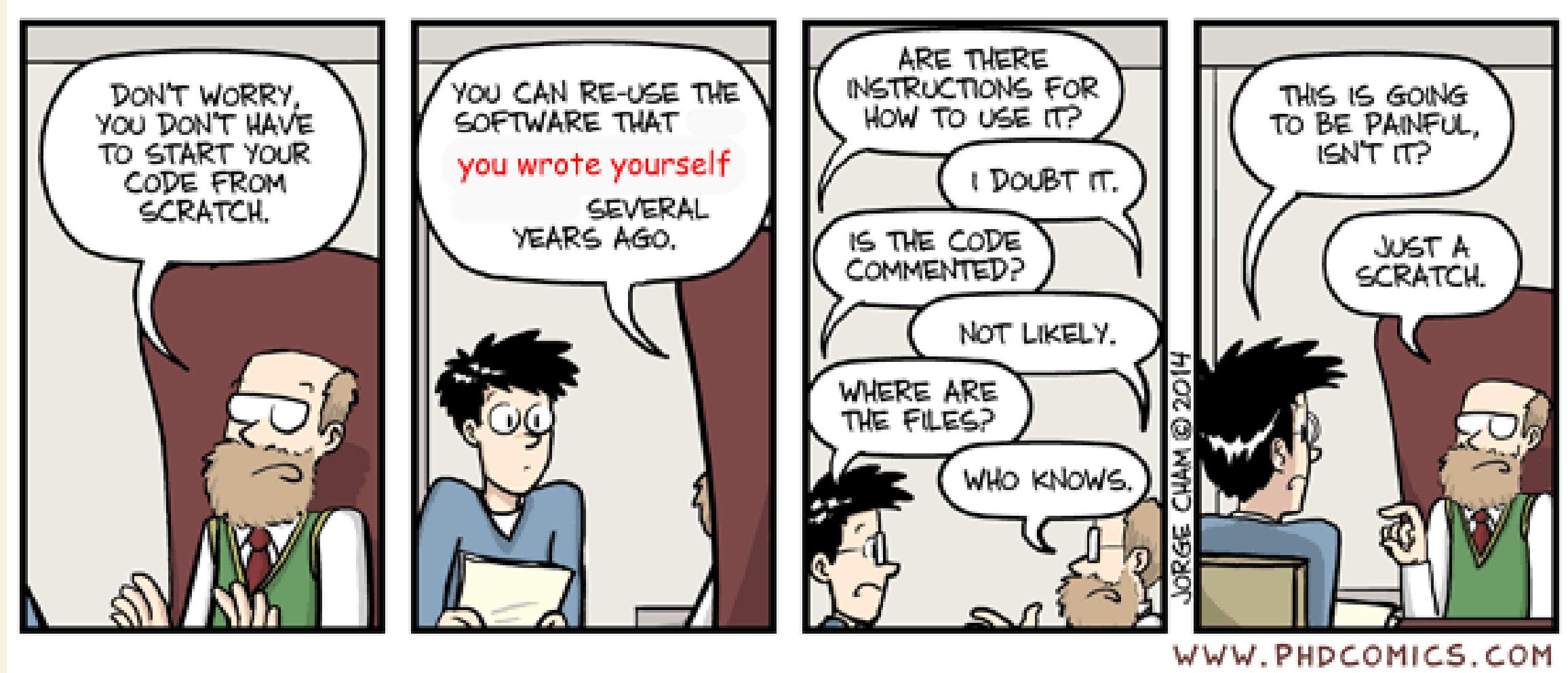
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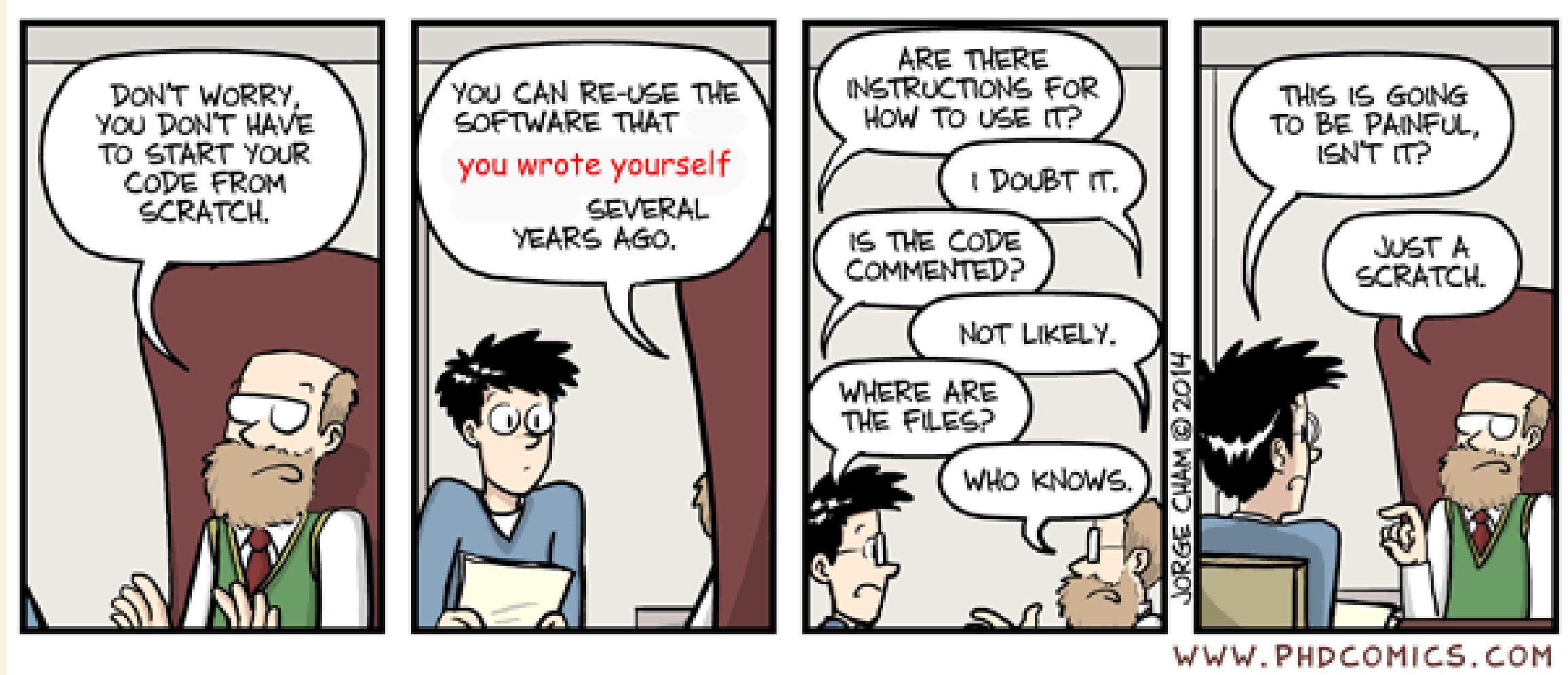
The superdataset records only the *version state* of the subdataset.

REPRODUCIBLE DATA ANALYSIS



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Image credit: Full comic at <http://phdcomics.com/comics.php?f=1979>



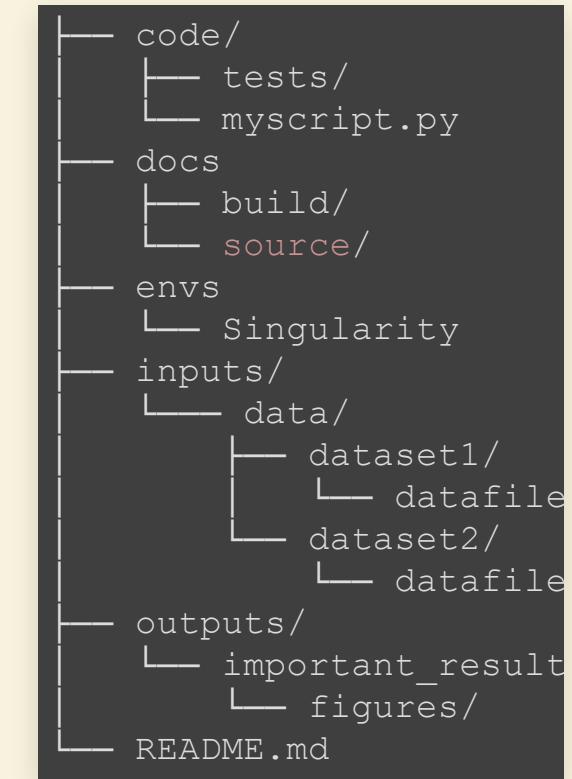
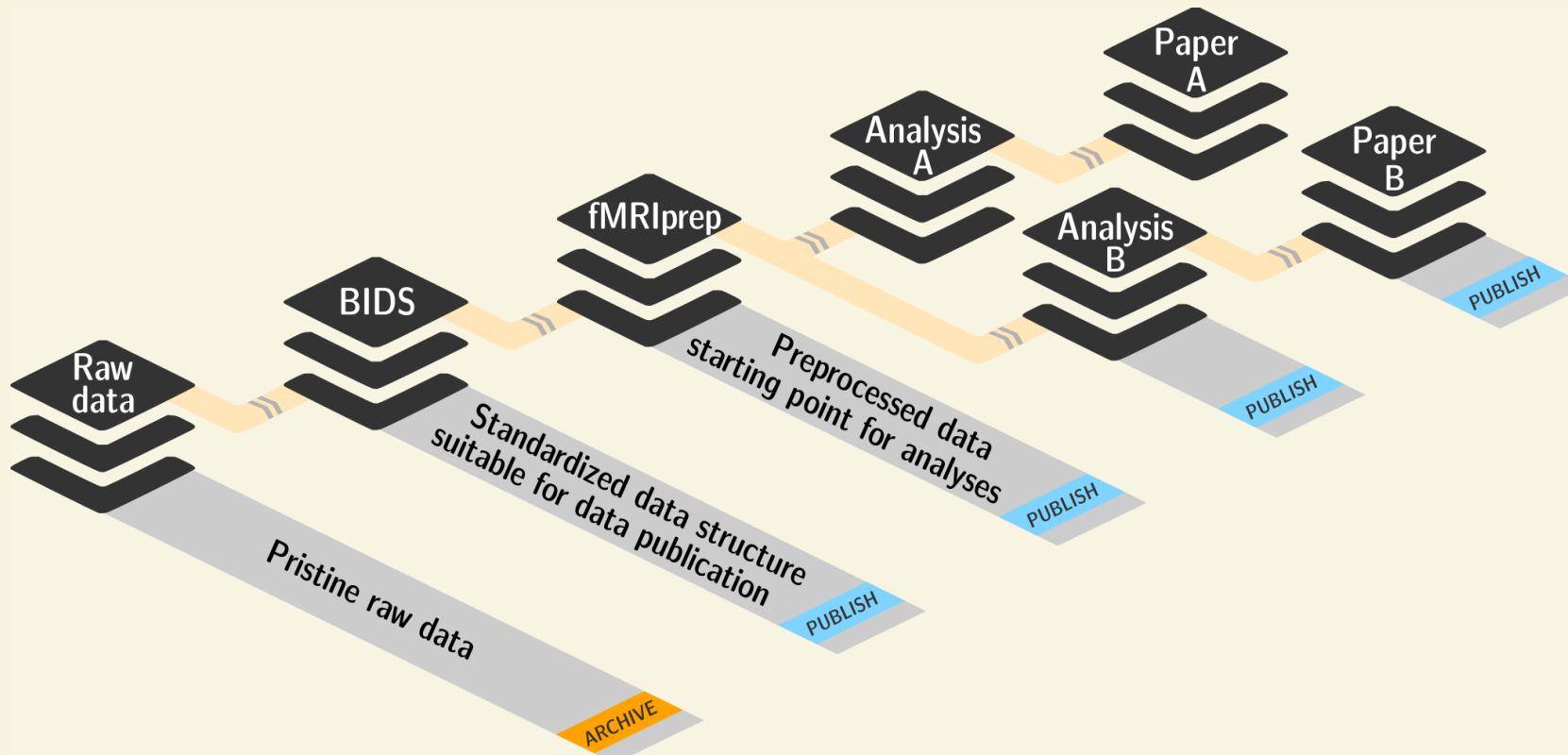
Code to follow along:

http://handbook.datalad.org/en/latest/code_from_chapters/10_yoda_code.html

BASIC ORGANIZATIONAL PRINCIPLES FOR DATASETS

Keep everything clean and modular

- An analysis is a superdataset, its components are subdatasets, and its structure modular

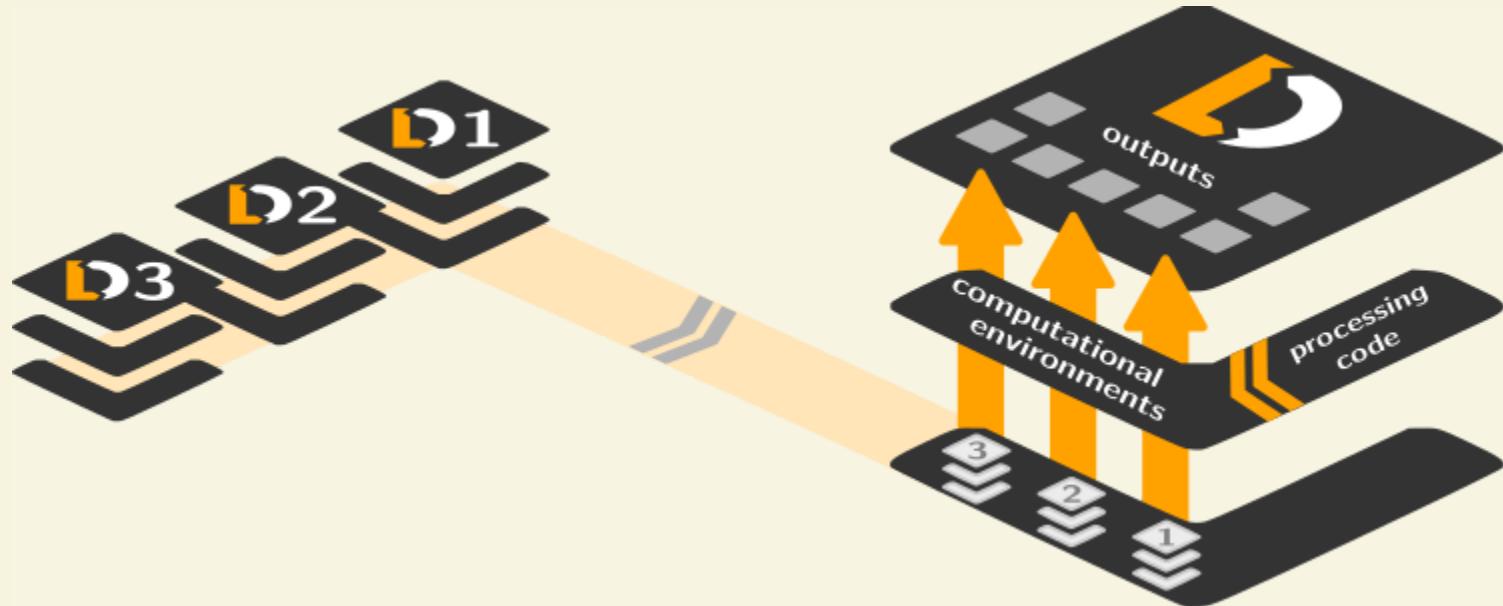


- do not touch/modify raw data: save any results/computations *outside* of input datasets
 - Keep a superdataset self-contained: Scripts reference subdatasets or files with *relative paths*

BASIC ORGANIZATIONAL PRINCIPLES FOR DATASETS

Record where you got it from, where it is now, and what you do to it

- Link datasets (as subdatasets), record data origin
- Collect and store provenance of all contents of a dataset that you create

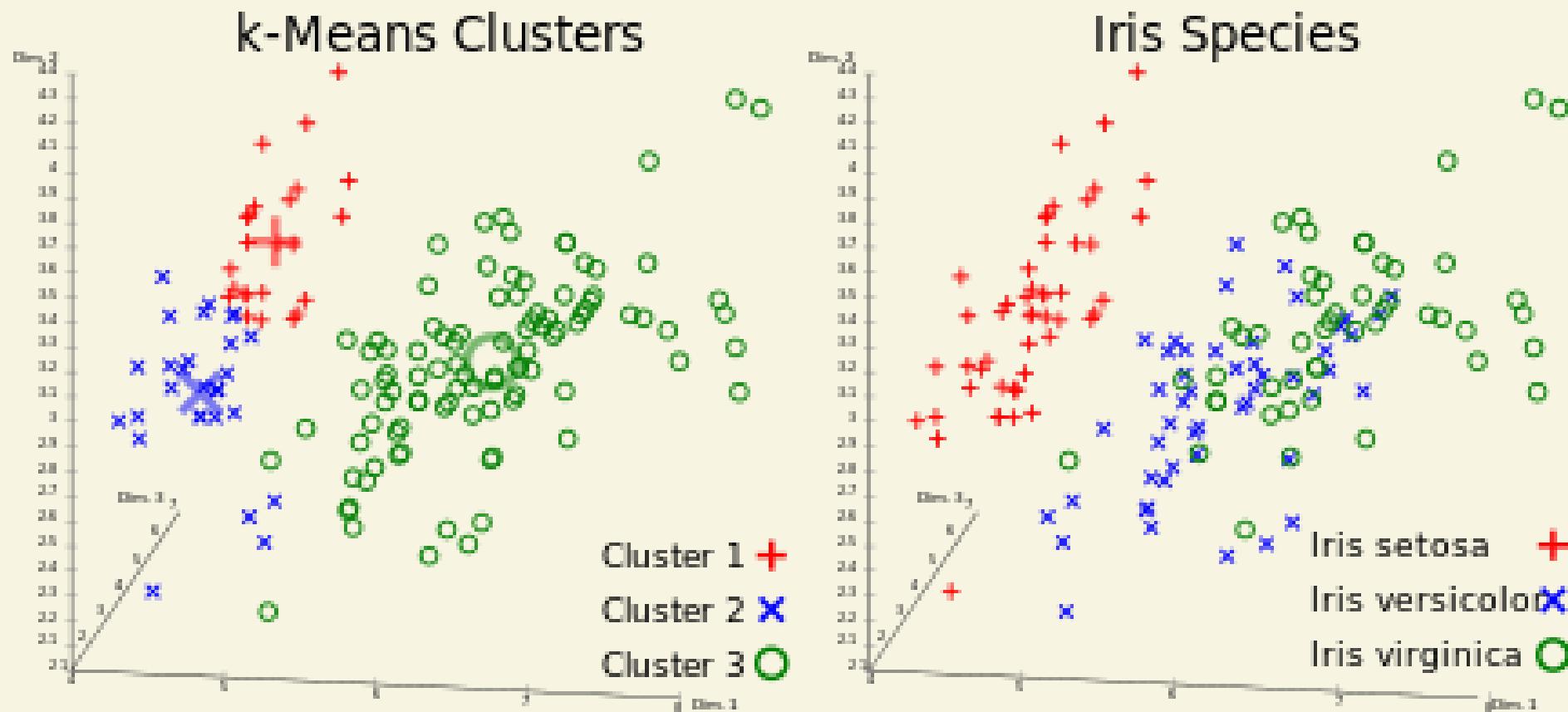
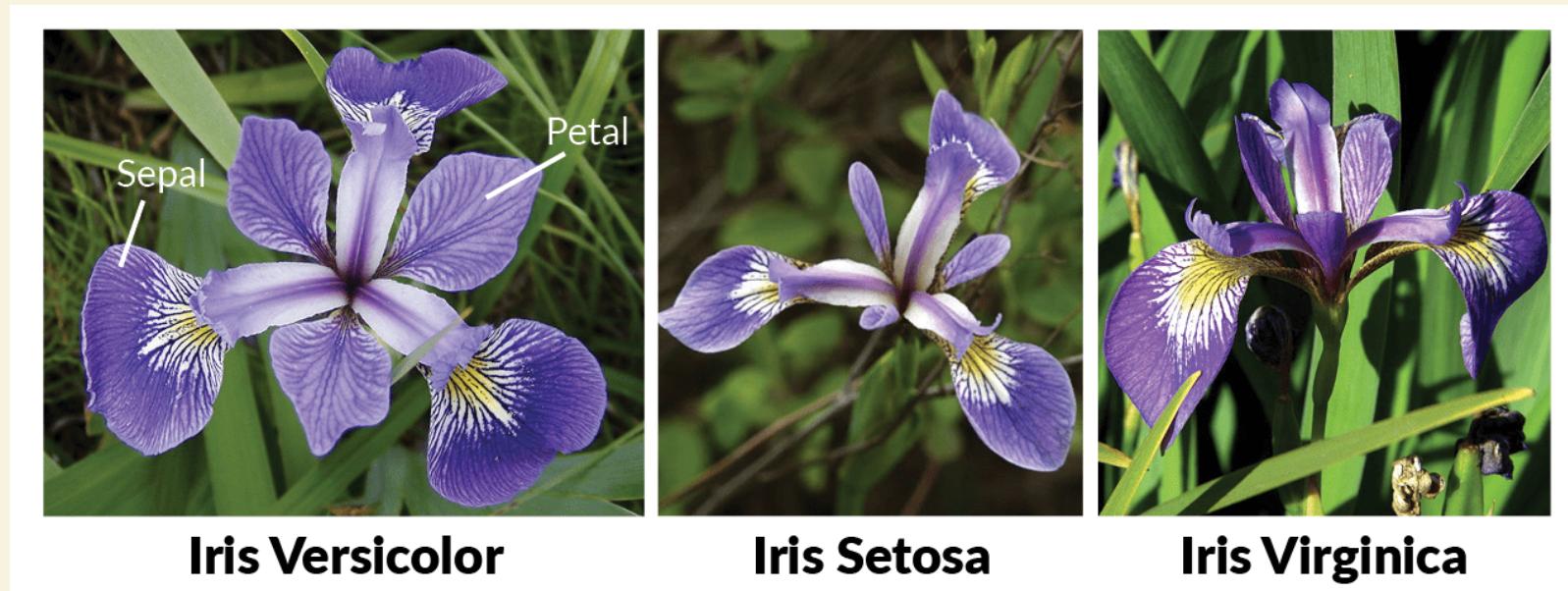


Document everything:

- Which script produced which output? From which data? In which software environment?...

Find out more about organizational principles in the [YODA principles](#)!

A CLASSIFICATION ANALYSIS ON THE IRIS FLOWER DATASET

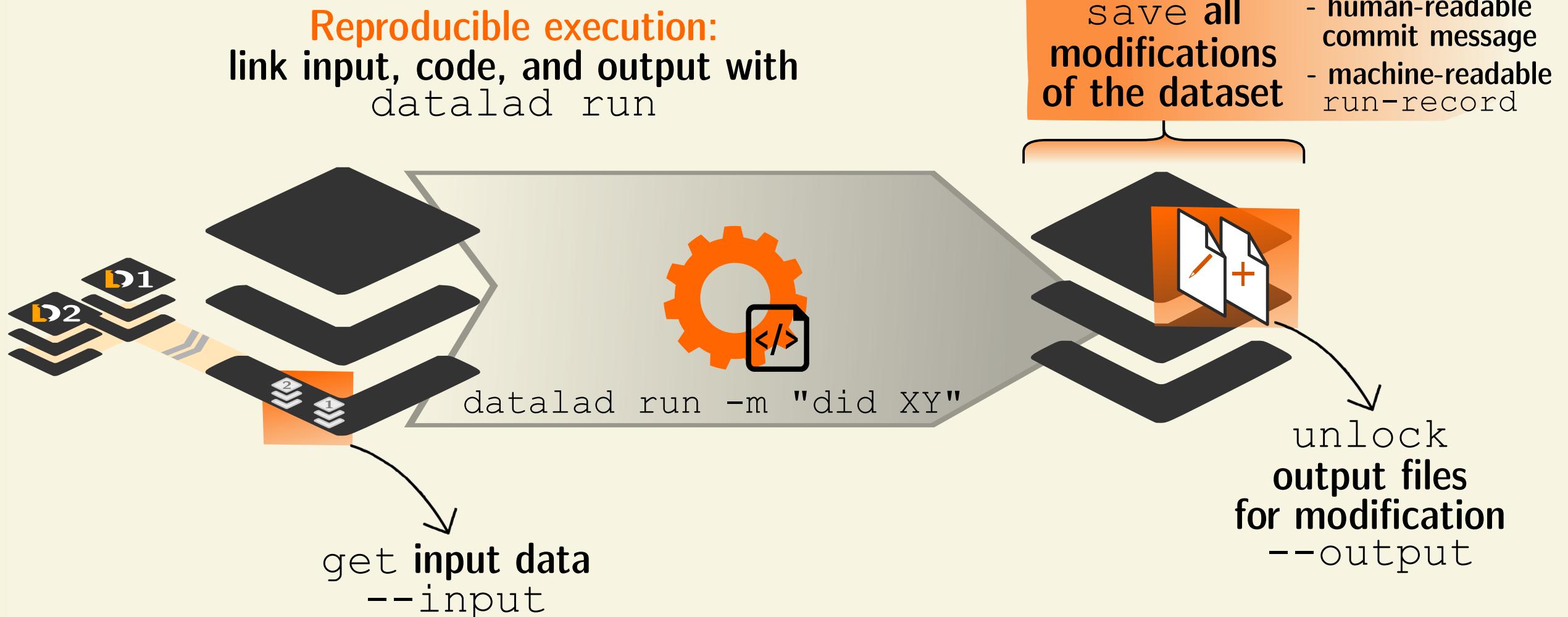


REPRODUCIBLE EXECUTION & PROVENANCE CAPTURE

datalad run

REPRODUCIBLE EXECUTION & PROVENANCE CAPTURE

datalad run



COMPUTATIONAL REPRODUCIBILITY

- Code may produce different results or fail if run in a different software environment
- DataLad datasets can store (and share) software environments (Docker or Singularity containers) and reproducibly execute code inside of the software container, capturing software as additional provenance
- DataLad extension: `datalad-container`

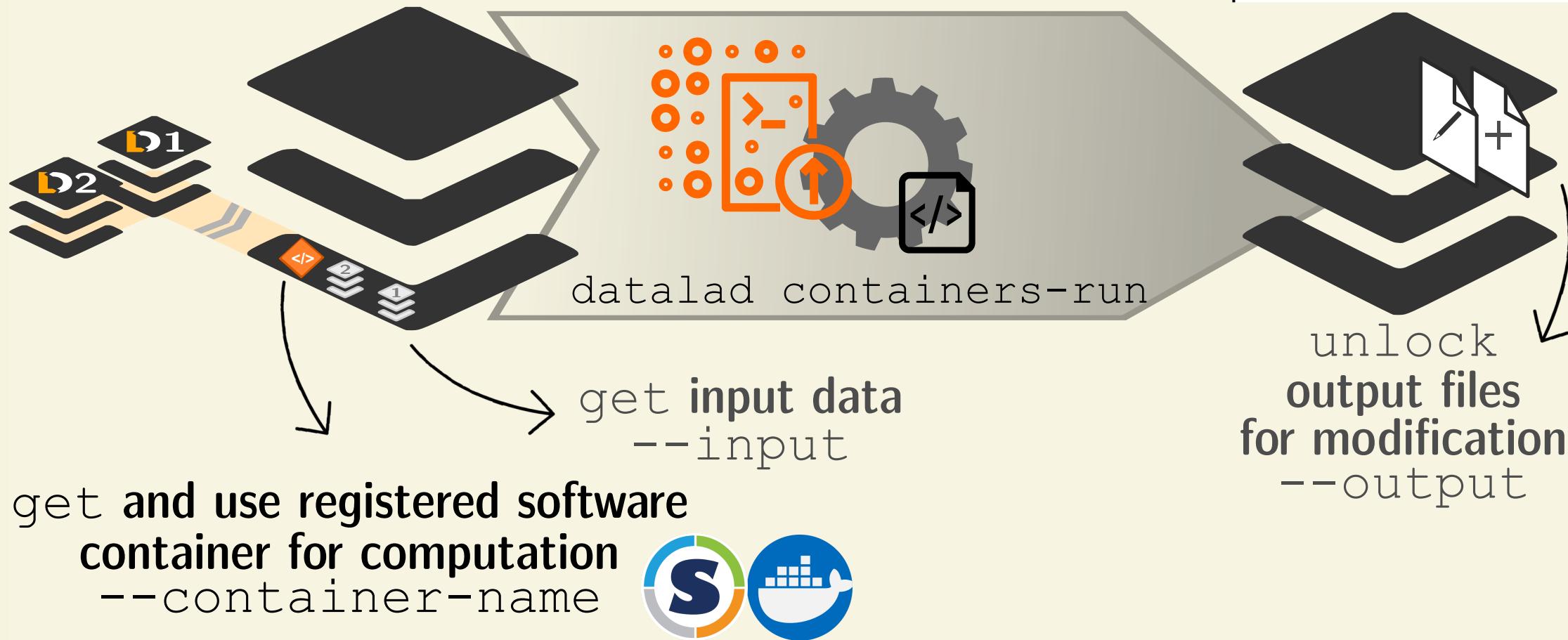
`datalad-containers run`

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`datalad-containers run`

**link input, code, output, and software with
datalad containers-run**



HOW TO GET STARTED WITH DATALAD

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```
$ datalad clone ///openneuro/ds000001
[INFO    ] Cloning http://datasets.datalad.org/openneuro/ds000001 [1 other candidates] into '/tmp
[INFO    ] access to 1 dataset sibling s3-PRIVATE not auto-enabled, enable with:
|           datalad siblings -d "/tmp/ds000001" enable -s s3-PRIVATE
install(ok): /tmp/ds000001 (dataset)

$ cd ds000001
$ ls sub-01/*
sub-01/anat:
sub-01_inplaneT2.nii.gz  sub-01_T1w.nii.gz

sub-01/func:
sub-01_task-balloonanalogrisktask_run-01_bold.nii.gz
sub-01_task-balloonanalogrisktask_run-01_events.tsv
sub-01_task-balloonanalogrisktask_run-02_bold.nii.gz
sub-01_task-balloonanalogrisktask_run-02_events.tsv
sub-01_task-balloonanalogrisktask_run-03_bold.nii.gz
sub-01_task-balloonanalogrisktask_run-03_events.tsv
```

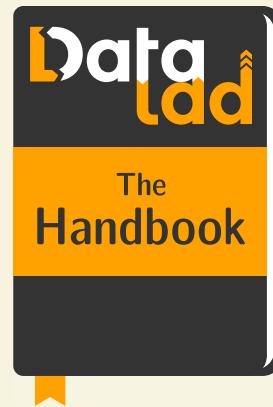
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- 22+ additional contributors

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- Michael Hanke
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THANK YOU!

QUESTIONS?