DATA MANAGEMENT WITH DATALAD

AN INTRODUCTION

Adina Wagner
@AdinaKrik

JÜLICH
Forschungszentrum

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

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

WHAT IS (RESEARCH) DATA MANAGEMENT?

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

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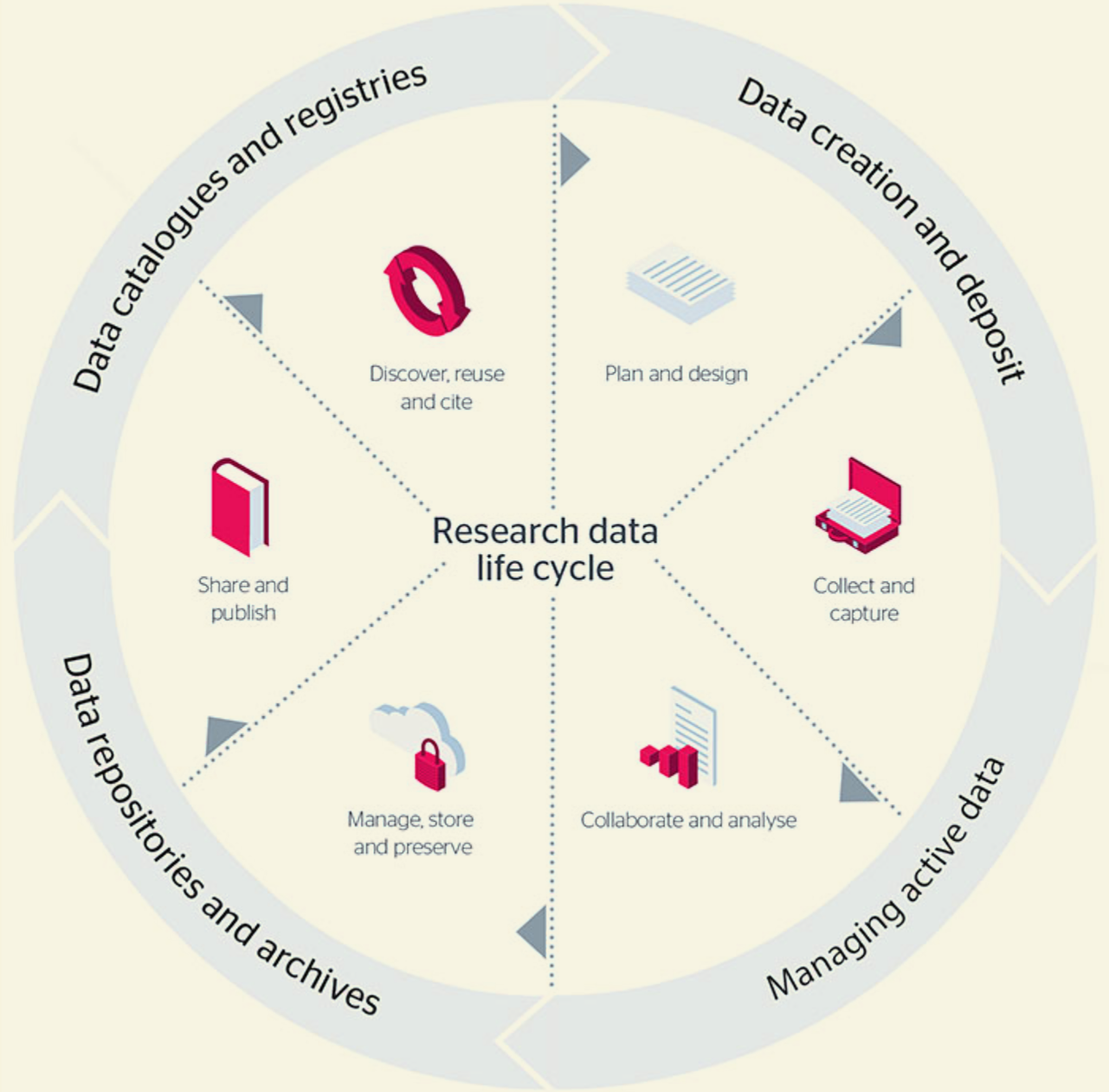

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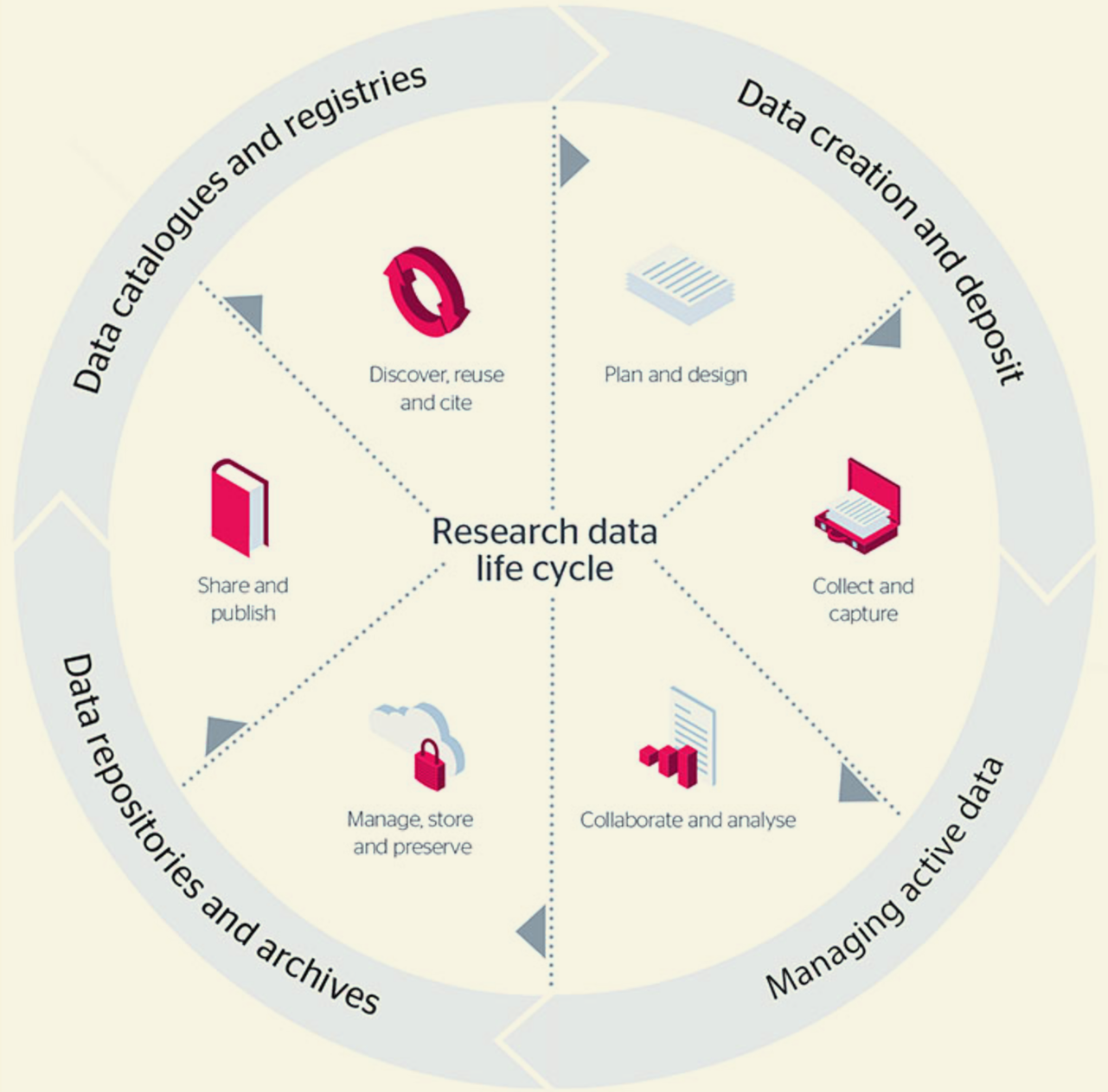

- Research data management is a key component for reproducibility, efficiency, and impact/reach of data analysis projects

WHY DATA MANAGEMENT?

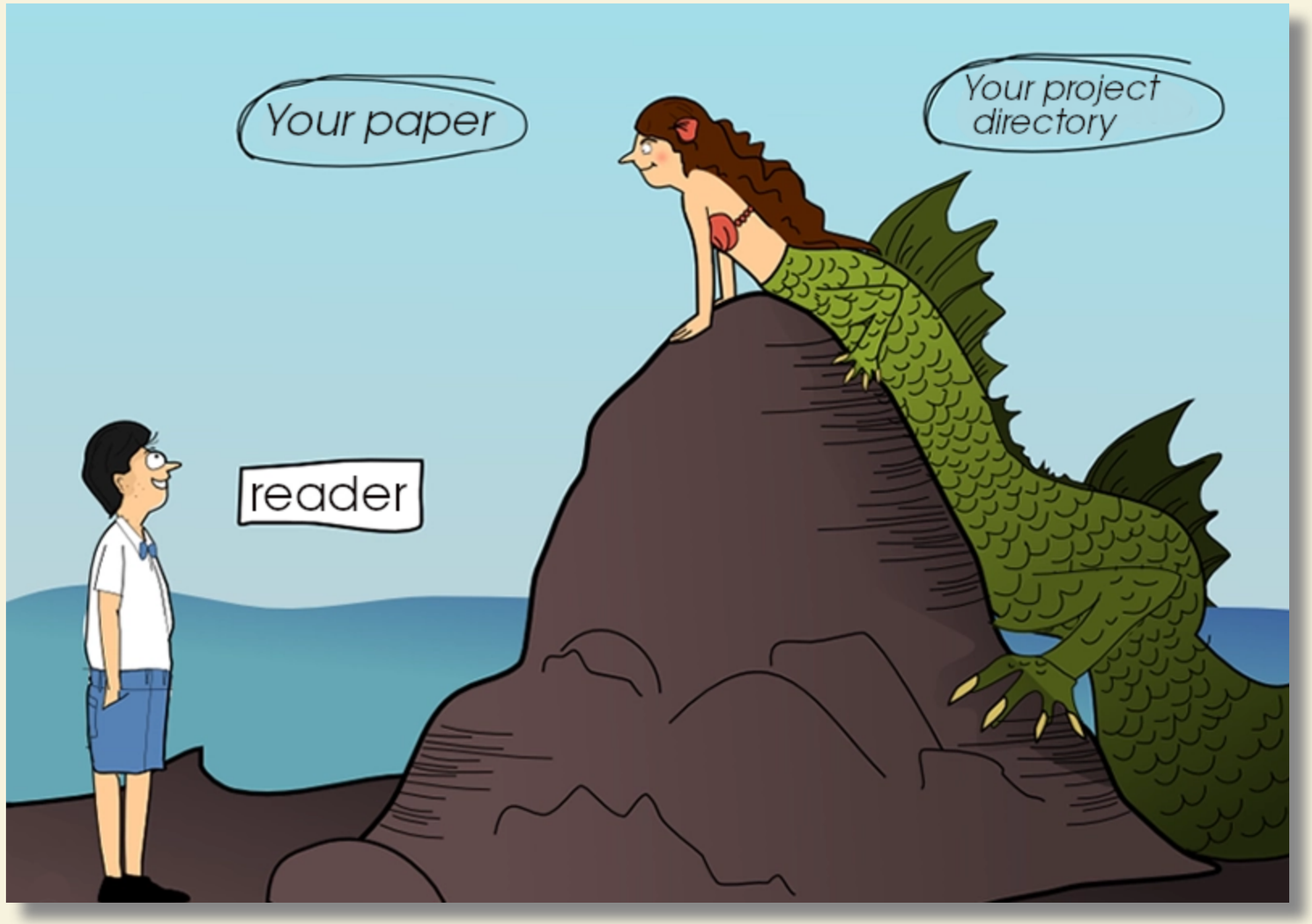

Image credit: adapted from https://dribbble.com/shots/3090048-Front-end-vs-Back-end

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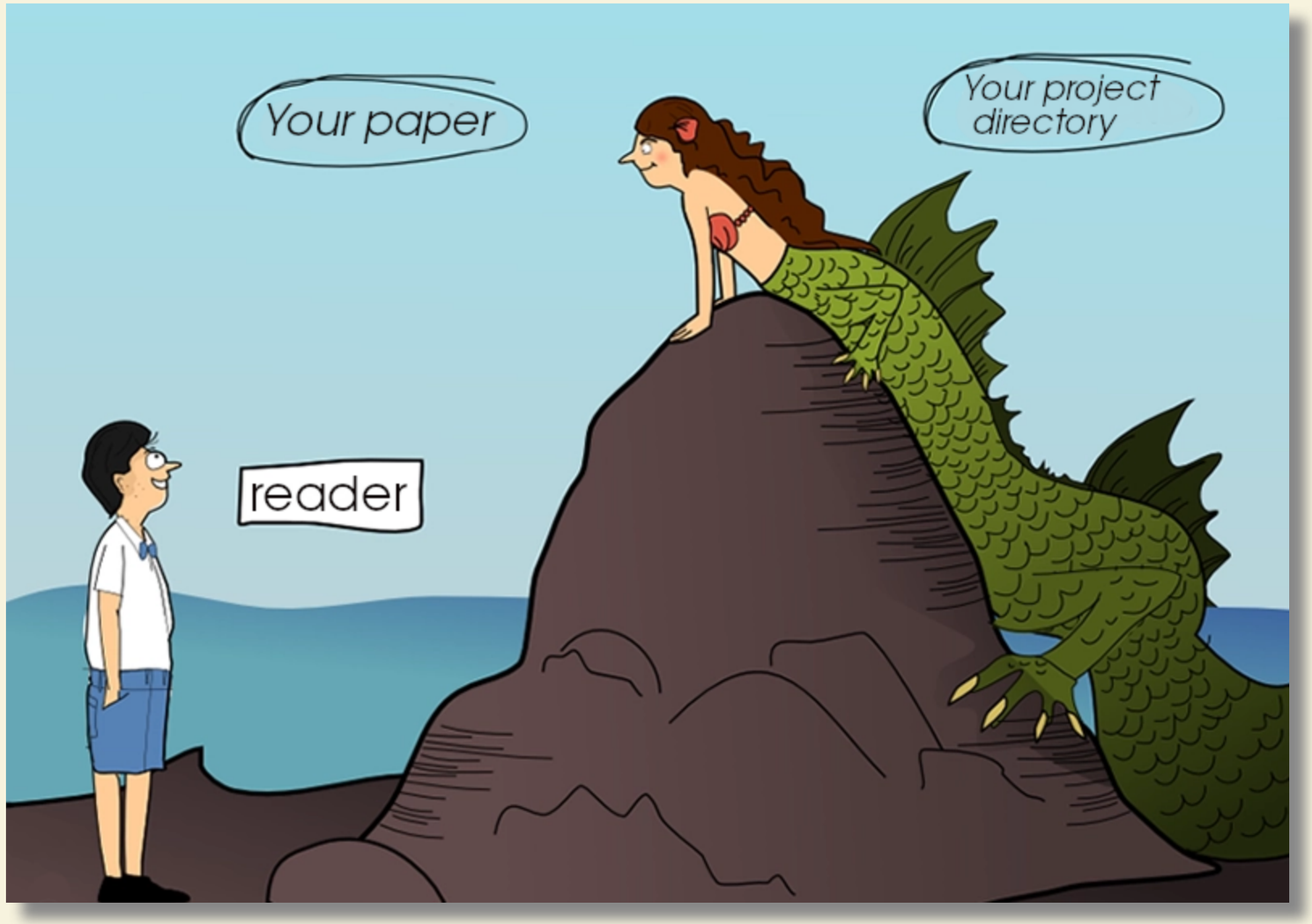

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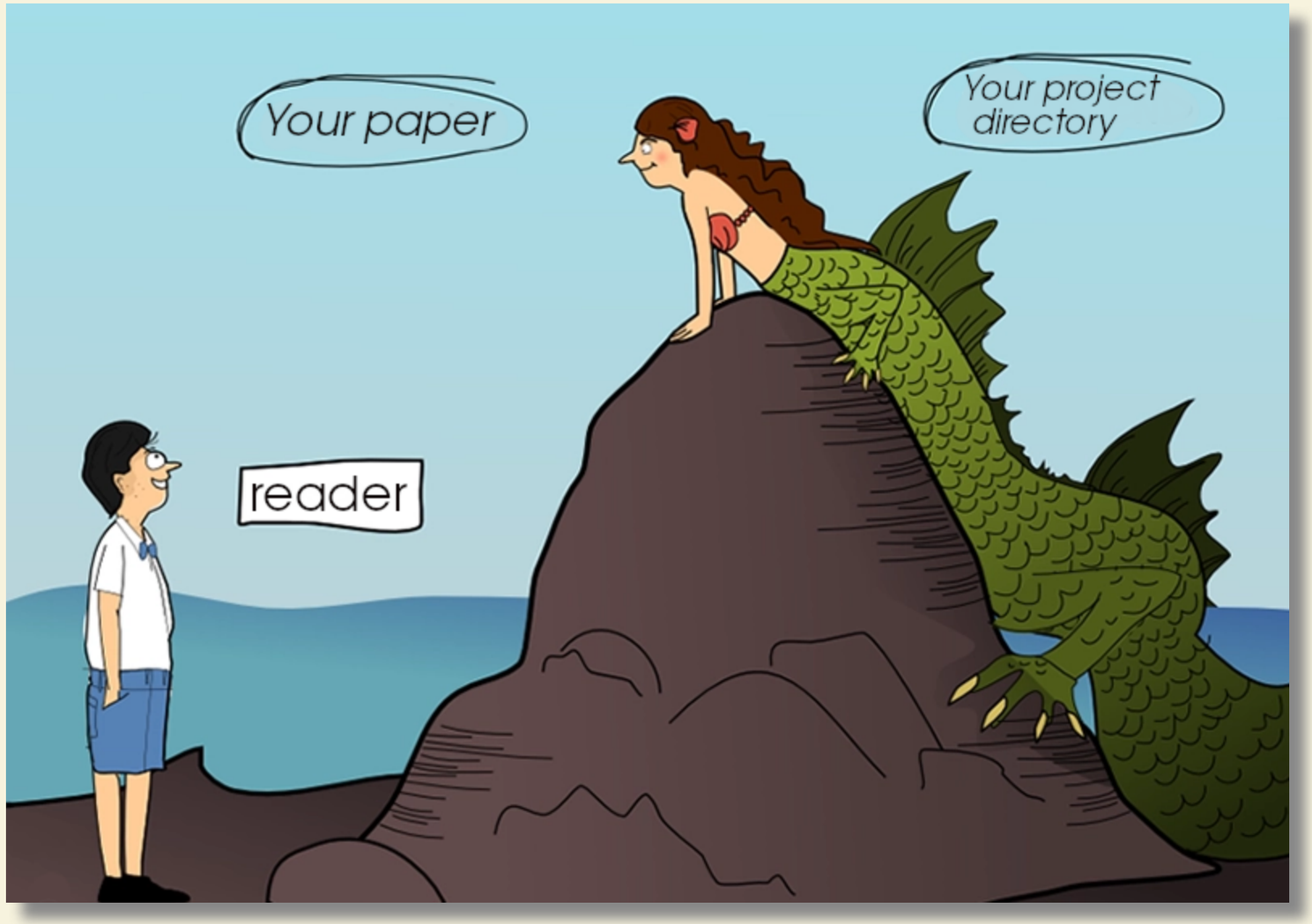

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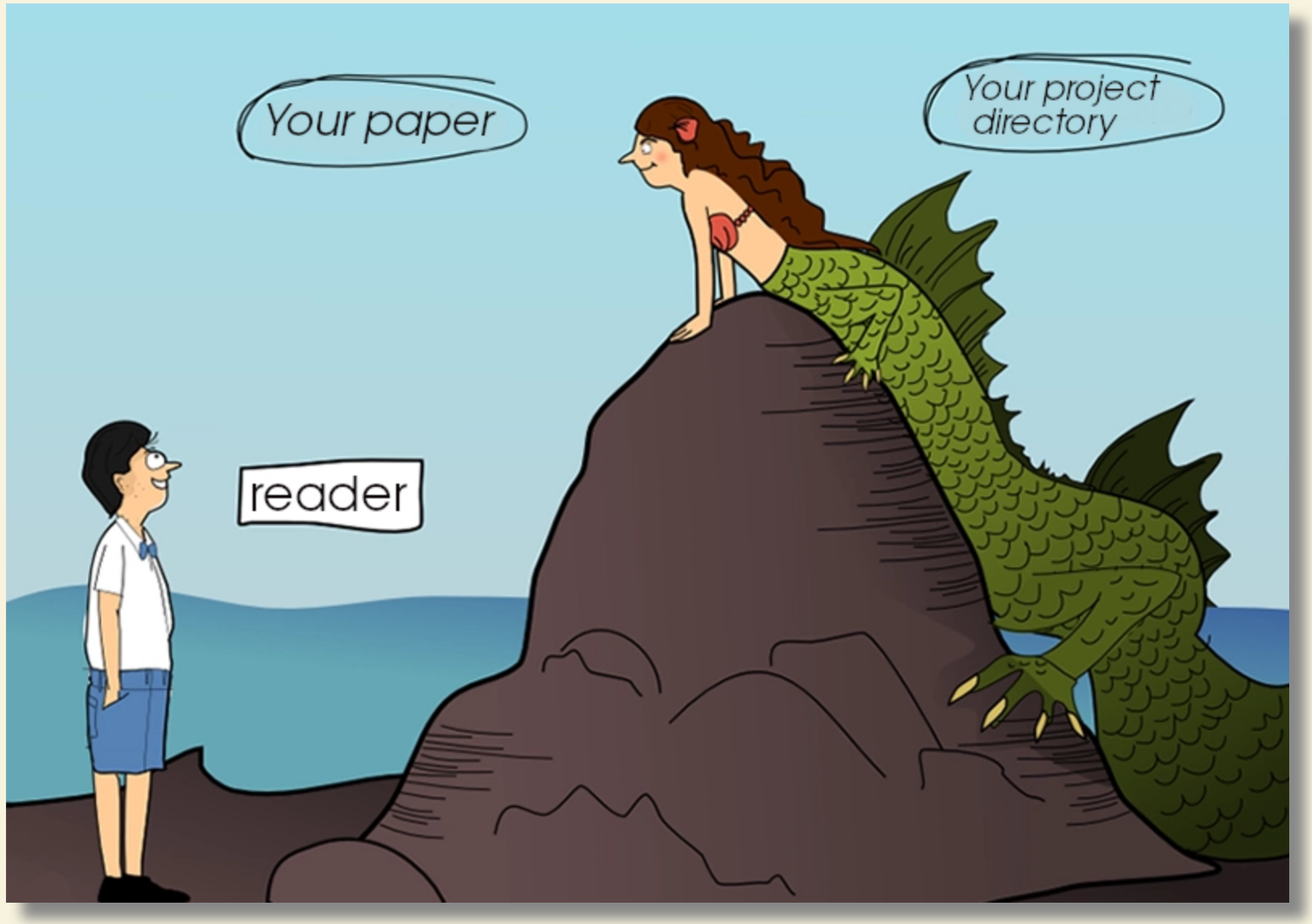

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- Funders & publishers require it
- Scientific peers increasingly expect it
- The quality and efficiency of your work improves

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 then 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)

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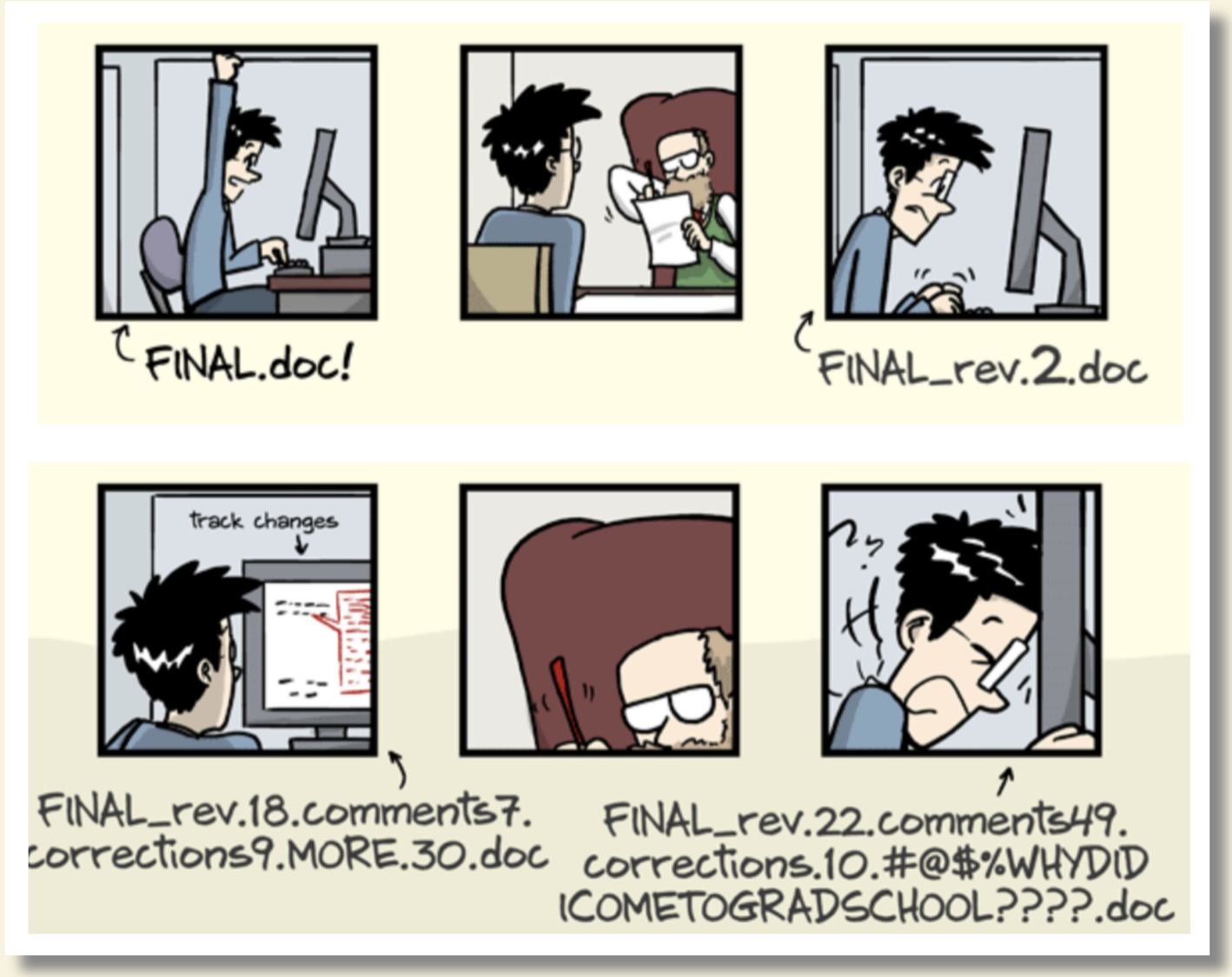

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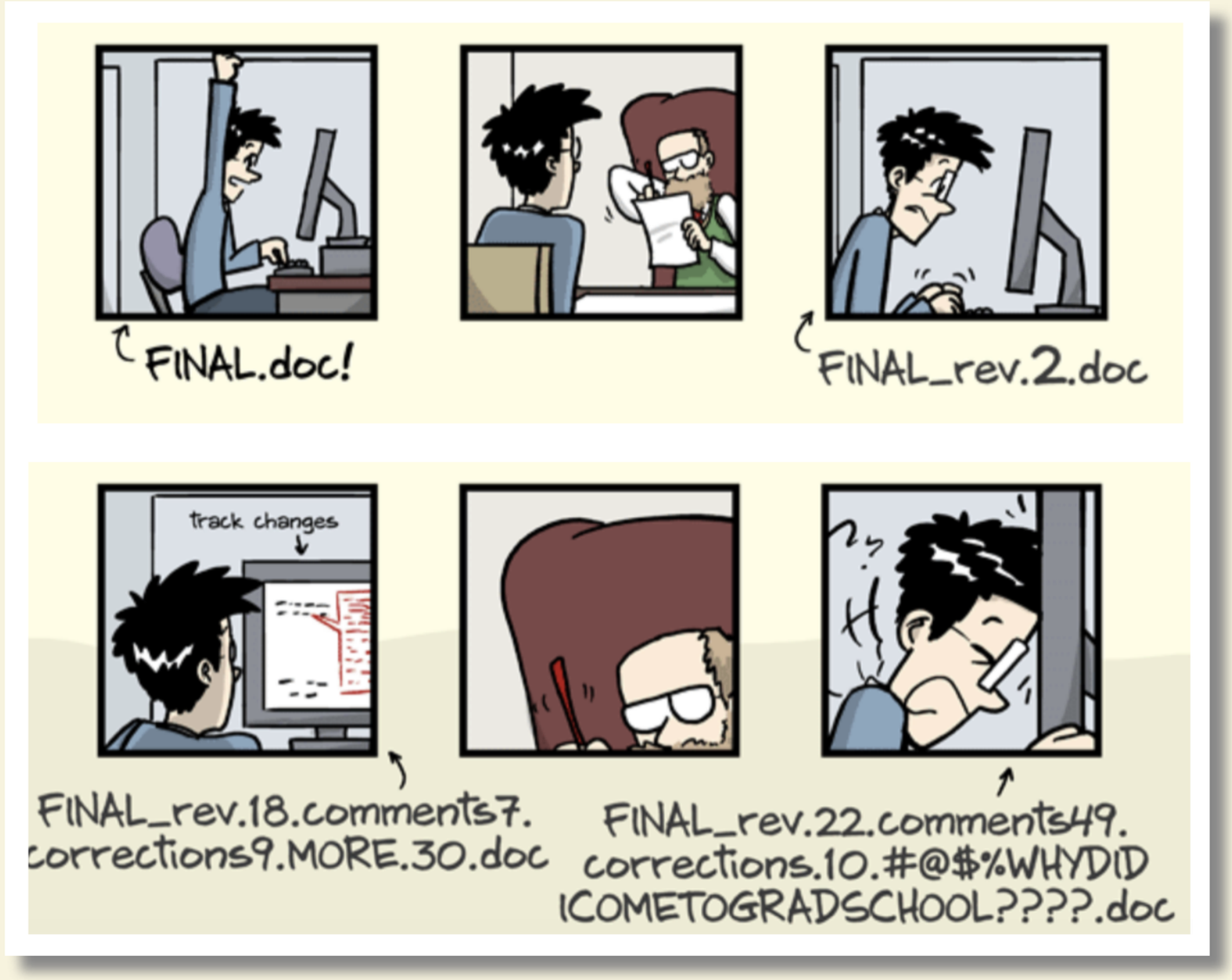

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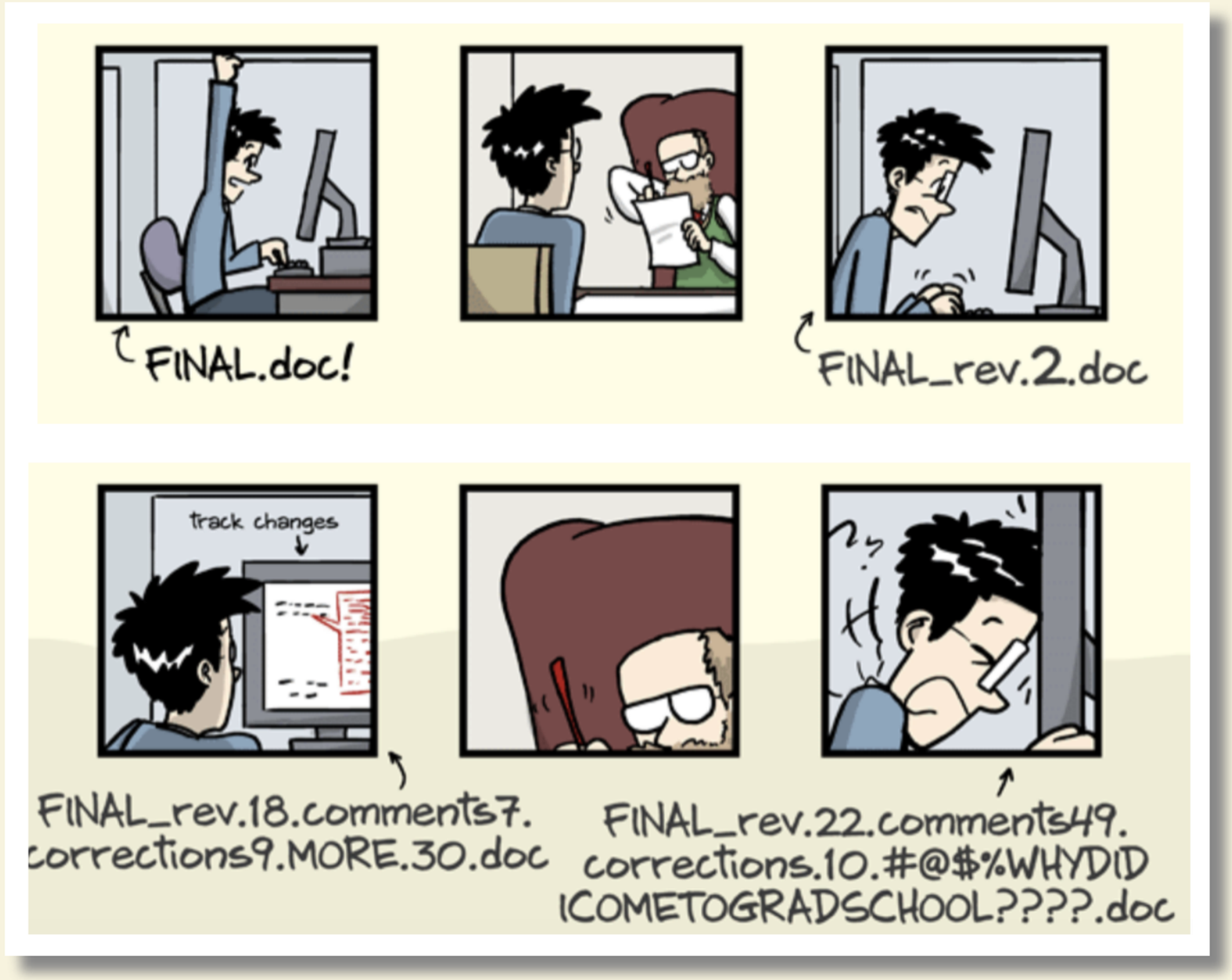

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- Mostly done for code, but **data** changes as well!

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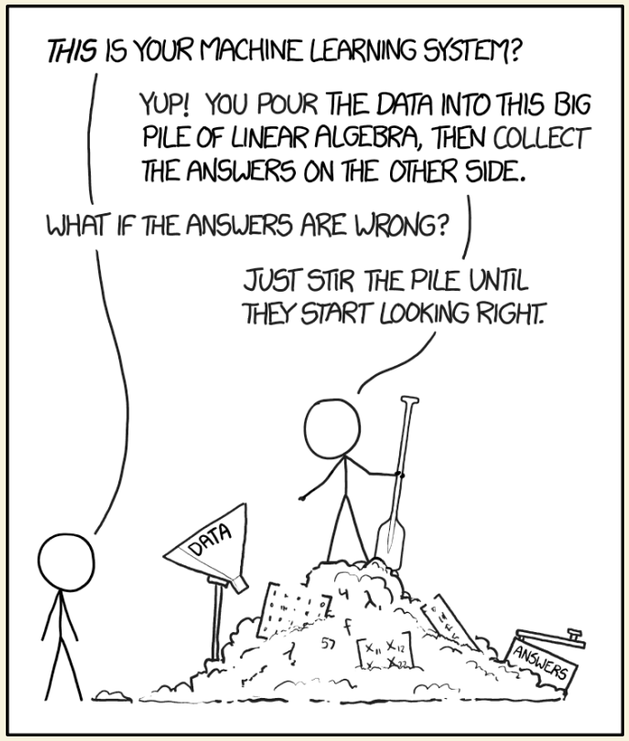

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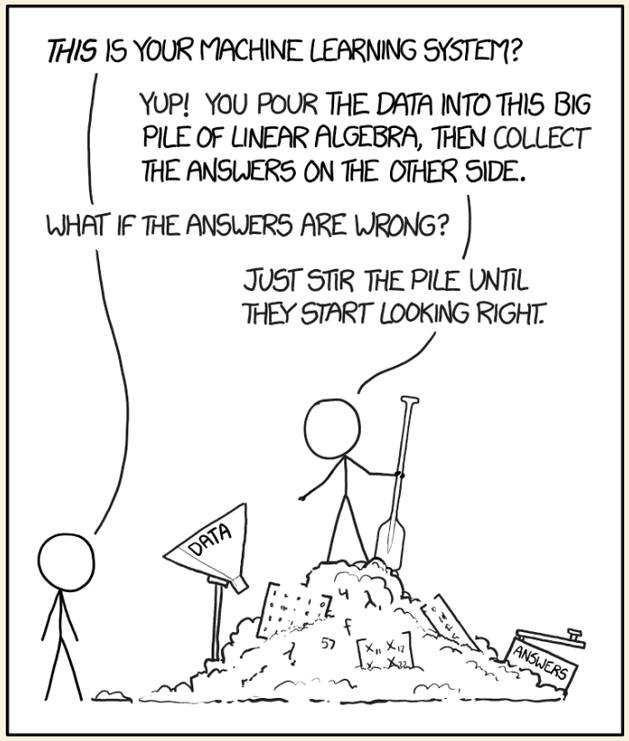

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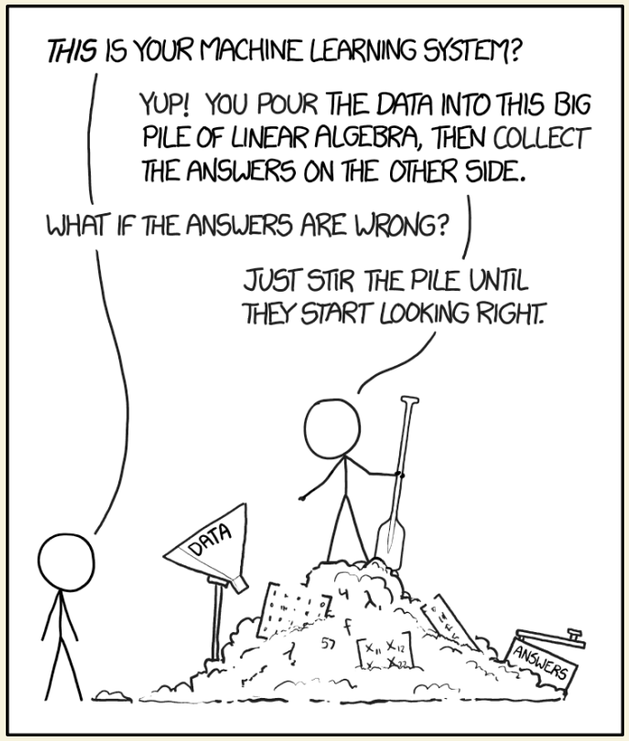

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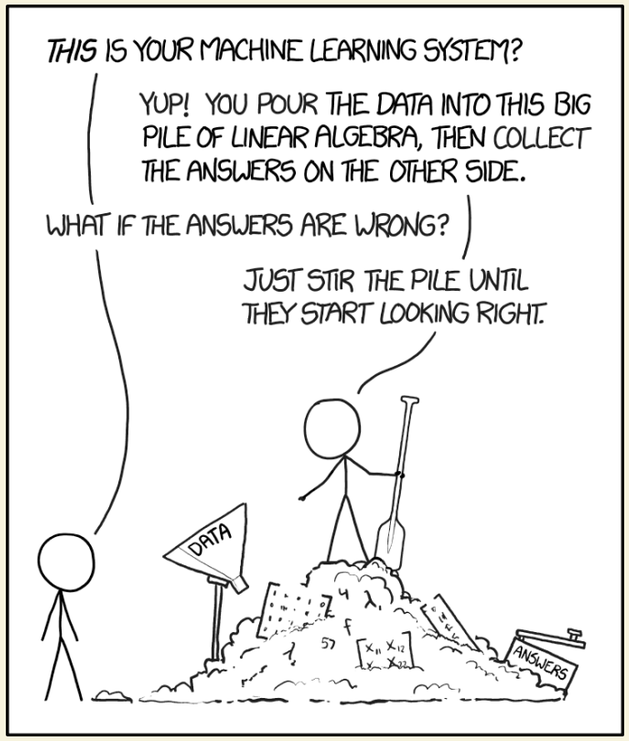

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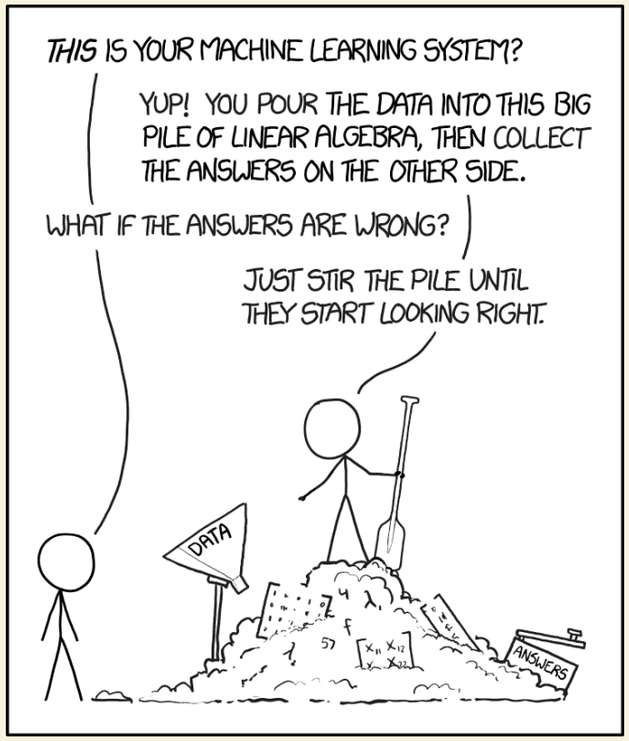

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    - What is the software (libraries, environment) used for a computation and its dependencies to data or code?

DATALAD CAN HELP WITH DATA MANAGEMENT

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What is it?
Why should I use it?
How can I use it?

DataLad

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.

DataLad 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!),
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➲ **For more:** Read the DataLad Handbook

DATALAD DATASETS

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  - Datasets can be *created* (from scratch) or *installed*
  - 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

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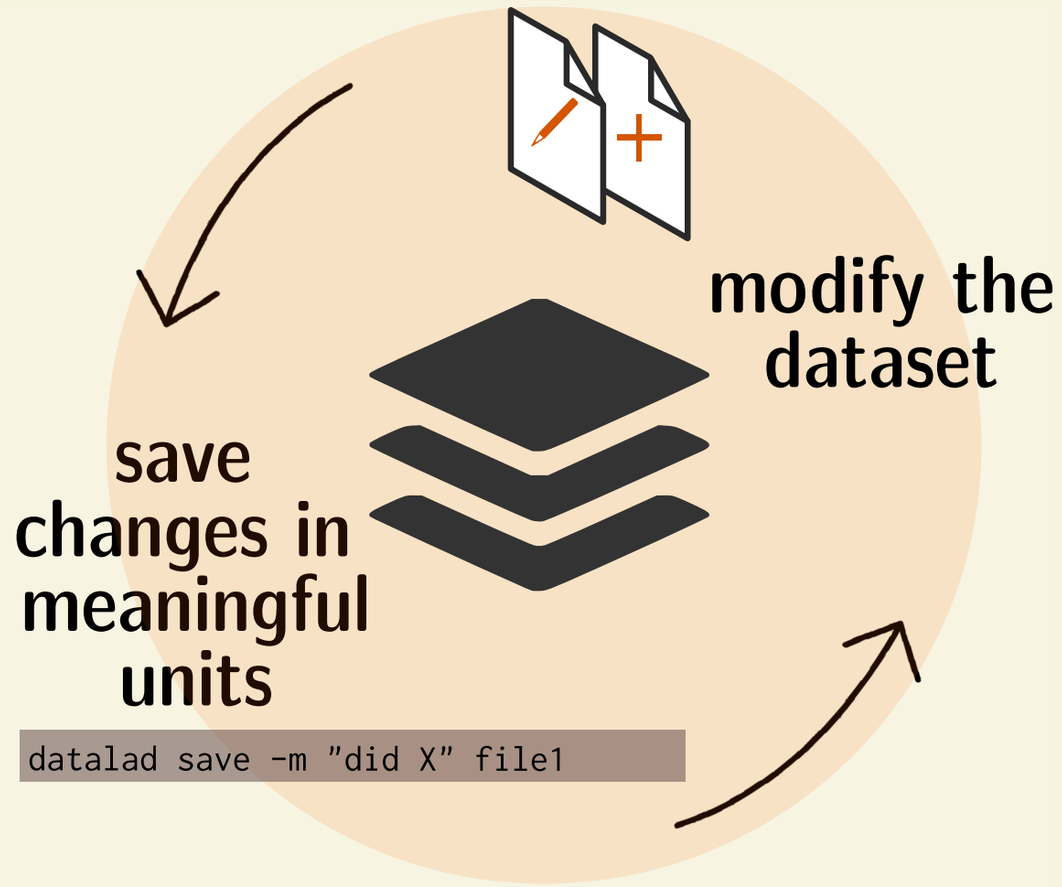

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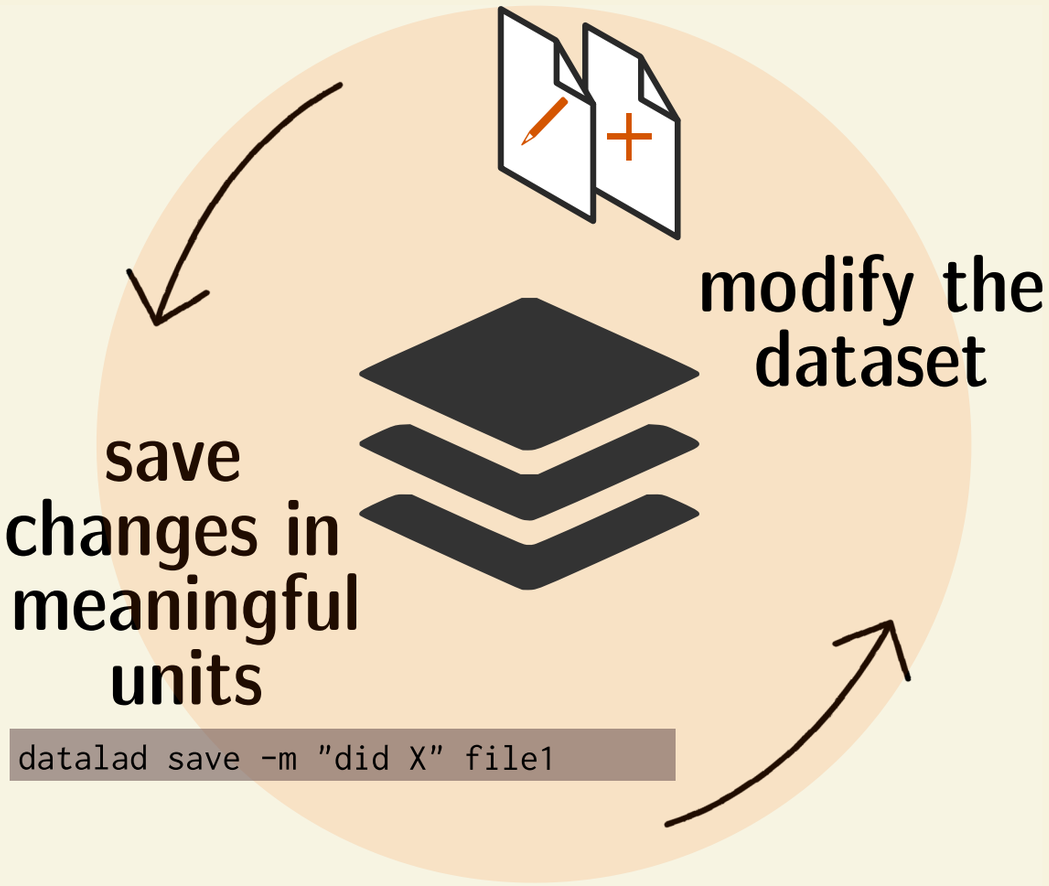

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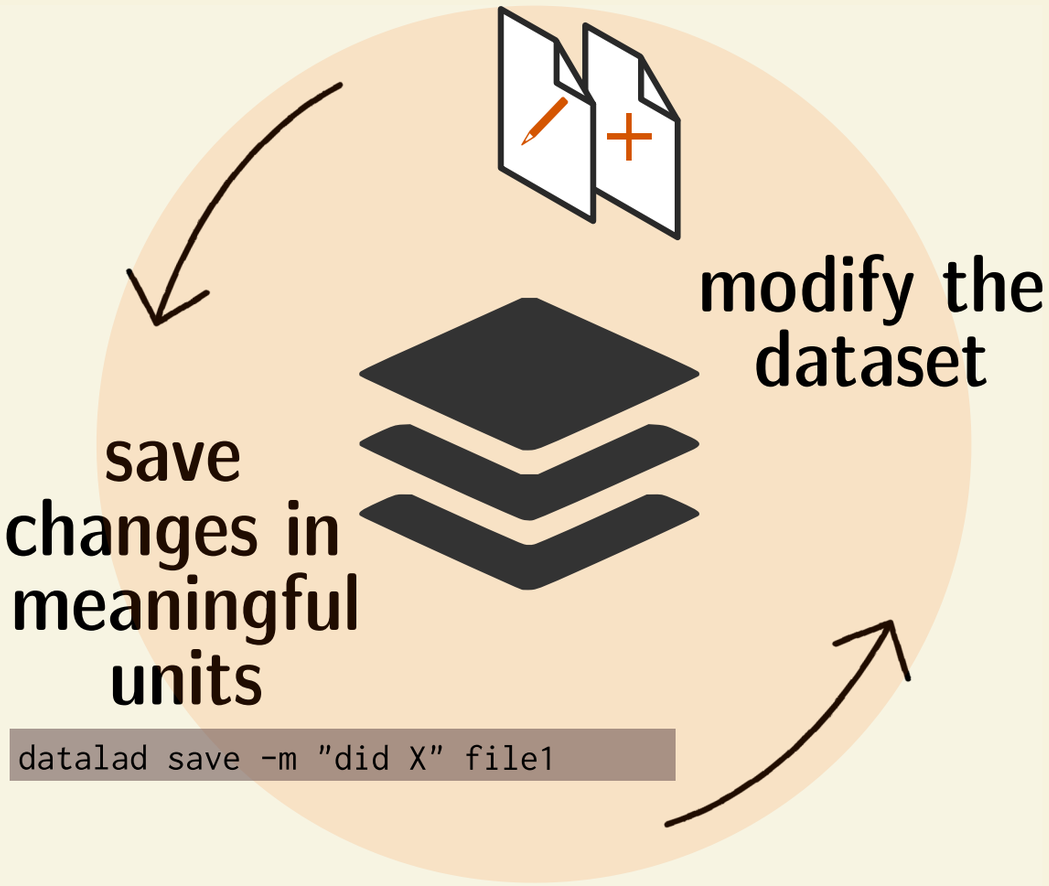

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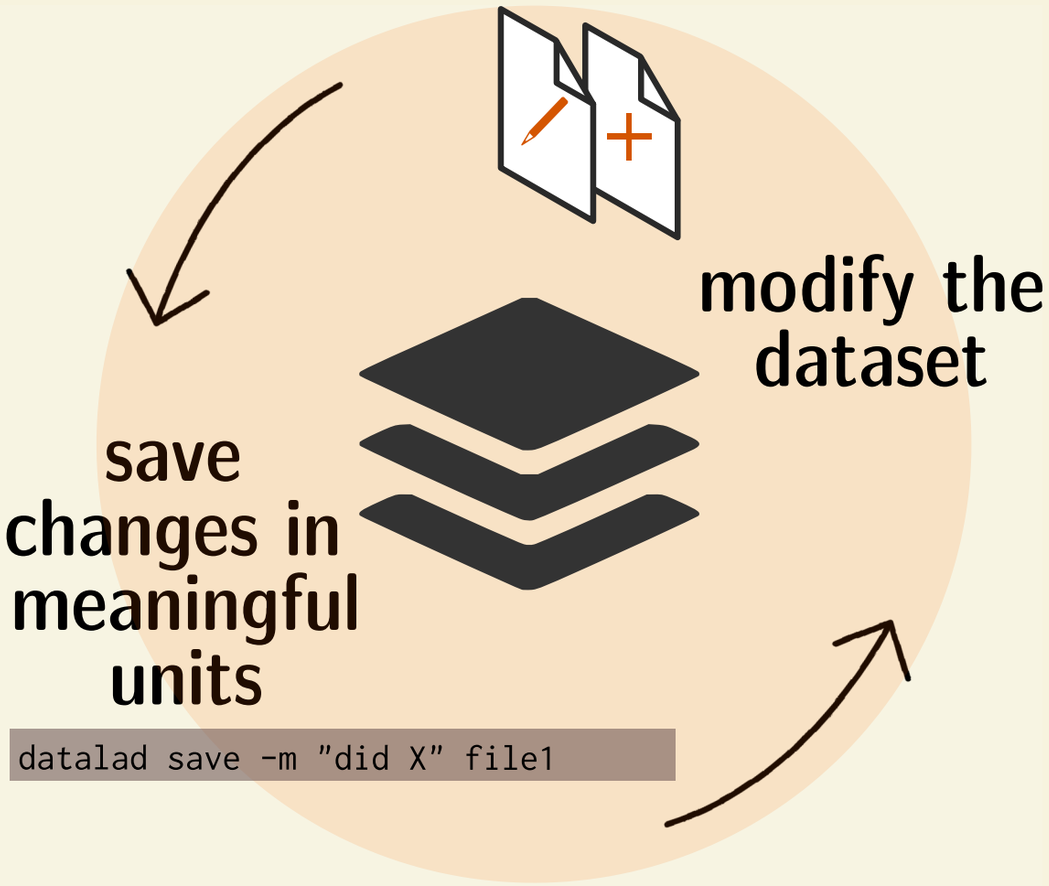

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A clean dataset status is good practice.

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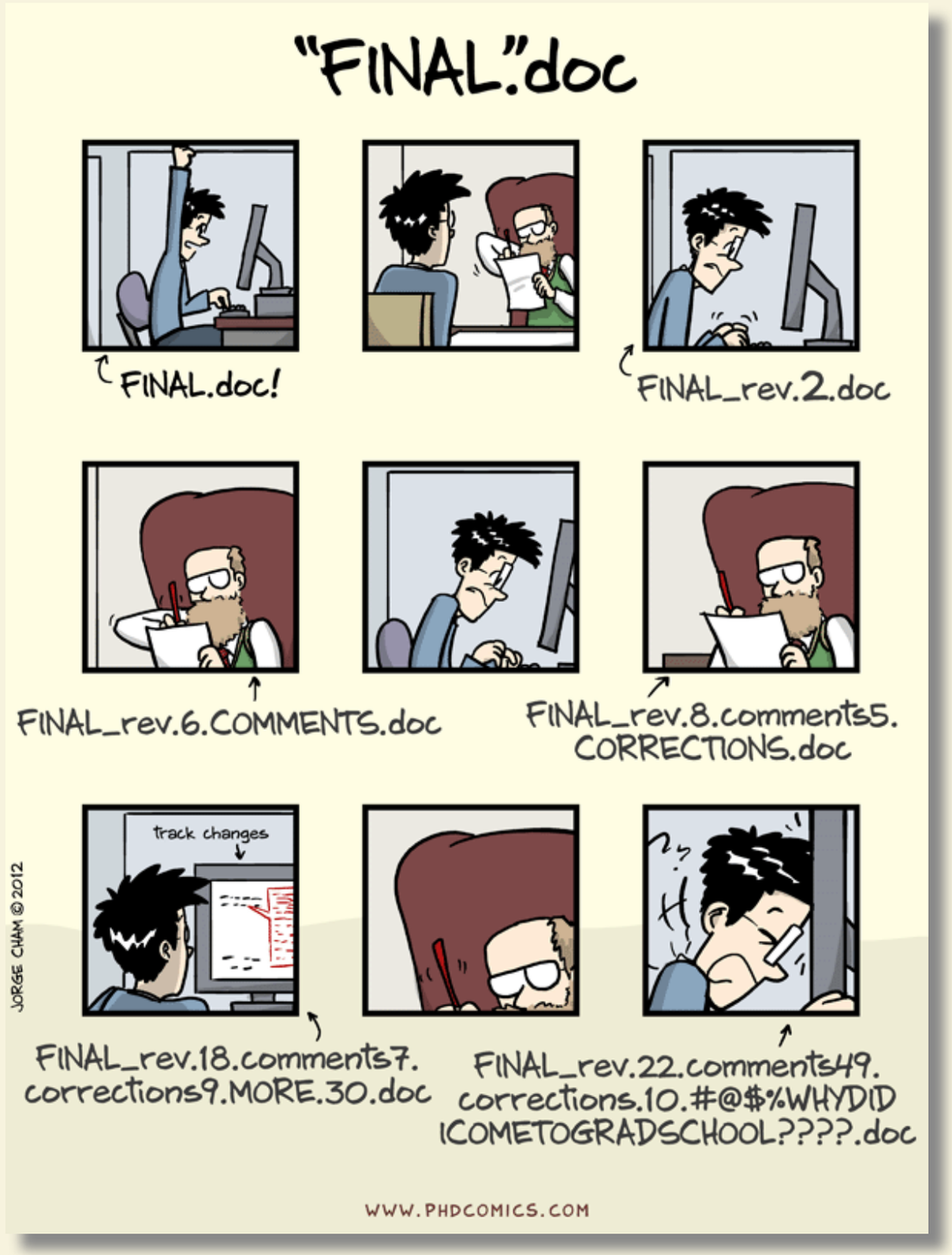

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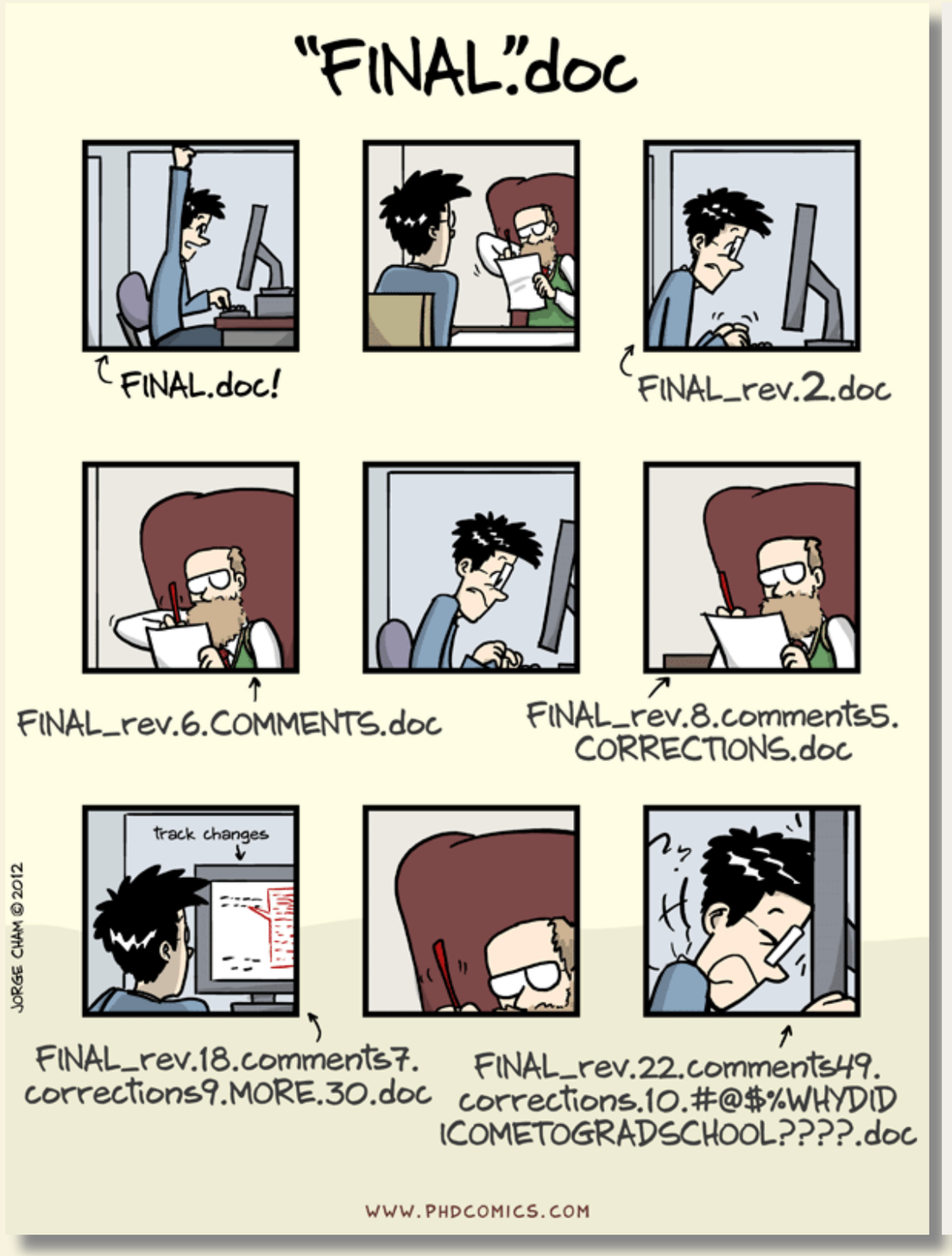

Image credit: www.phdcomics.com www.linode.com

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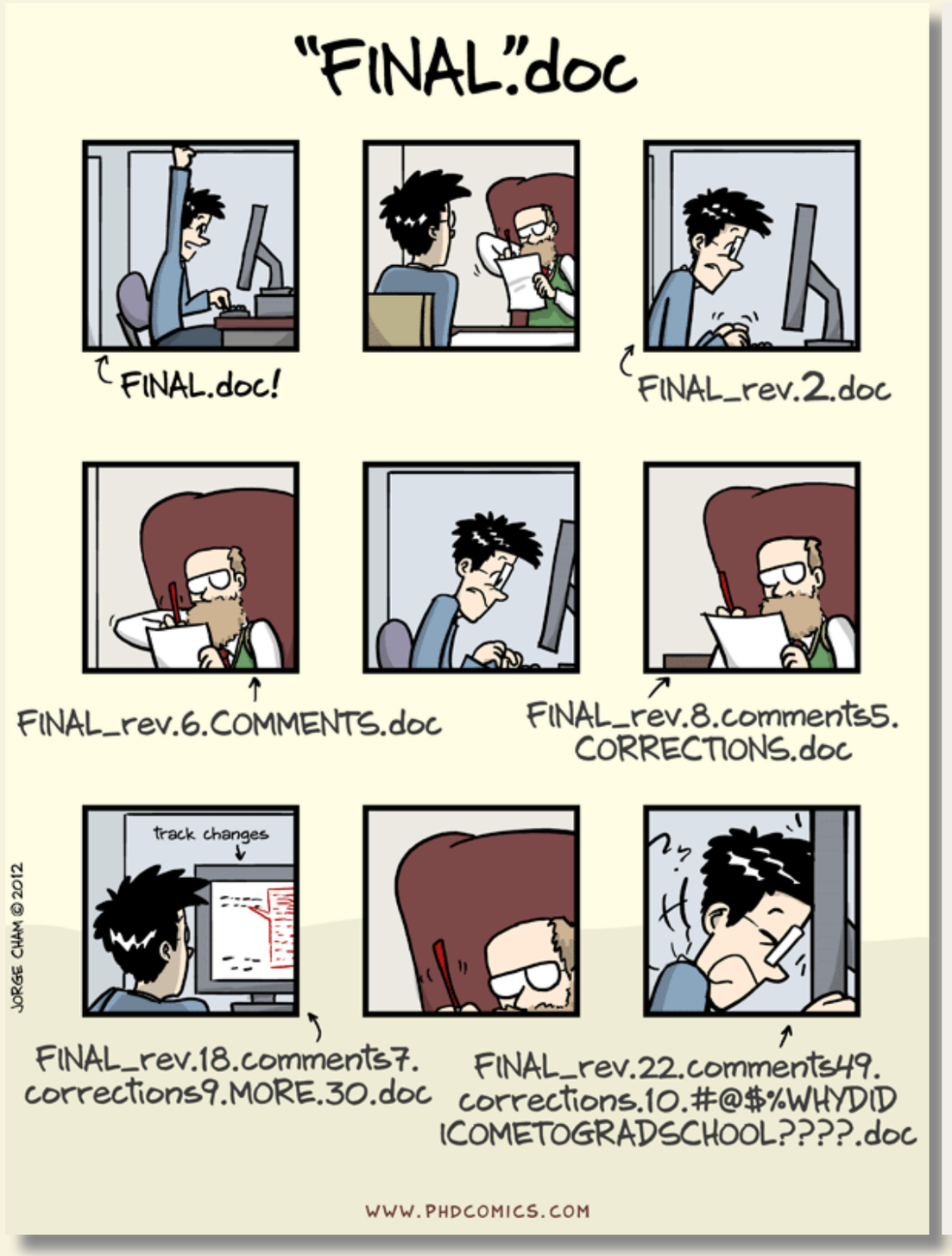

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TO THIS:

BUT: Version control is only one aspect of data management

CONSUMING DATASETS

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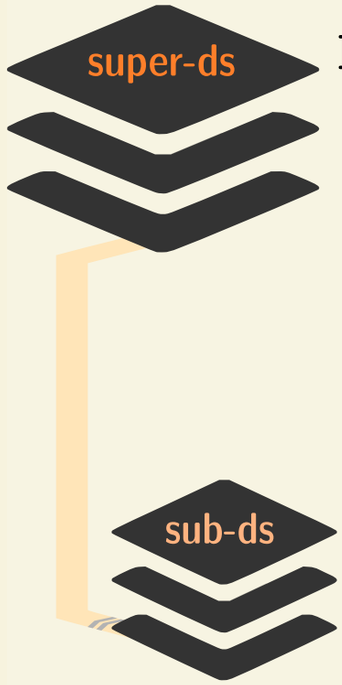

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    progit.pdf
    TLCL.pdf
  recordings/
    longnow/
      Long_Now___Conv[...]/
        ...
      Long_Now___Seminars[...]/
        2003_12_13[...]
        2003_11_15[...]
        ...
  notes.txt

Dataset structure is fully flexible to be able to accommodate domain standards or personal preferences.

A dataset can be populated with any type of files, and these files can be saved to the dataset.

Published repositories can be installed as subdatasets. This nesting can be arbitrily deep. Datasets can be installed from a path, URL., or data collection.

DataLad can obtain required subdataset content on demand. Only content elements actually required for an analysis are present. Directory structure is expanded recursively as needed.

Any content is referenced via the dataset that contains it. Dataset state provides unambiguous version specification for the subdataset.

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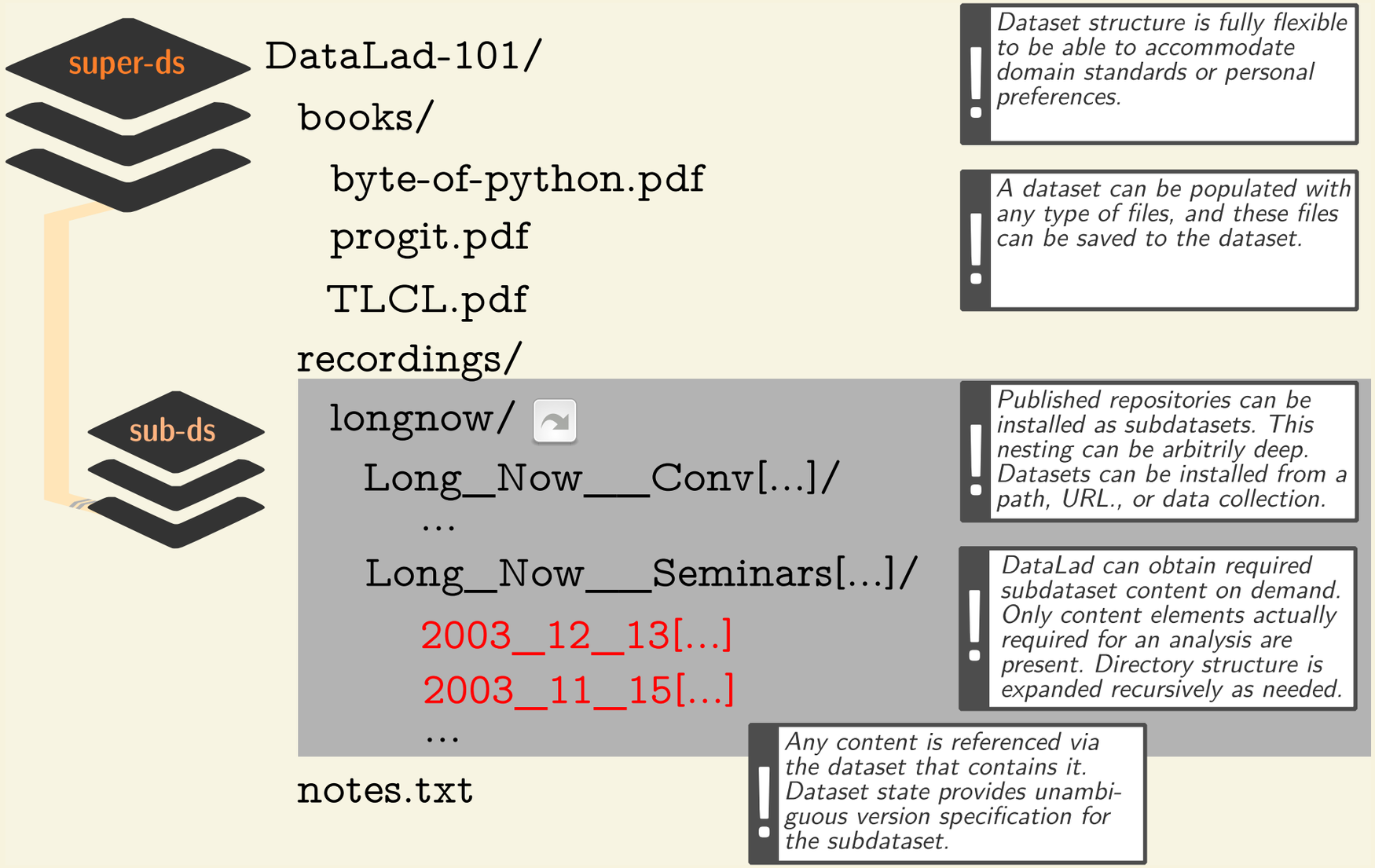

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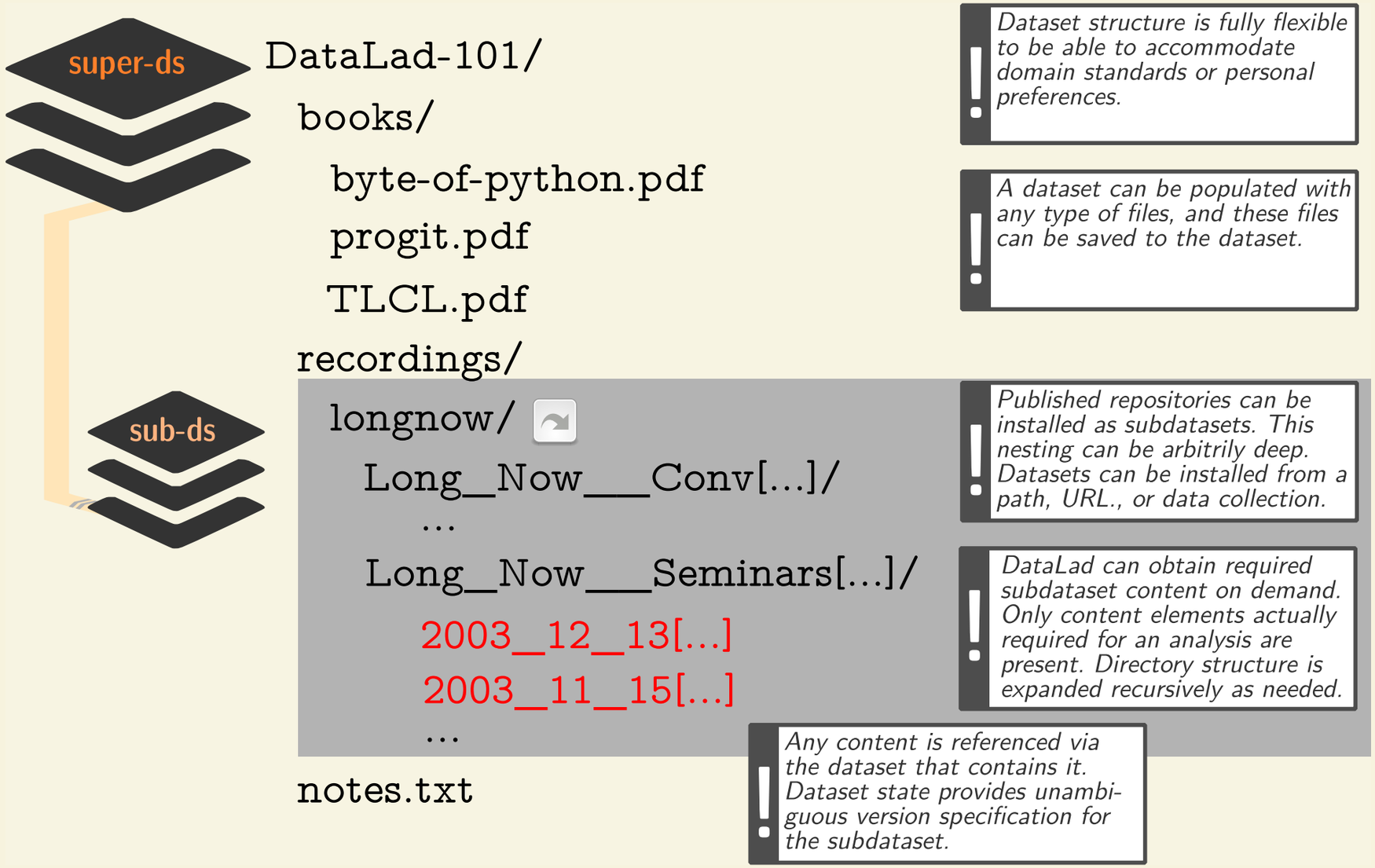

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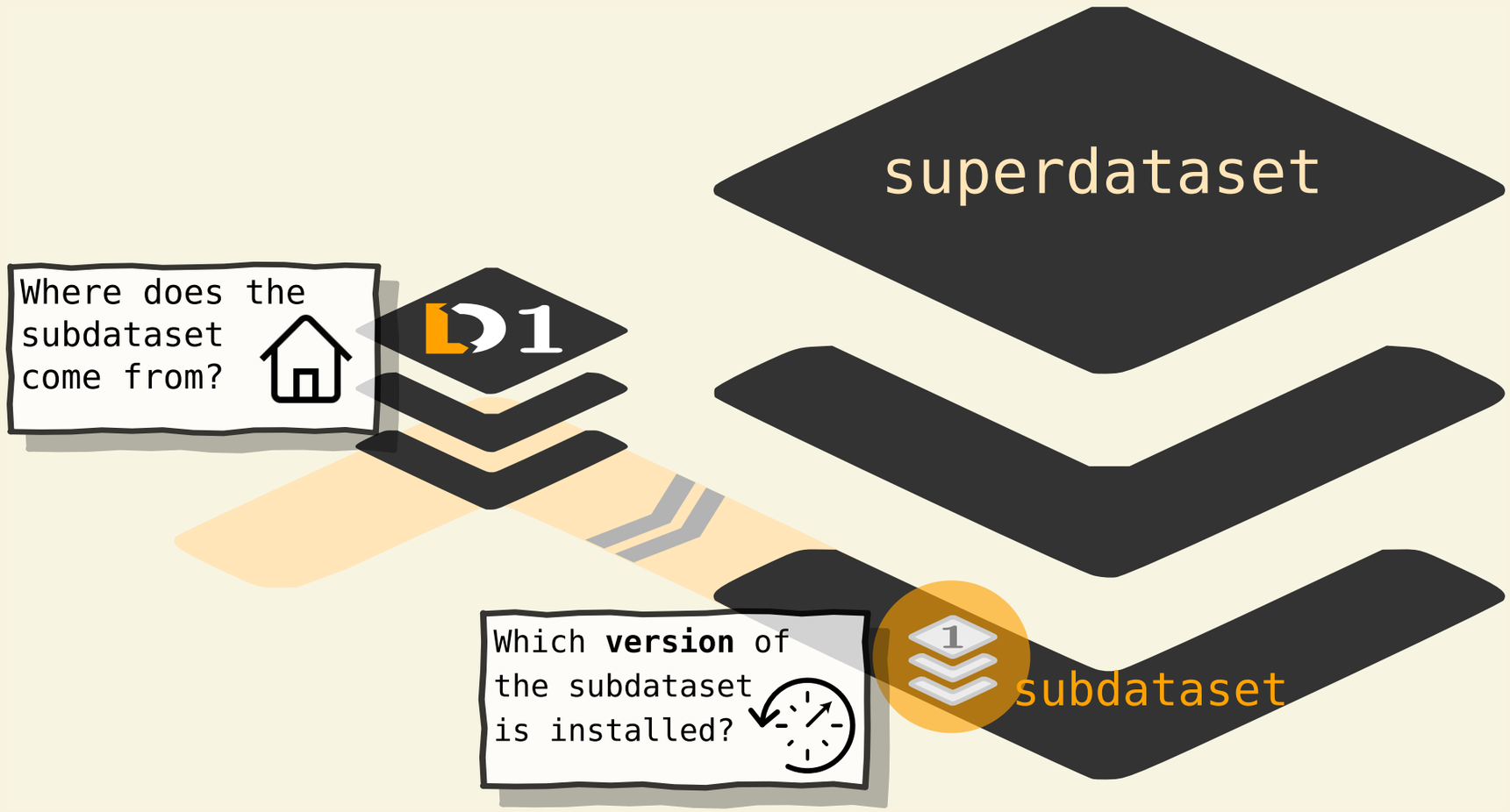

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Datasets preserve their history.

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

REPRODUCIBLE DATA ANALYSIS

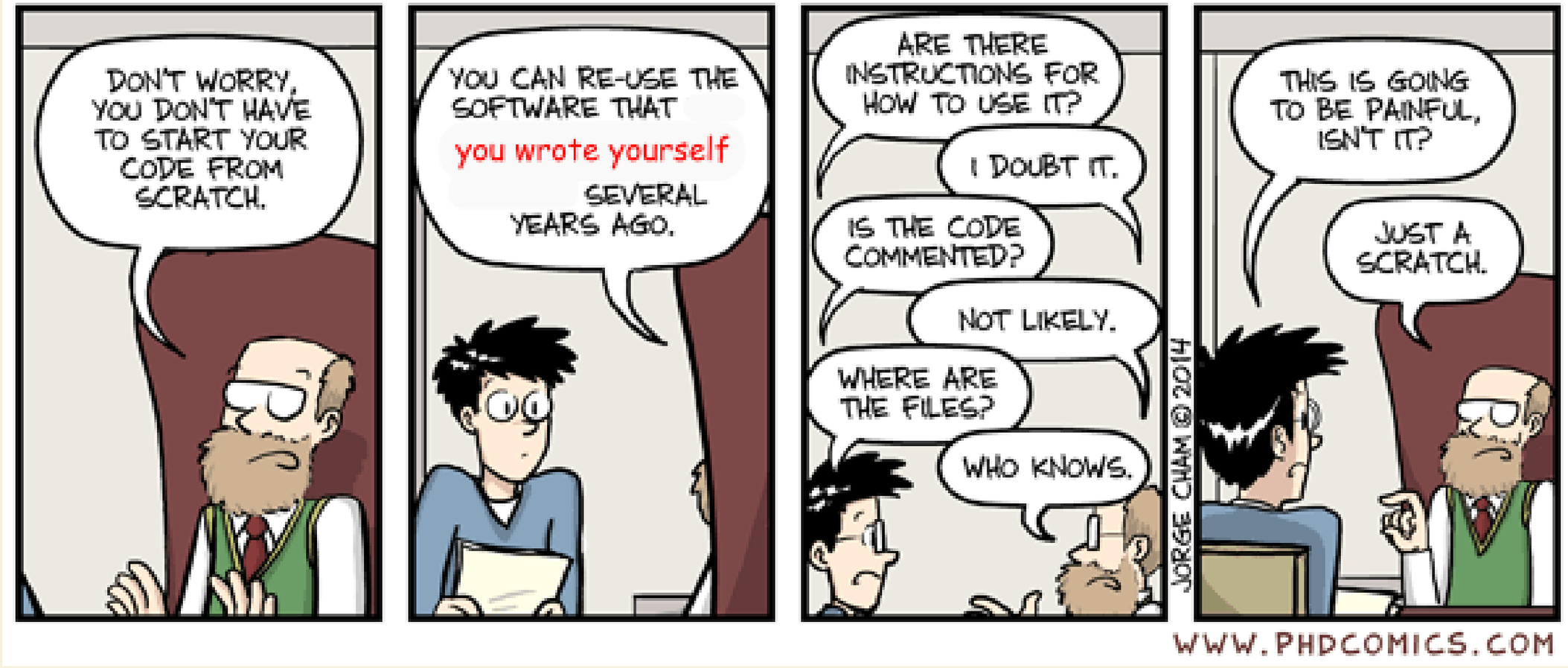

Image credit: Full comic at http://phdcomics.com/comics.php?f=1979

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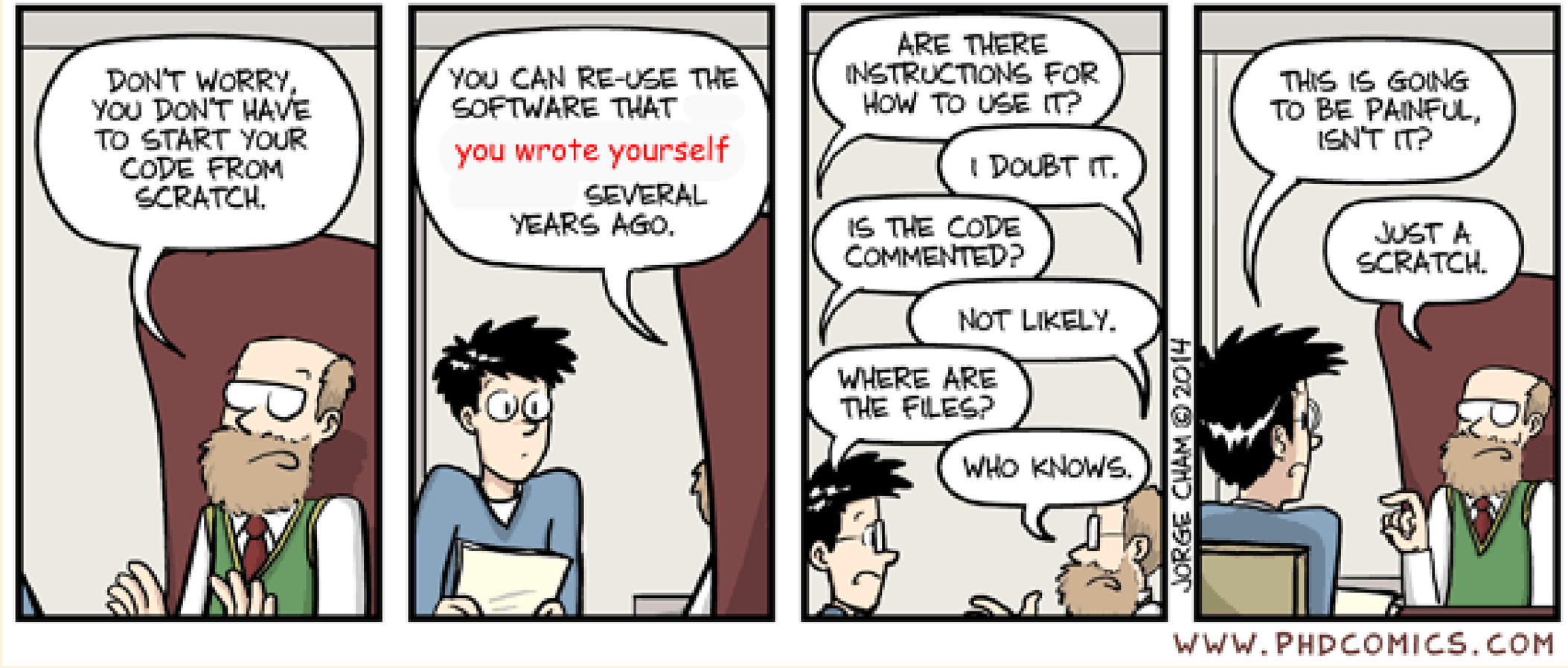


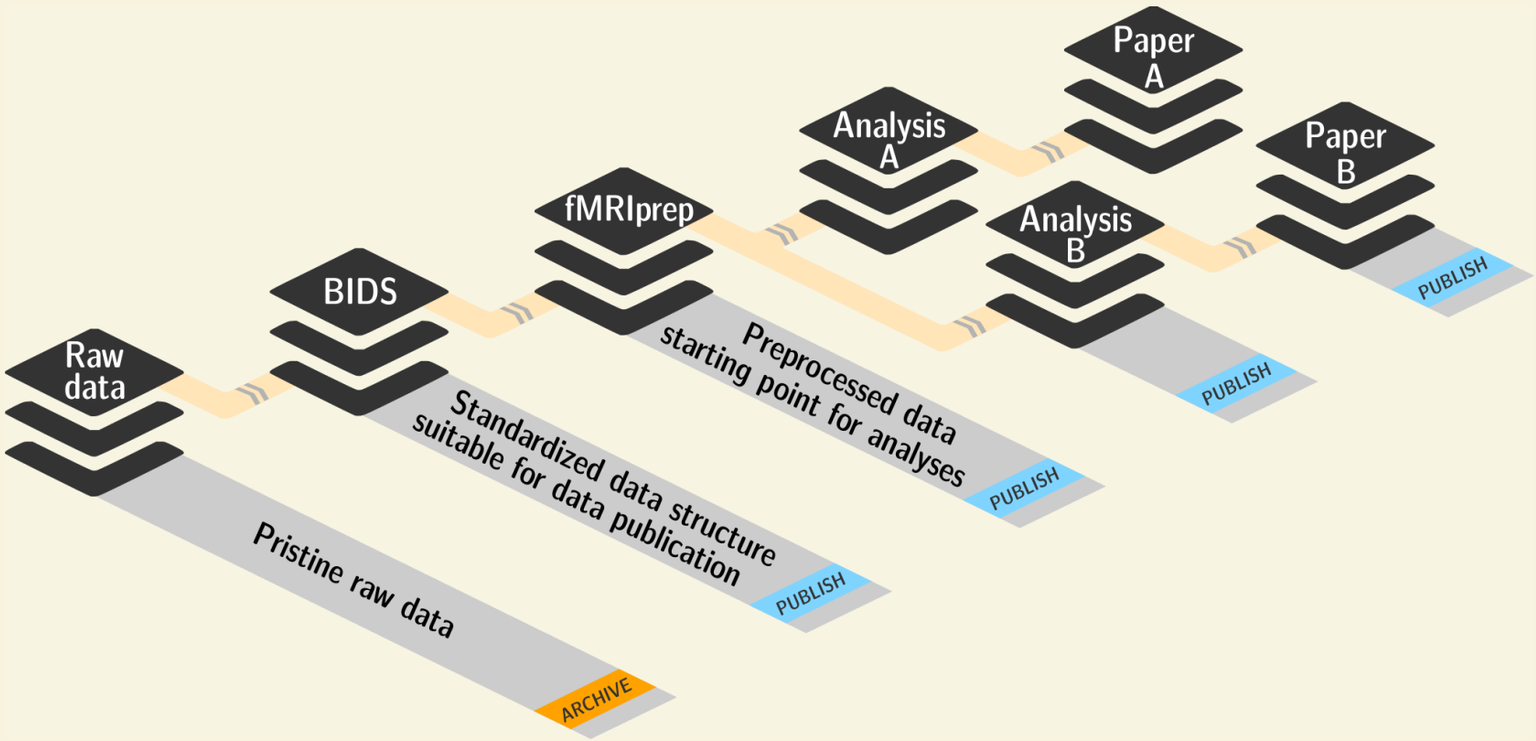
Image credit: Full comic at http://phdcomics.com/comics.php?f=1979

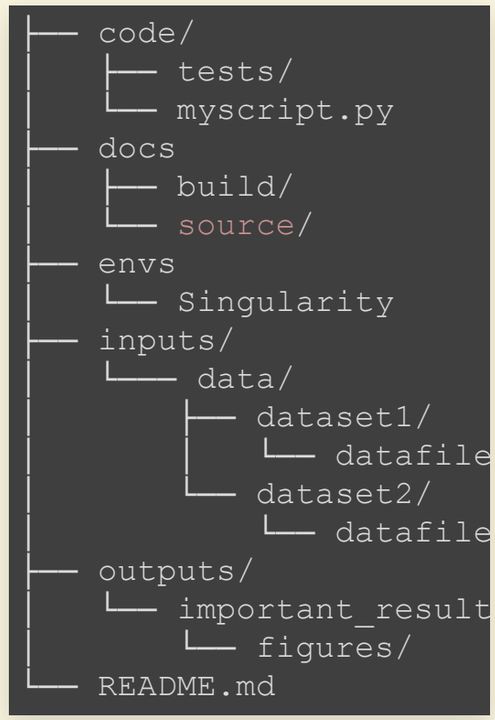
Code to follow along:
http://handbook.datalad.org/en/latest/code_from_chapters/10_yoda_code.html

BASIC ORGANIZATIONAL PRINCIPLES FOR DATASETS

Keep everything clean and modular

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



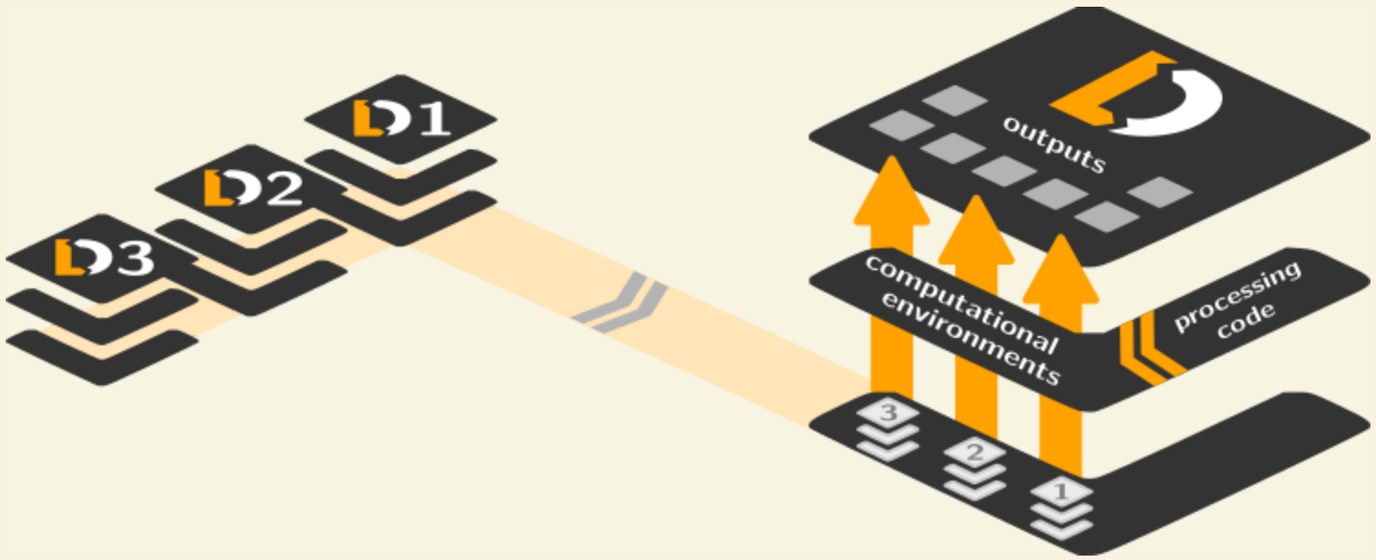


- do not touch/modify raw data: save any results/computations *outside* of input datasets
- Keep a superdataset self-contained: Scripts reference subdatasets or files with *relative paths*

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

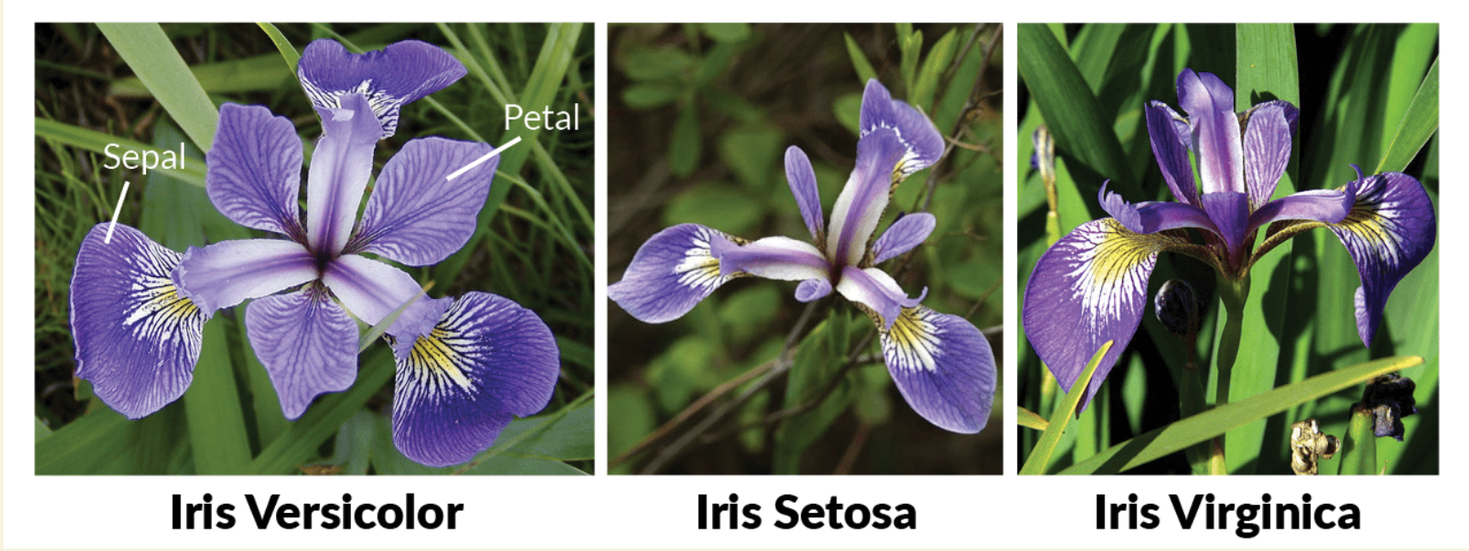


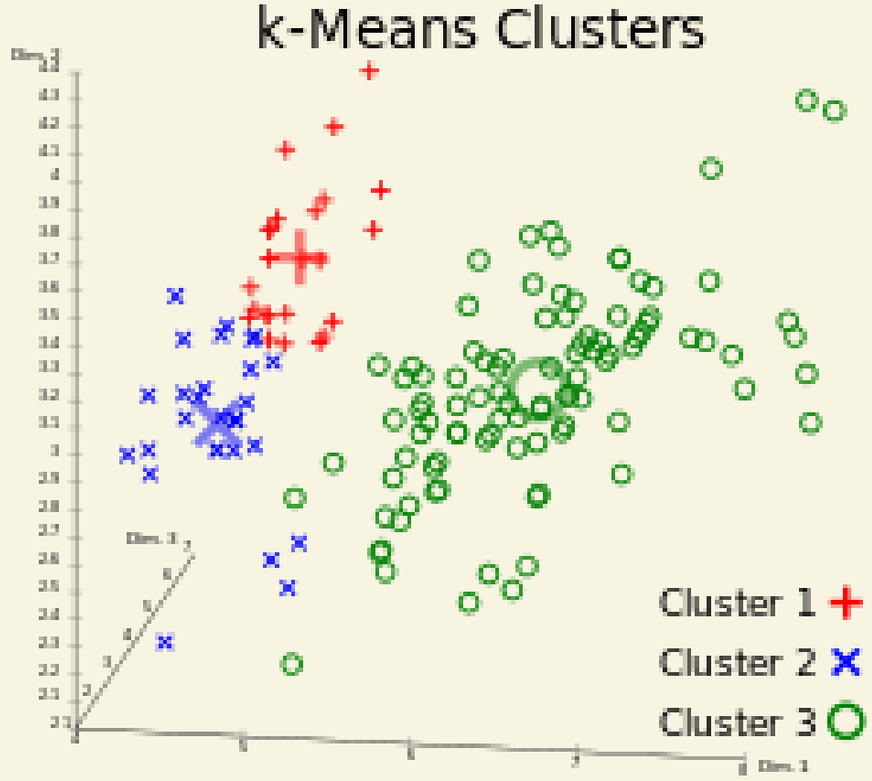
Document everything:

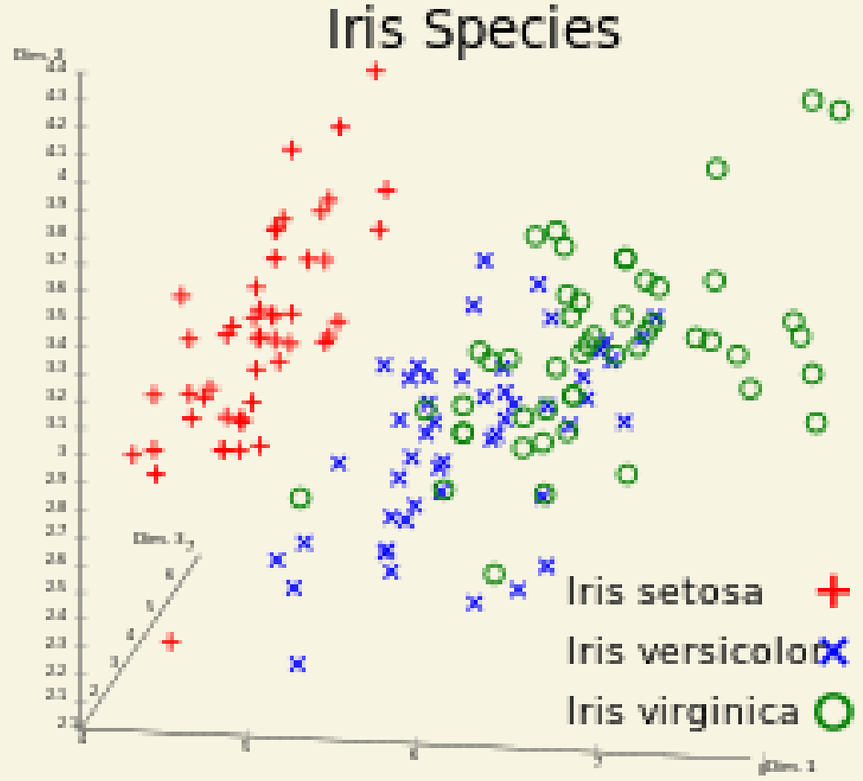
- Which script produced which output? From which data? In which software environment? …

Find out more about organizational principles in the YODA principles!

A CLASSIFICATION ANALYSIS ON THE IRIS FLOWER DATASET







REPRODUCIBLE EXECUTION & PROVENANCE CAPTURE

datalad run

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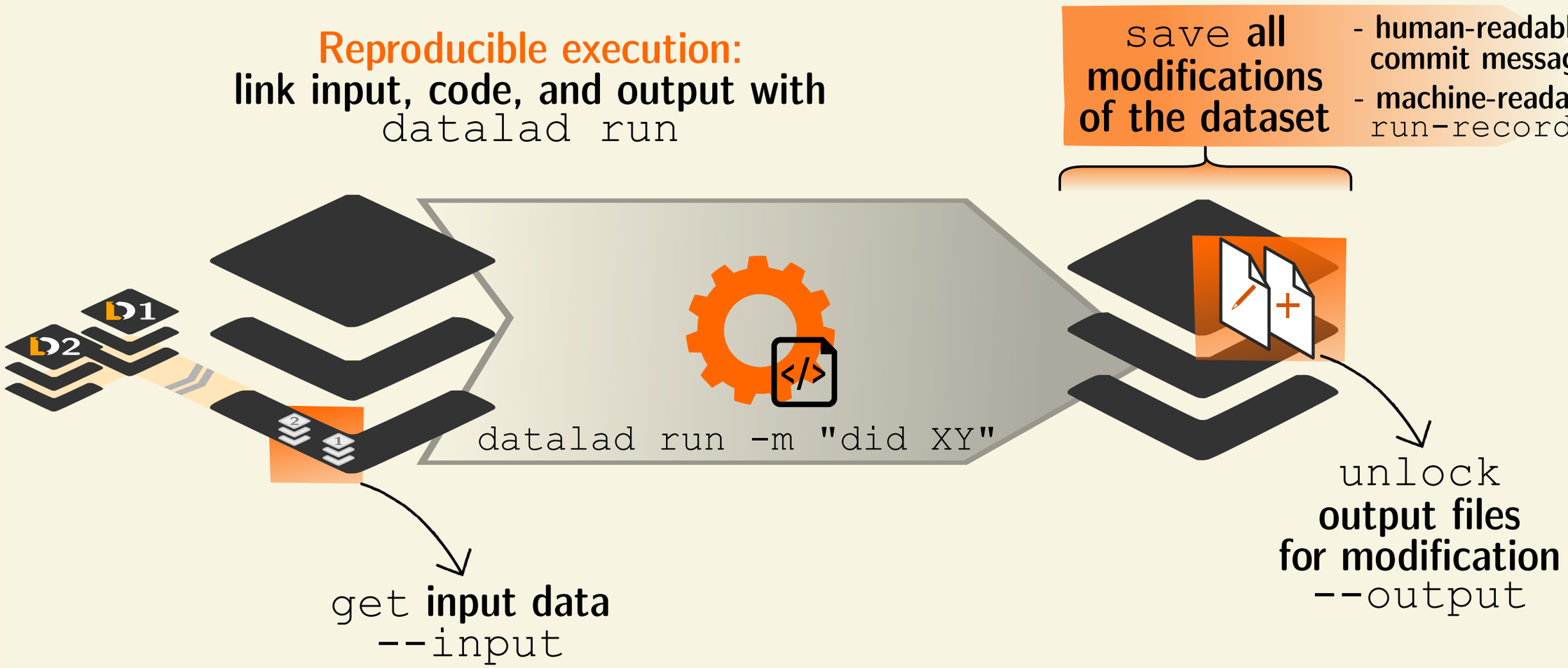

COMPUTATIONAL REPRODUCIBILITY

- 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`

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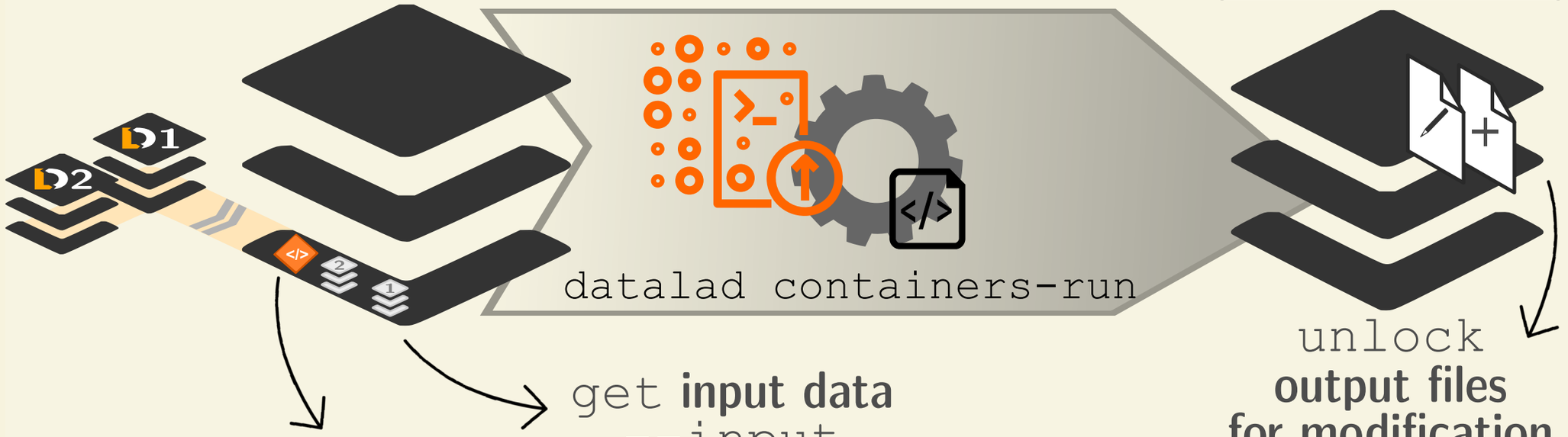
datalad-containers run

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

save all
modifications
of the dataset



get input data
--input

unlock
output files
for modification
--output

get and use registered software
container for computation
--container-name

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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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- 17+ additional contributors

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- Benjamin Poldrack
- Kyle Meyer
- 22+ additional contributors

THANK YOU!

QUESTIONS?