DATALAD BASICS

Code to follow along: handbook.datalad.org/r.html?MPIBerlin

PREREQUISITES: INSTALLATION AND CONFIGURATION

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$ git config --list
user.name=Adina Wagner
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[...]
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```

Else, find installation and configuration instructions at handbook.datalad.org

USING DATALAD

- DataLad can be used from the command line

```
datalad create mydataset
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- ... or with its Python API

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import datalad.api as dl
dl.create(path="mydataset")
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import datalad.api as dl
dl.create(path="mydataset")
```

- ... and other programming languages can use it via system call

```
# in R
> system("datalad create mydataset")
```

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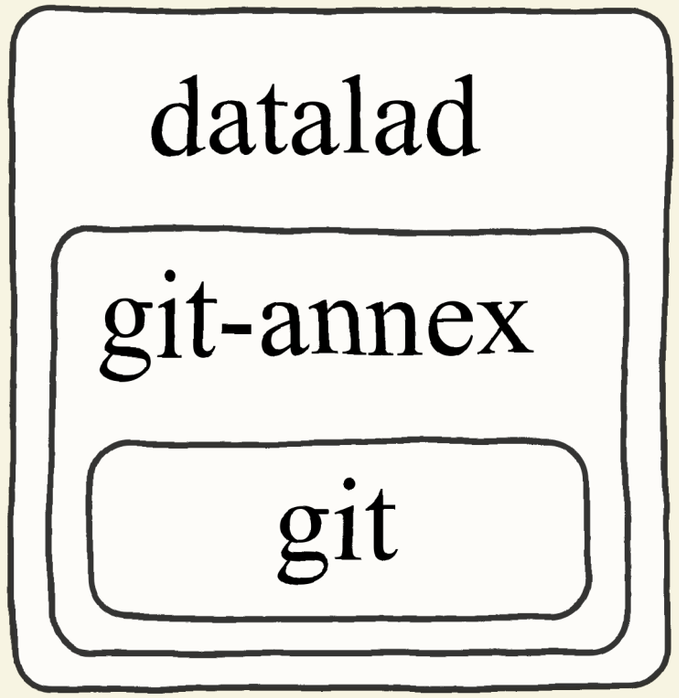
  - Datasets can be nested: *linked subdirectories*
- Let's start by creating a dataset

DATALAD DATASETS



A DataLad dataset is a joined Git + git-annex repository

WHY VERSION CONTROL?

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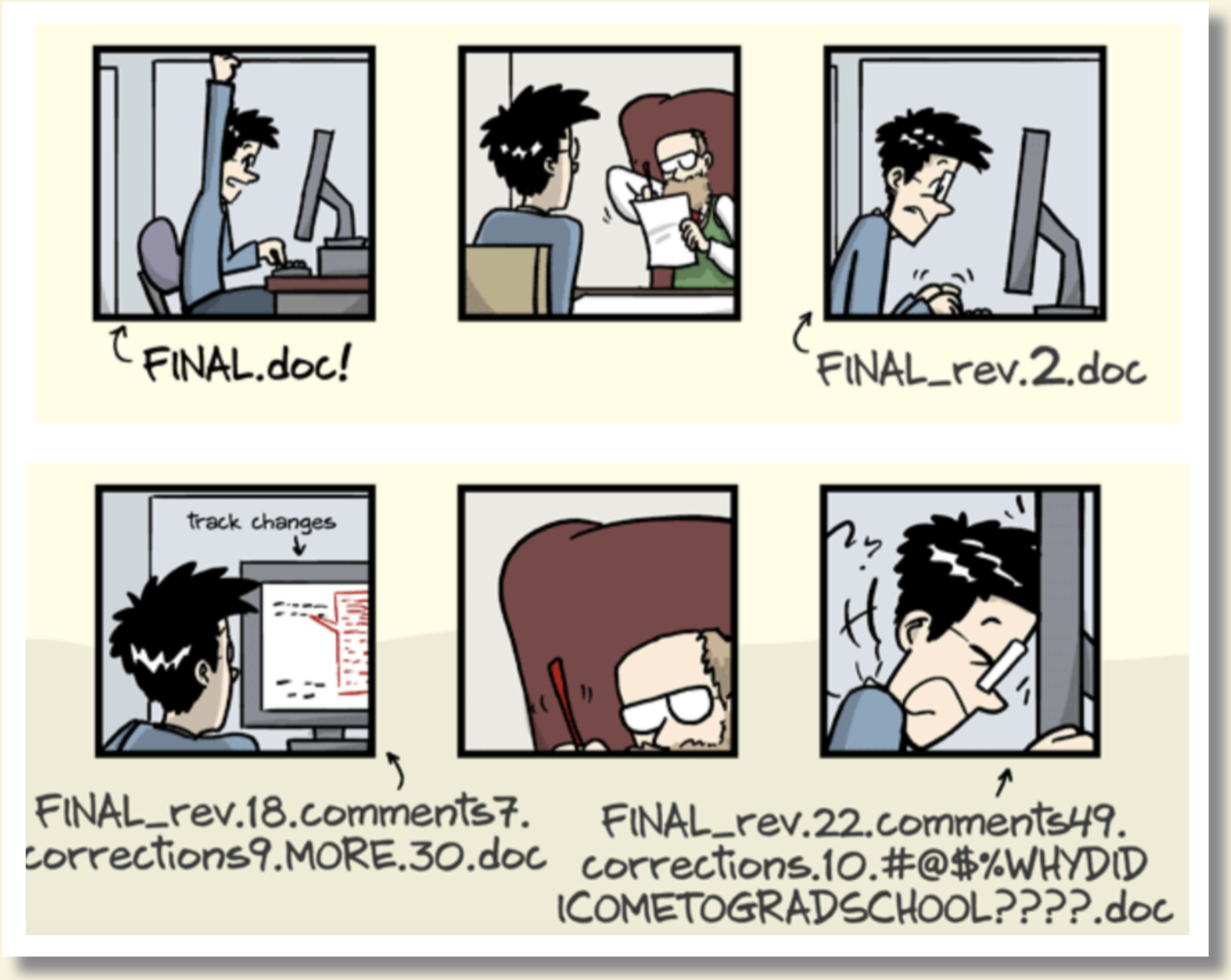

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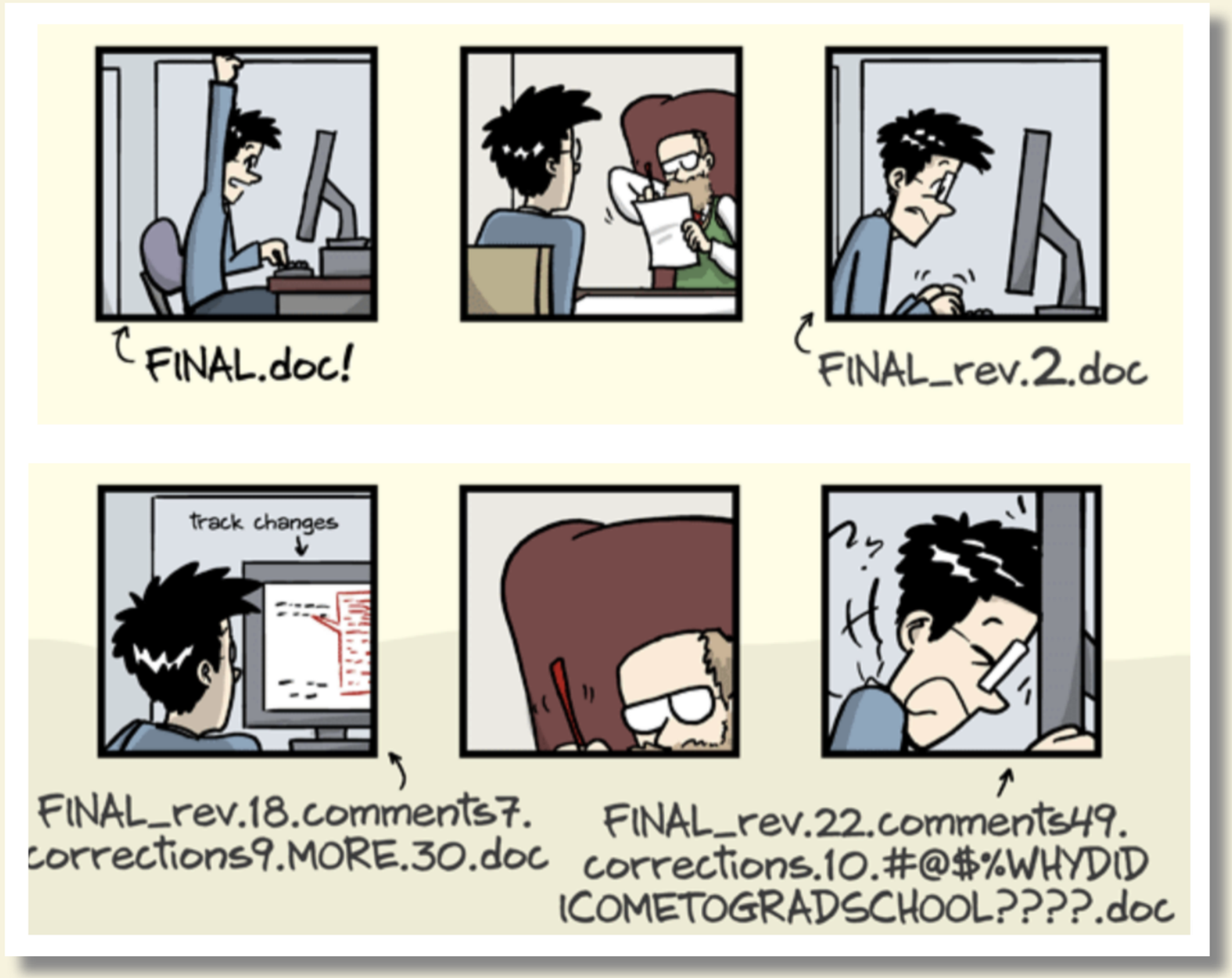

- keep things organized
- keep track of changes

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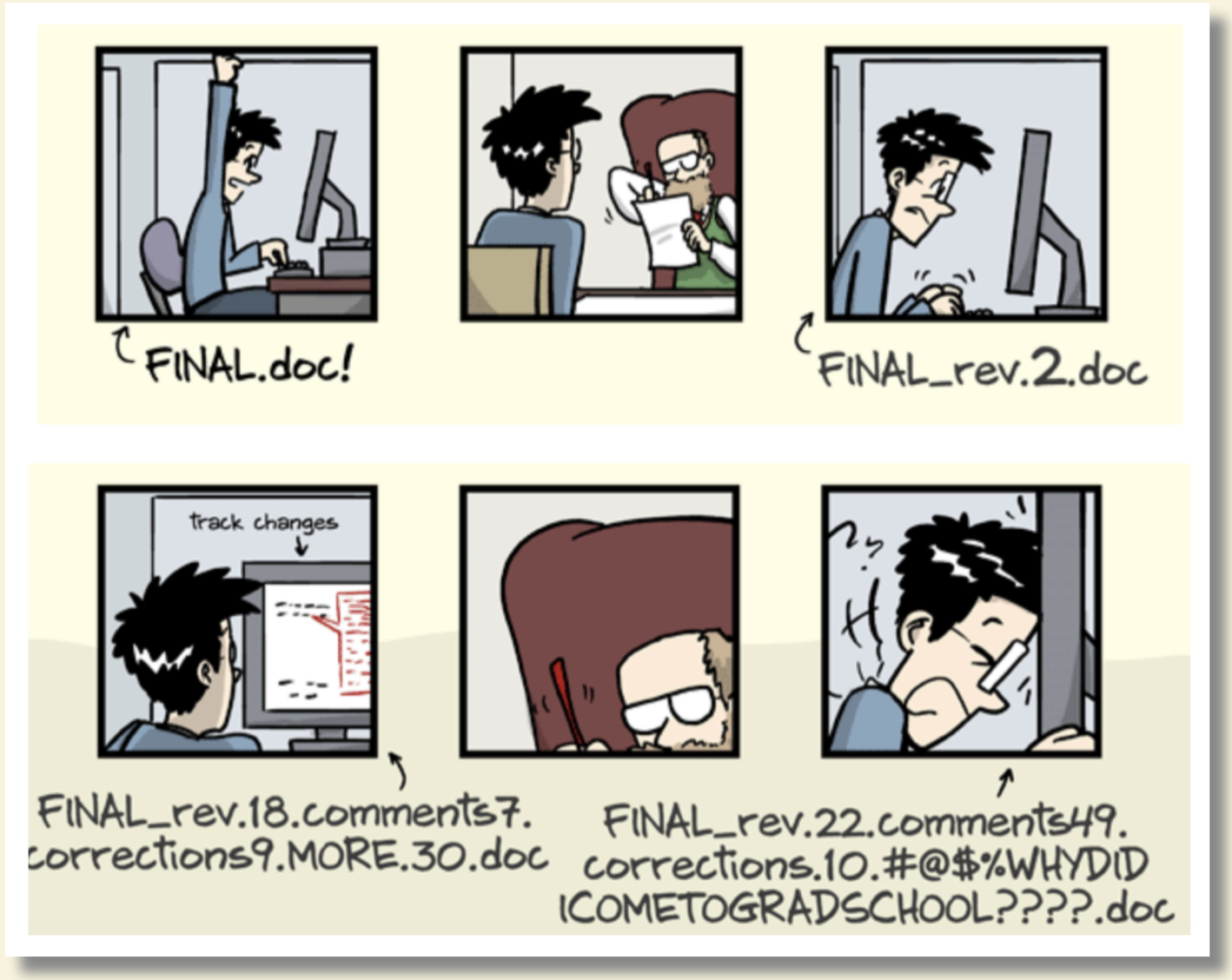

- keep things organized
- keep track of changes
- revert changes or go back to previous states

VERSION CONTROL

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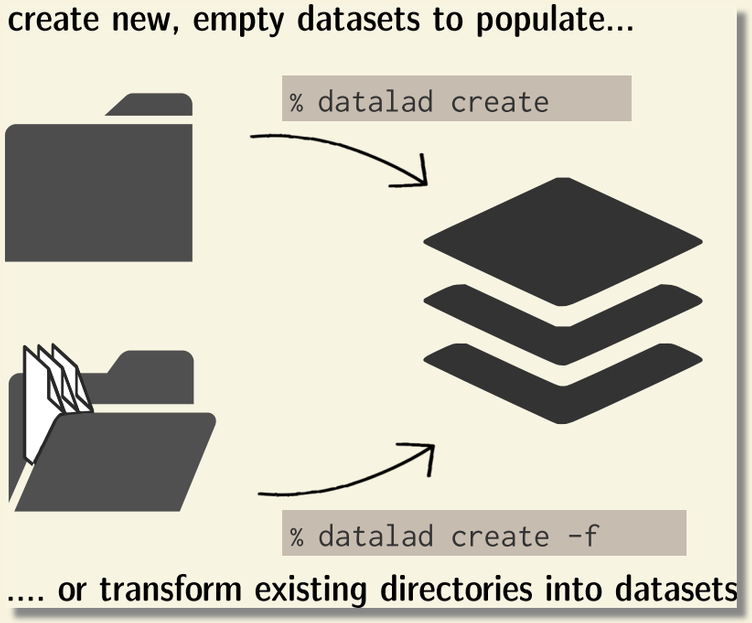

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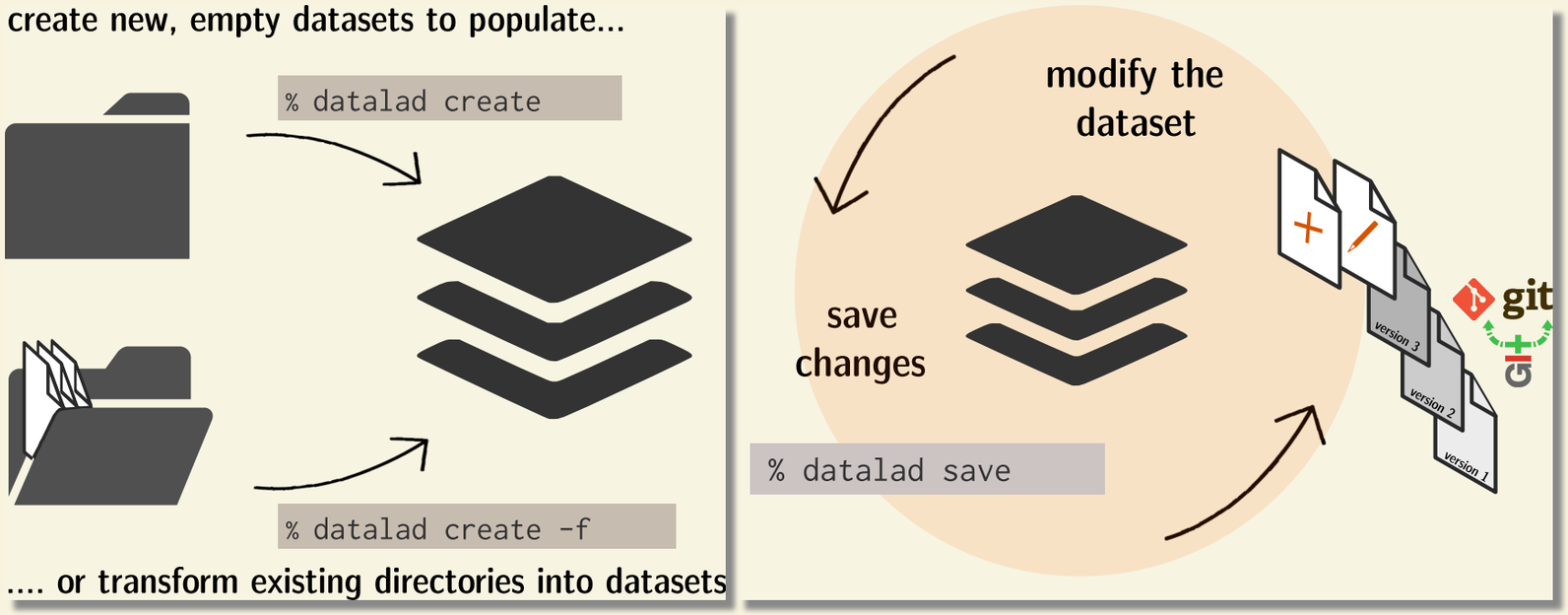

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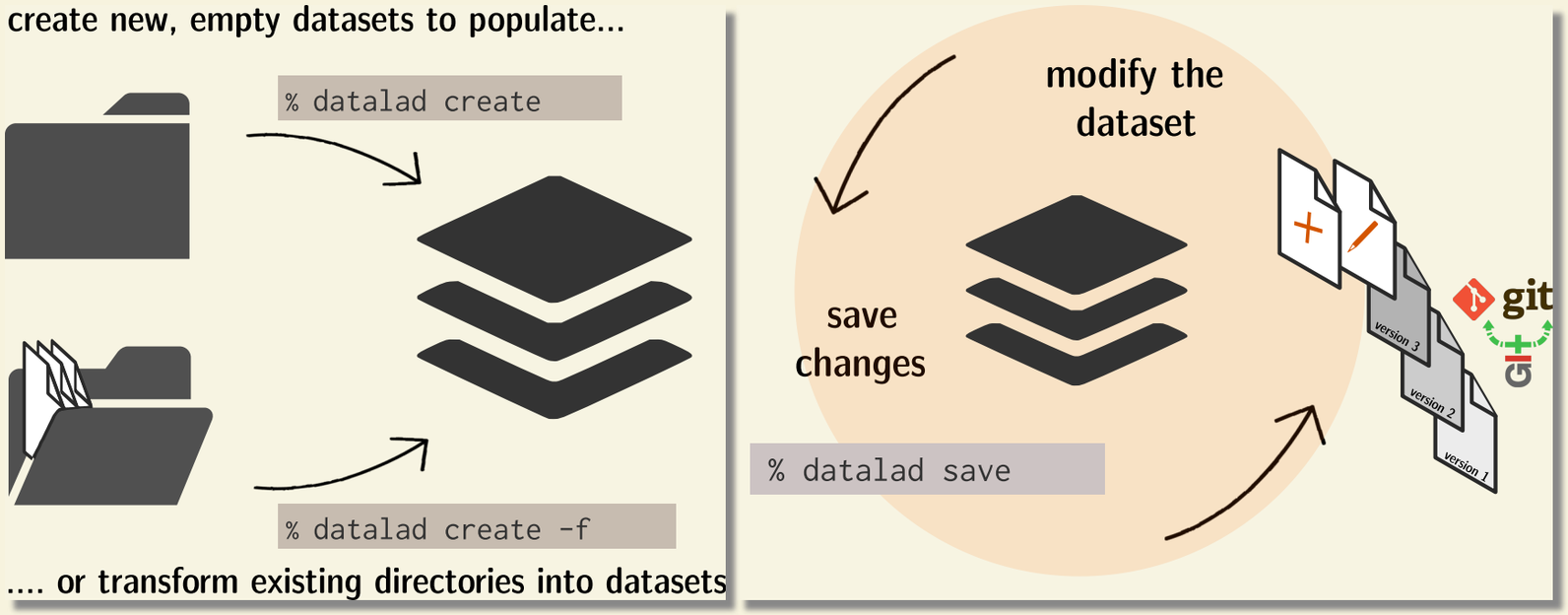

- Every file you put into a in a dataset can be easily version-controlled, regardless of size, with the same command.

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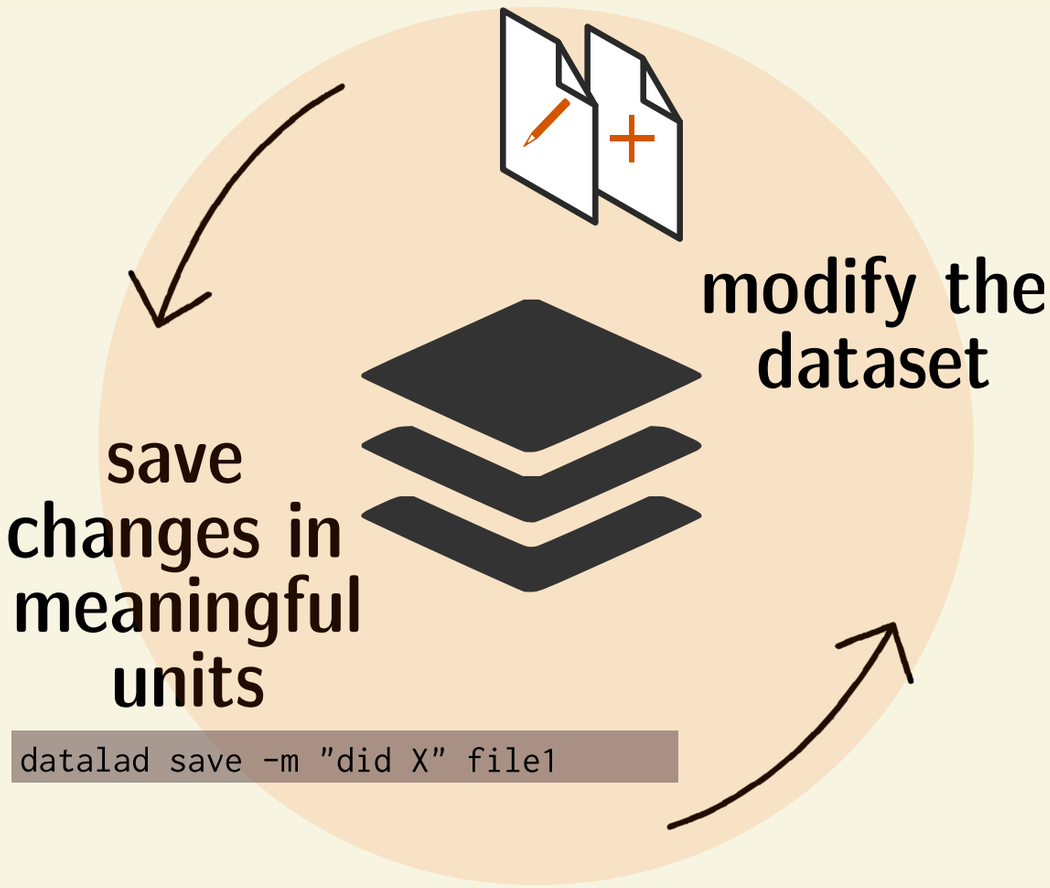

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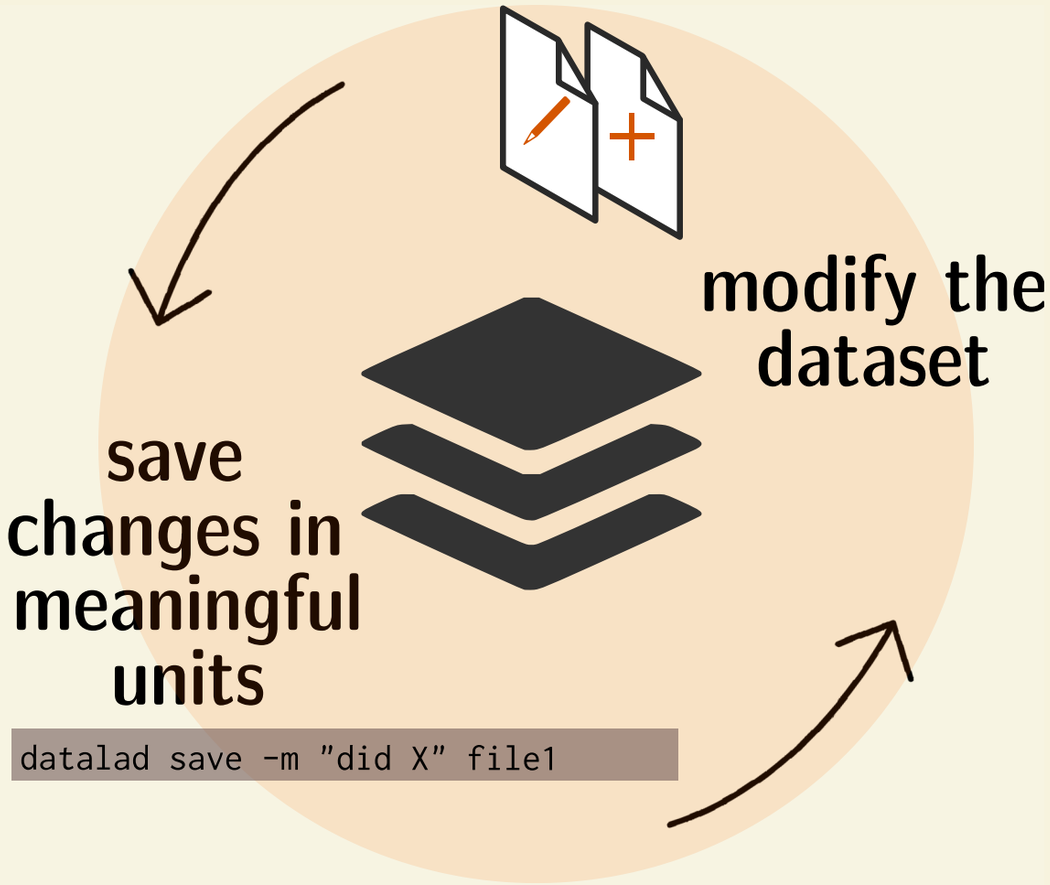

Advice:

LOCAL VERSION CONTROL

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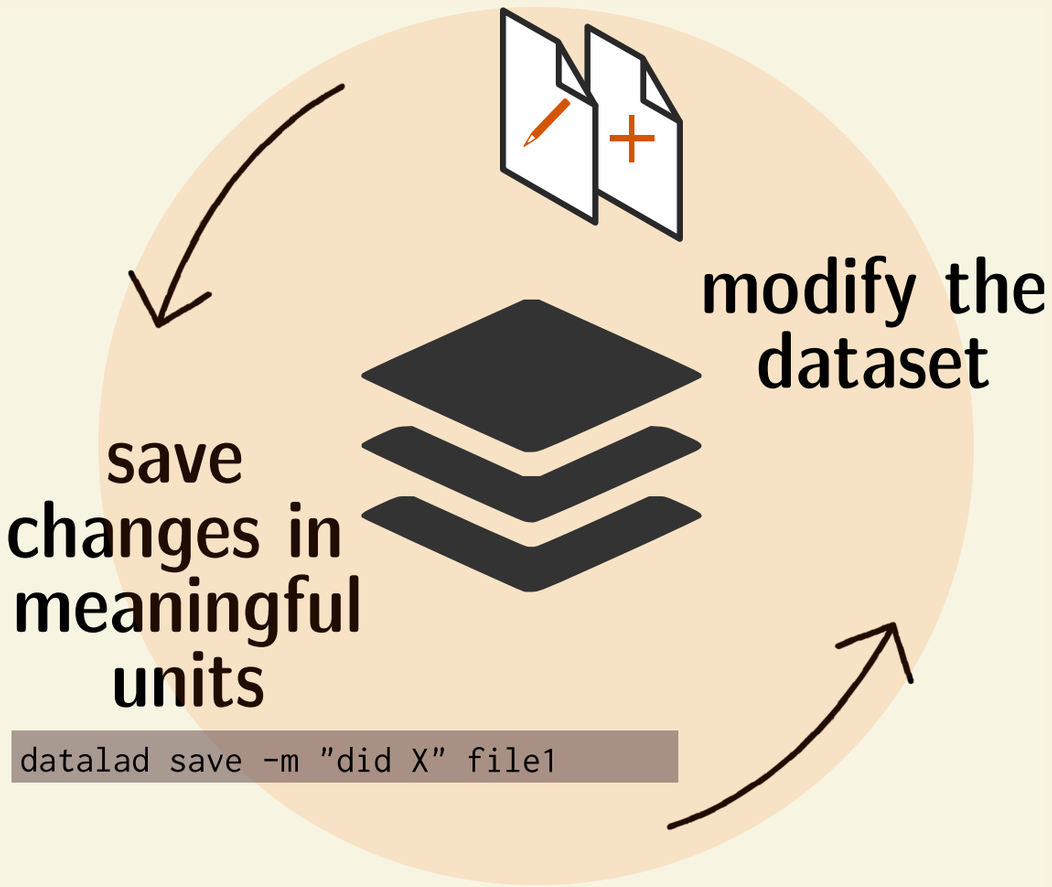

Advice:

- Save *meaningful* units of change

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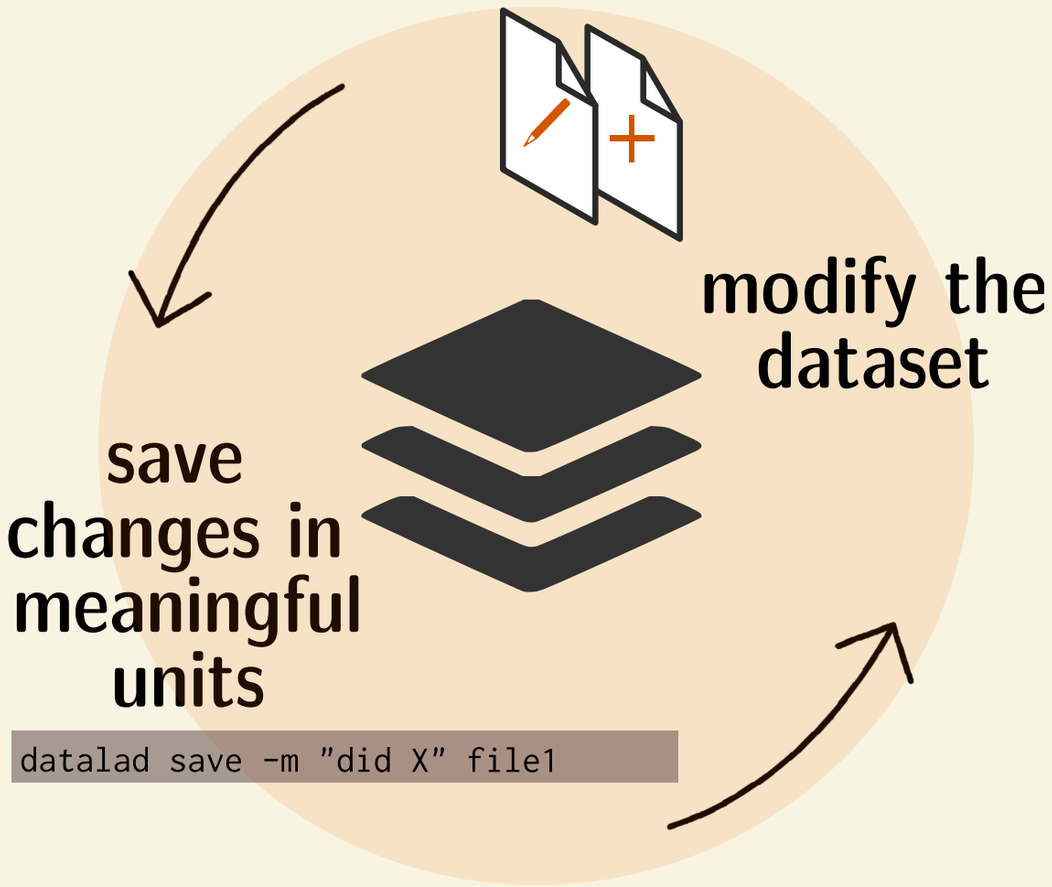

Advice:

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

THIS MEANS: YOU CAN ALSO VERSION CONTROL DATA!

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```
$ datalad save \
  -m "Adding raw data from neuroimaging study 1" \
  sub-*
  add(ok): sub-1/anat/T1w.json (file)
  add(ok): sub-1/anat/T1w.nii.gz (file)
  add(ok): sub-1/anat/T2w.json (file)
  add(ok): sub-1/anat/T2w.nii.gz (file)
  add(ok): sub-1/func/sub-1-run-1_bold.json (file)
  add(ok): sub-1/func/sub-1-run-1_bold.nii.gz (file)
  add(ok): sub-10/anat/T1w.json (file)
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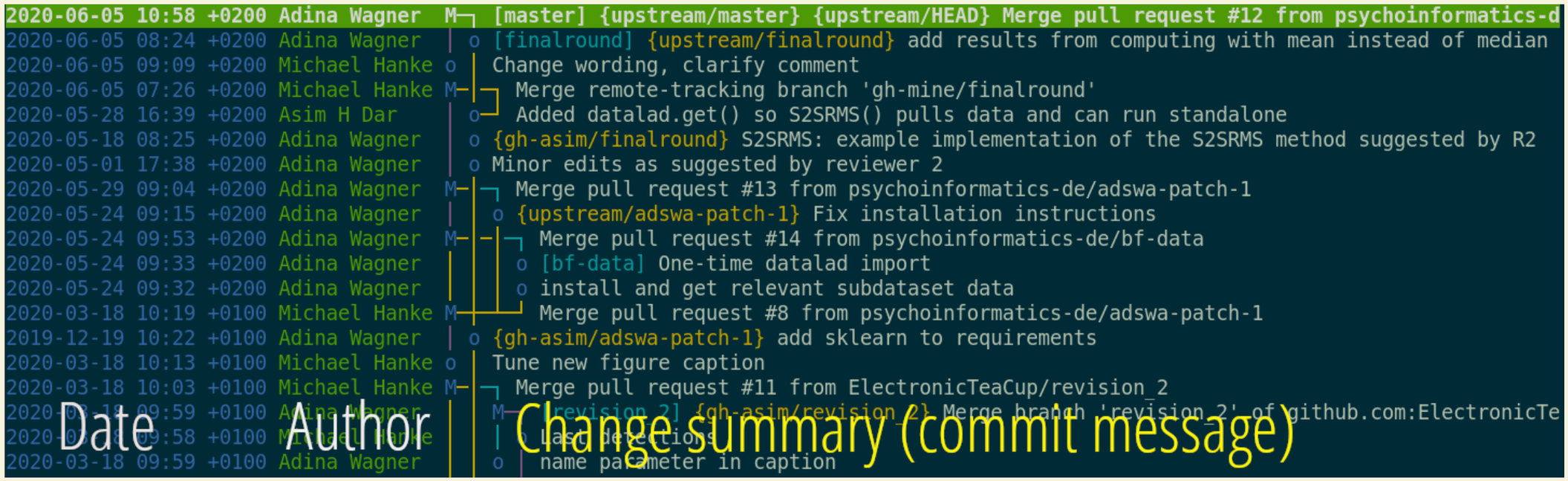
[110 similar messages have been suppressed]
  save(ok): . (dataset)
  action summary:
add (ok: 120)
save (ok: 1)
```

VERSION CONTROL

- Your dataset can be a complete research log, capturing everything that was done, when, by whom, and how



- Interact with the history:
- reset your dataset (or subset of it) to a previous state,
- throw out changes or bring them back,
- find out what was done when, how, why, and by whom
- Identify precise versions: Use data in the most recent version, or the one from 2018, or...
- ...

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- Have you ever saved a PDF to read later onto your computer, but forgot where you got it from?
- Digital Provenance = *"The tools and processes used to create a digital file, the responsible entity, and when and where the process events occurred"*
- The history of a dataset already contains provenance, but there is more to record - for example: Where does a file come from? `datalad download-url` is helpful

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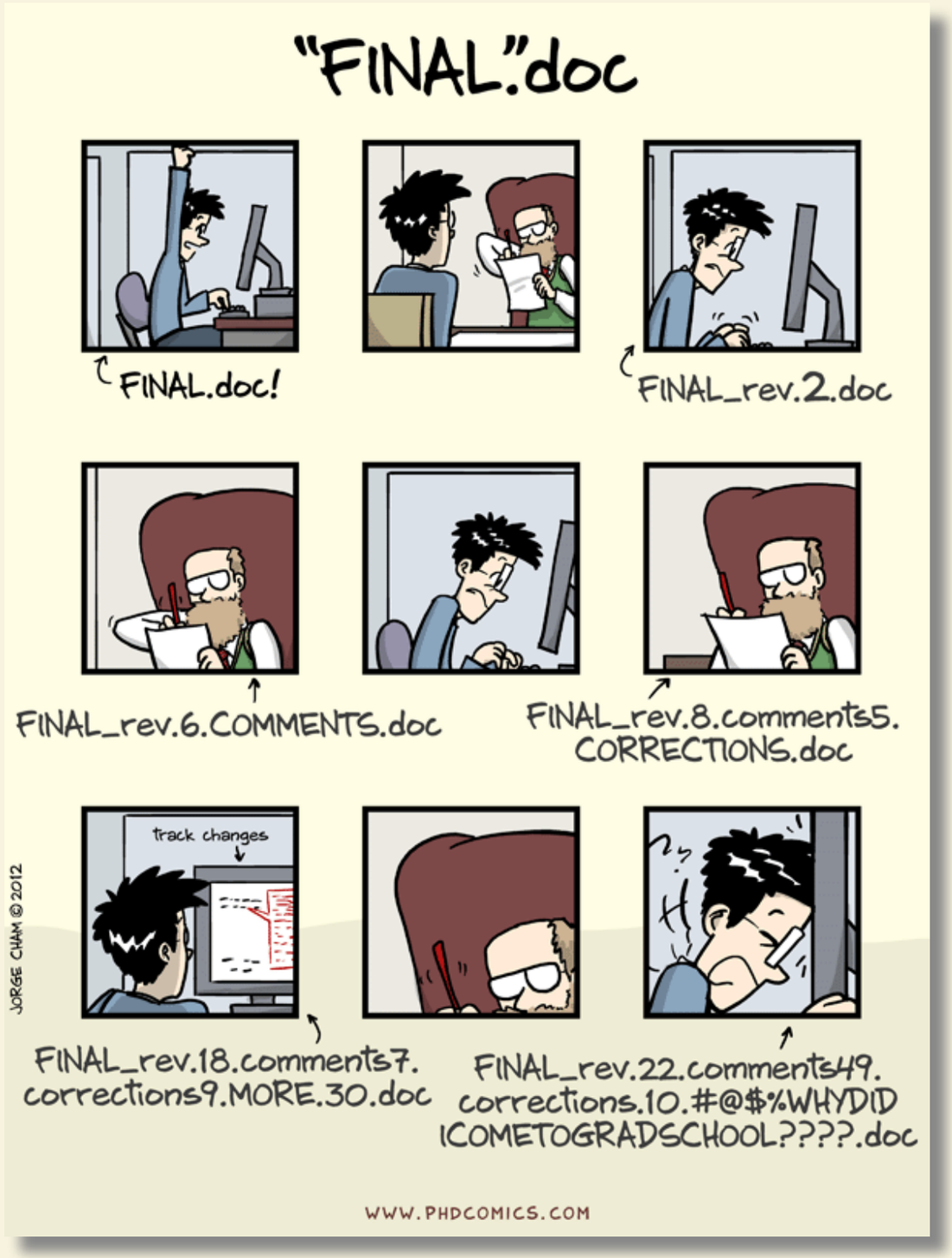
A clean dataset status (no modifications, not untracked files) is good practice.

FROM HERE


"FINAL".doc
FINAL.doc!
FINAL_rev.2.doc
FINAL_rev.6.COMMENTS.doc
FINAL_rev.8.comments5.
CORRECTIONS.doc
track changes
FINAL_rev.18.comments7.
corrections9.MORE.30.doc
FINAL_rev.22.comments49.
corrections.10.#@$%WHYDID
ICOMETOGRADSCHOOL????.doc
JORGE CHAM © 2012
WWW.PHDCOMICS.COM

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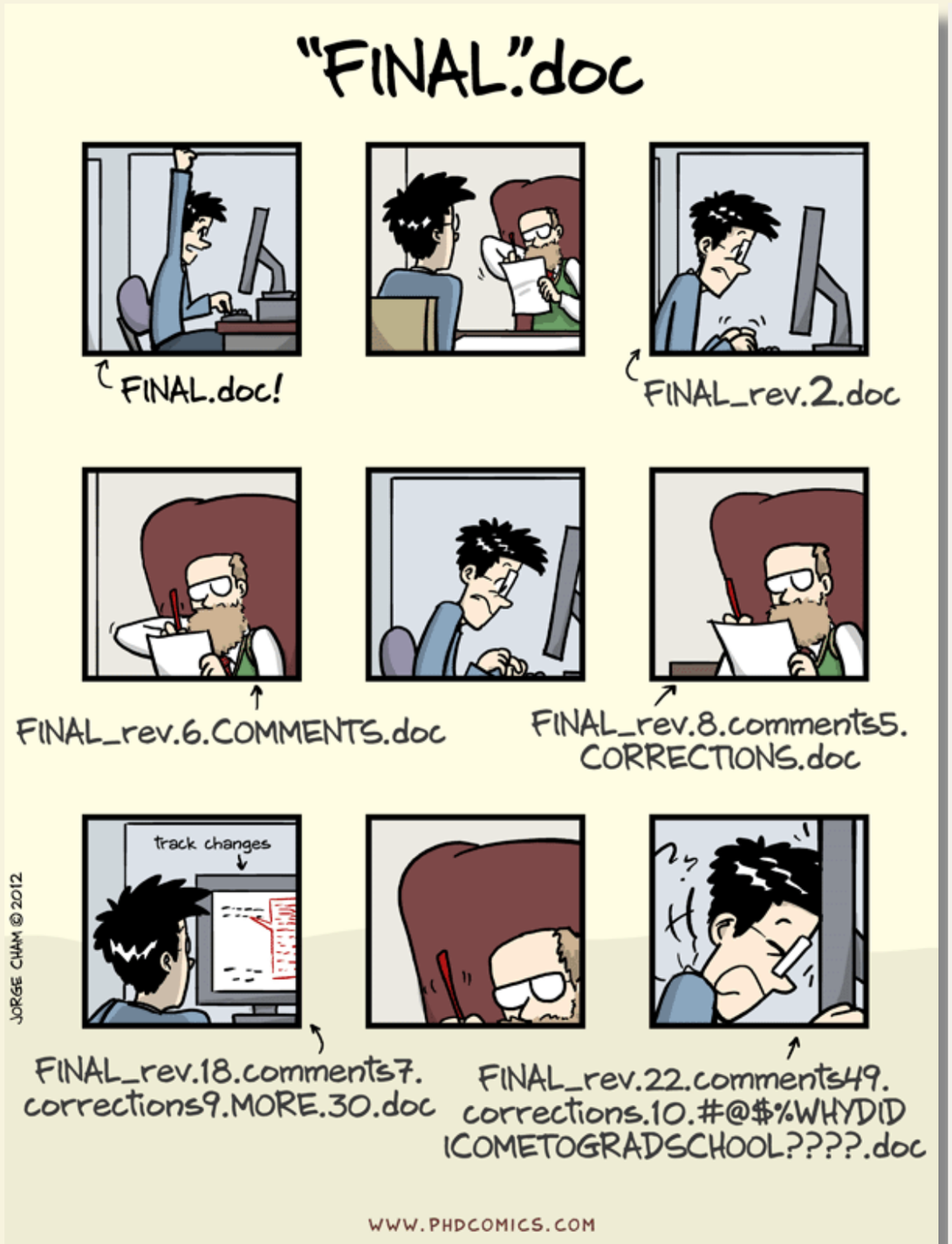

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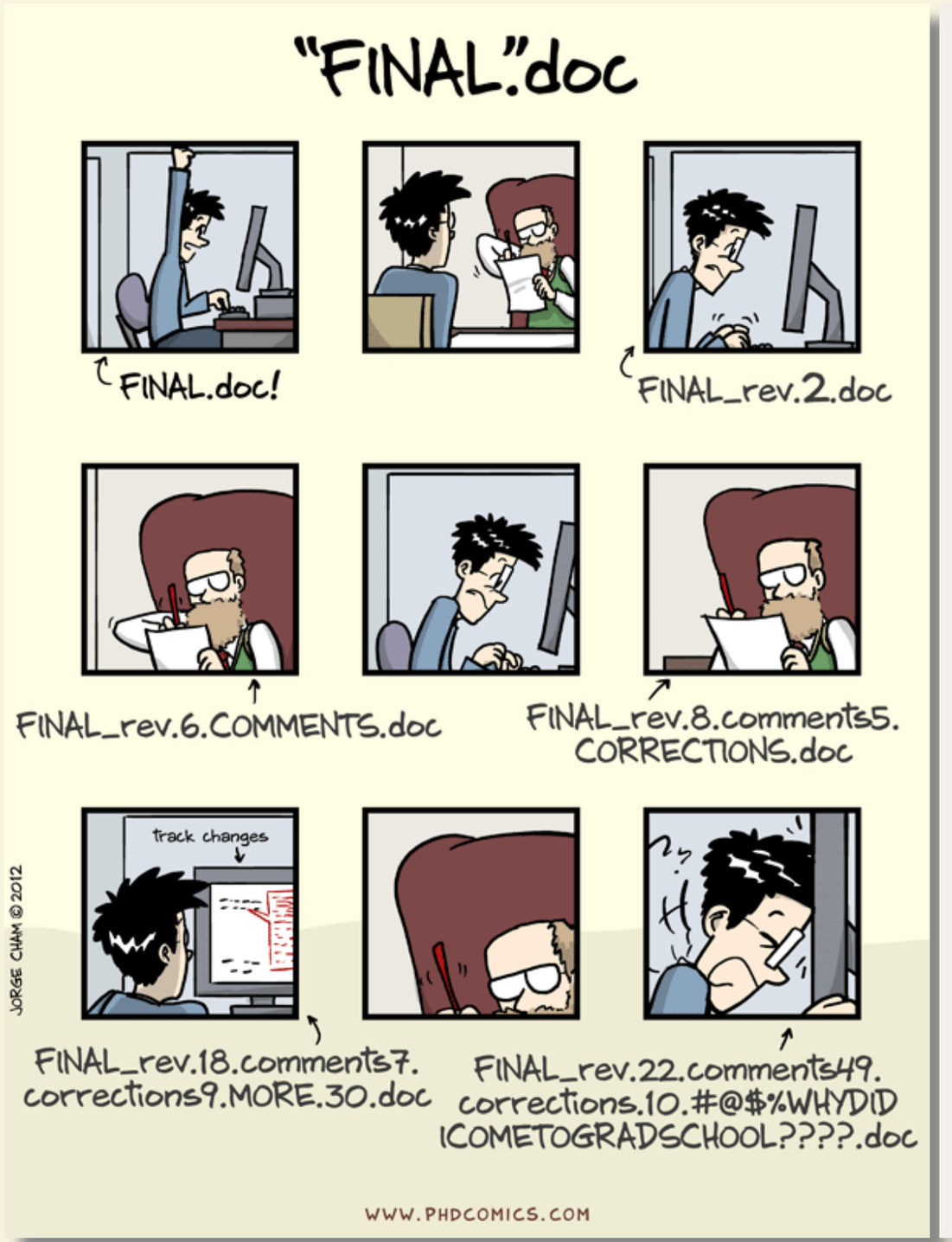

TO THIS:

BUT: Version control is only one aspect of data management

QUESTIONS!

http://etc.ch/5xo7

CONSUMING DATASETS

- A dataset can be created from scratch/existing directories:

```
$ datalad create mydataset
[INFO
] Creating a new annex repo at /home/adina/mydataset
create(ok): /home/adina/mydataset (dataset)
```

- but datasets can also be installed from paths or from URLs:

```
$ datalad clone https://github.com/datalad-datasets/human-connectome-project-openac
install(ok): /tmp/HCP (dataset)
```

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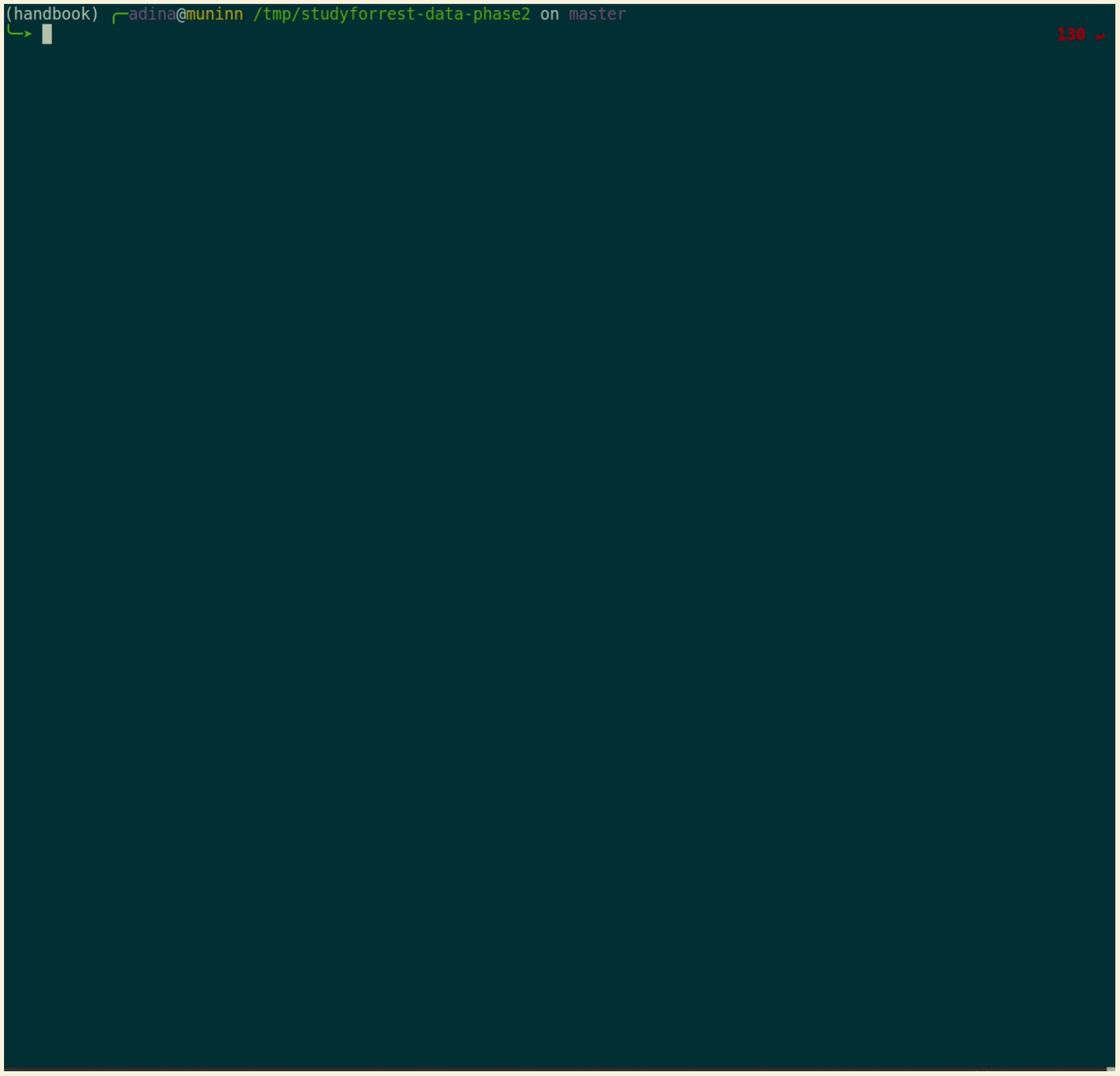

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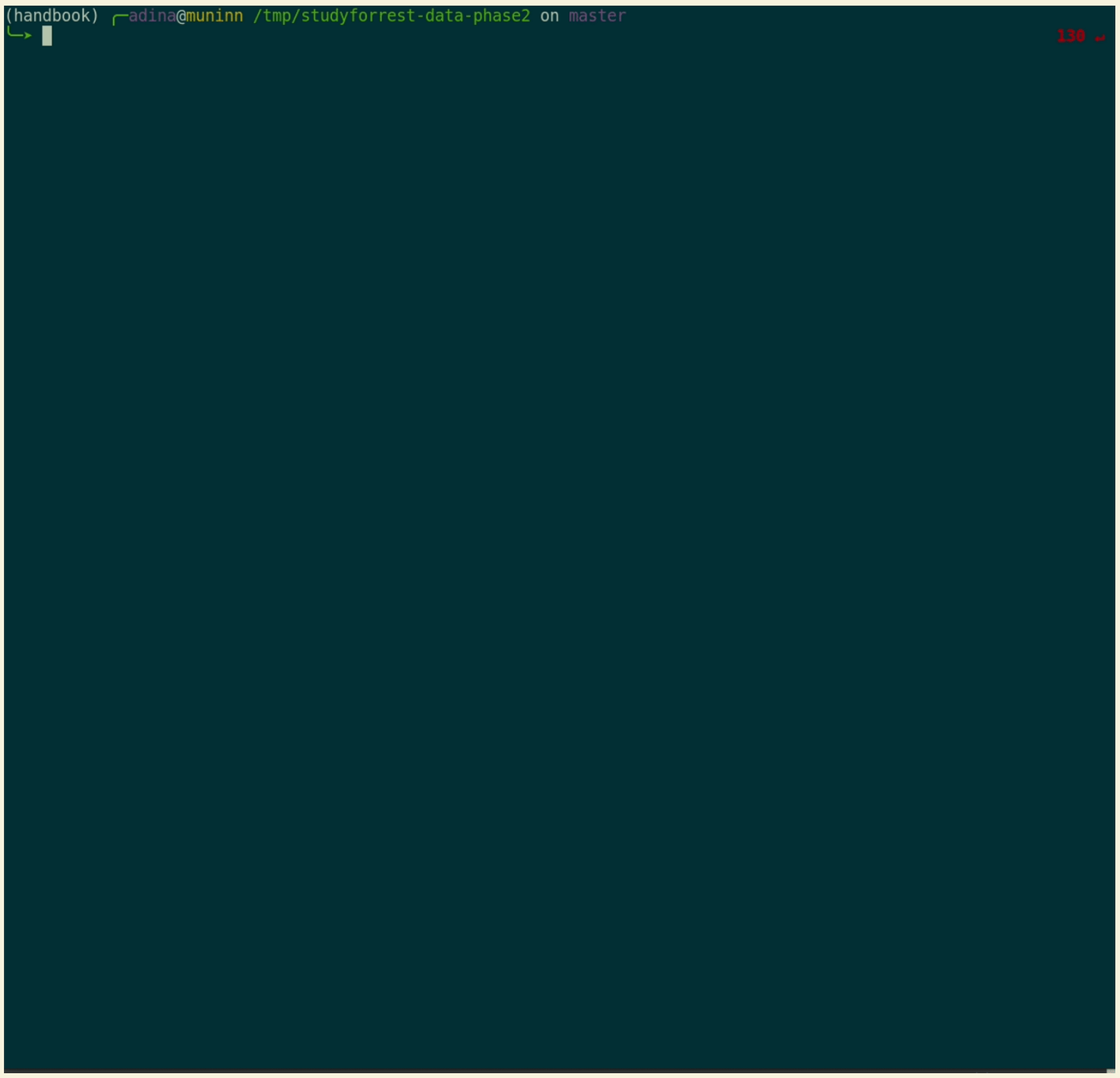

- Datasets are light-weight: Upon installation, only small files and meta data about file availability are retrieved.

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$ datalad get sub-01/ses-movie/func/sub-01_ses-movie_task-movie_run-1_bold.nii.gz
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```
# eNKI dataset (1.5TB, 34k files):
  $ du -sh
    1.5G        .
  # HCP dataset (80TB, 15 million files)
  $ du -sh
  48G   .
```

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➡ *compute your results*

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Install your input data

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➡ *drop input data (and potentially all automatically re-computable results)*

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```
$ datalad drop sub-01/ses-movie/func/sub-01_ses-movie_task-movie_run-1_bold.nii.gz
drop(ok): /tmp/studyforrest-data-phase2/sub-01/ses-movie/func/sub-01_ses-movie_task-movie_run-1_bold.nii.g
```

When files are dropped, only "meta data" stays behind, and they can be re-obtained on demand. This allows disk-space aware computations:

Install your input data

➡ *get the data you need*

➡ *compute your results*

➡ *drop input data (and potentially all automatically re-computable results)*

```
dl.get('input/sub-01')

[really complex analysis]

dl.drop('input/sub-01')
```

GIT VERSUS GIT-ANNEX

Data in datasets is either stored in Git or git-annex

By default, everything is *annexed*, i.e., stored in a dataset annex by git-annex

Git	**git-annex**
handles **small** files well (text, code)	handles **all** types and sizes of files well
file contents are in the Git history and will be **shared** upon git/datalad push	file contents are in the annex. Not necessarily shared
Shared with every dataset clone	**Can be kept private** on a per-file level when sharing the dataset
Useful: Small, non-binary, frequently modified, need-to-be-accessible (DUA, README) files	Useful: Large files, private files

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- With annexed data, only content identity (hash) and location information is put into Git, rather than file content. The annex, and transport to and from it is managed with **git-annex**

GIT VERSUS GIT-ANNEX

Git

- dataset history (commit messages, run records)
- All files + content committed into Git (useful with code, text, ...)
- File identity information of all annexed files (file name, identity hash, storage locations where to retrieve it from)

git-annex

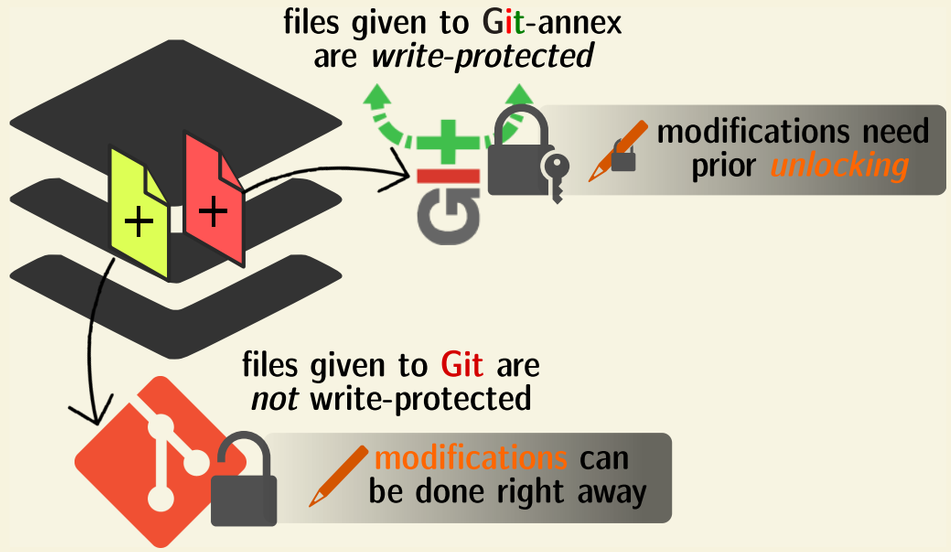
- contents of annexed files
- organized in the "annex" or "object tree" of the dataset

GIT VERSUS GIT-ANNEX

Useful background information for demo later. Read this handbook chapter for details

Git and Git-annex handle files differently: annexed files are stored in an annex. File content is hashed & only content-identity is committed to Git.

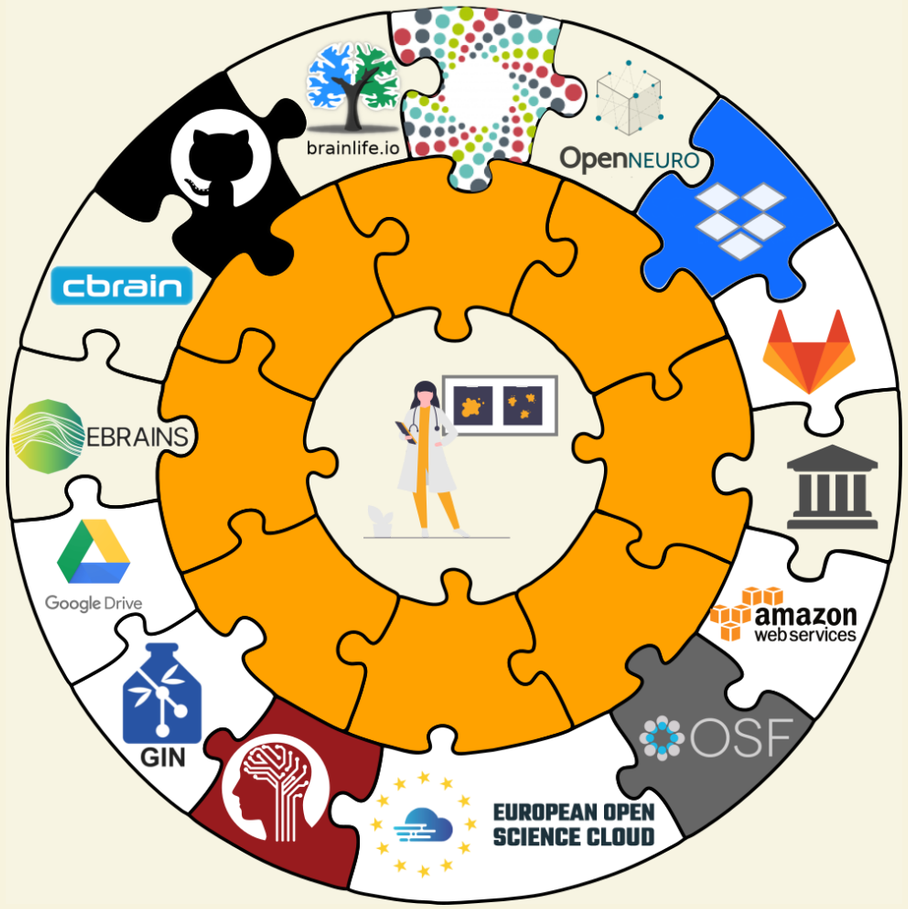
- Files stored in Git are modifiable, files stored in Git-annex are content-locked



- Annexed contents are not available right after cloning, only content identity and availability information (as they are stored in Git). Everything that is annexed needs to be retrieved with `datalad get` from whereever it is stored.

GIT VERSUS GIT-ANNEX

When sharing datasets with someone without access to the same computational infrastructure, annexed data is not necessarily stored together with the rest of the dataset (more in the **session on publishing**).



Transport logistics exist to interface with all major storage providers. If the one you use isn't supported, let us know!

GIT VERSUS GIT-ANNEX

Users can decide which files are annexed:

- **Pre-made run-procedures**, provided by DataLad (e.g., `text2git`, `yoda`) or created and shared by users (Tutorial)
- Self-made configurations in `.gitattributes` (e.g., based on file type, file/path name, size, ...; rules and examples)
- Per-command basis (e.g., via `datalad save --to-git`)

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  $ cd machinelearning-books && du -sh
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```

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```
$ ls
  A.Shashua-Introduction_to_Machine_Learning.pdf
  B.Efron_T.Hastie-Computer_Age_Statistical_Inference.pdf
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  drop(ok): /tmp/machinelearning-books/A.Shashua-Introduction_to_Machine_Learning.pdf (file) [checking htt
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```
$ datalad drop .easteregg
drop(ok): /demo/myanalysis/.easteregg (file) [checking https://imgs.xkcd.com/comics/fuck_grapefruit.png...
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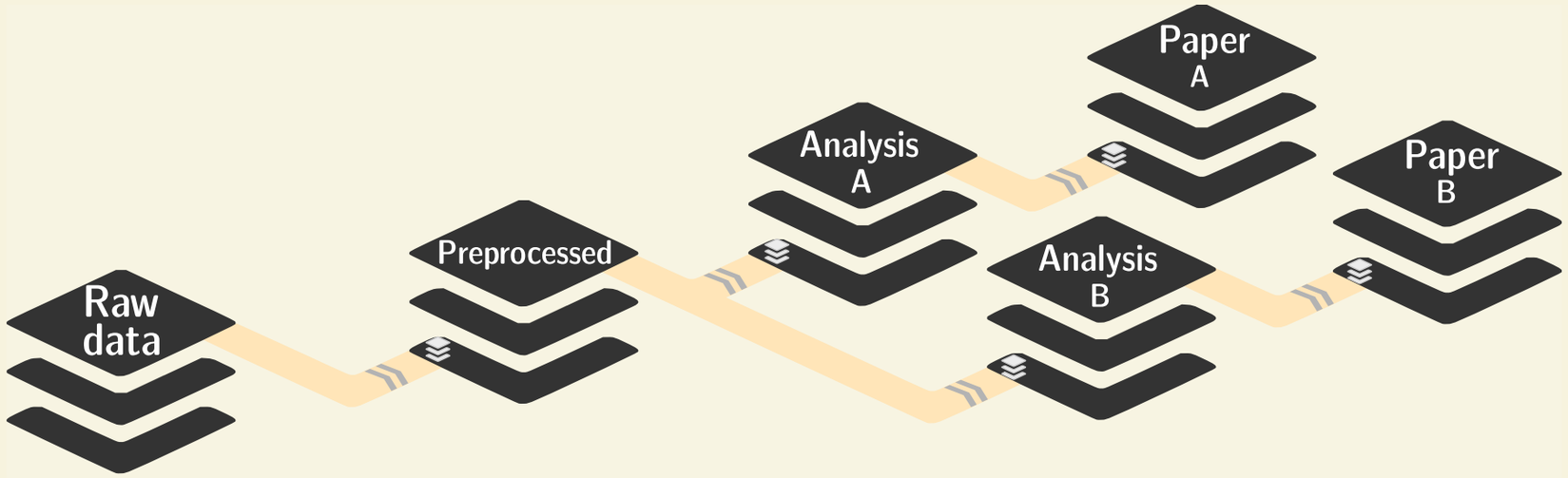
- If a different location for file content is known, `datalad get` can retrieve file content after dropping

DATASET NESTING

- Seamless nesting mechanisms:



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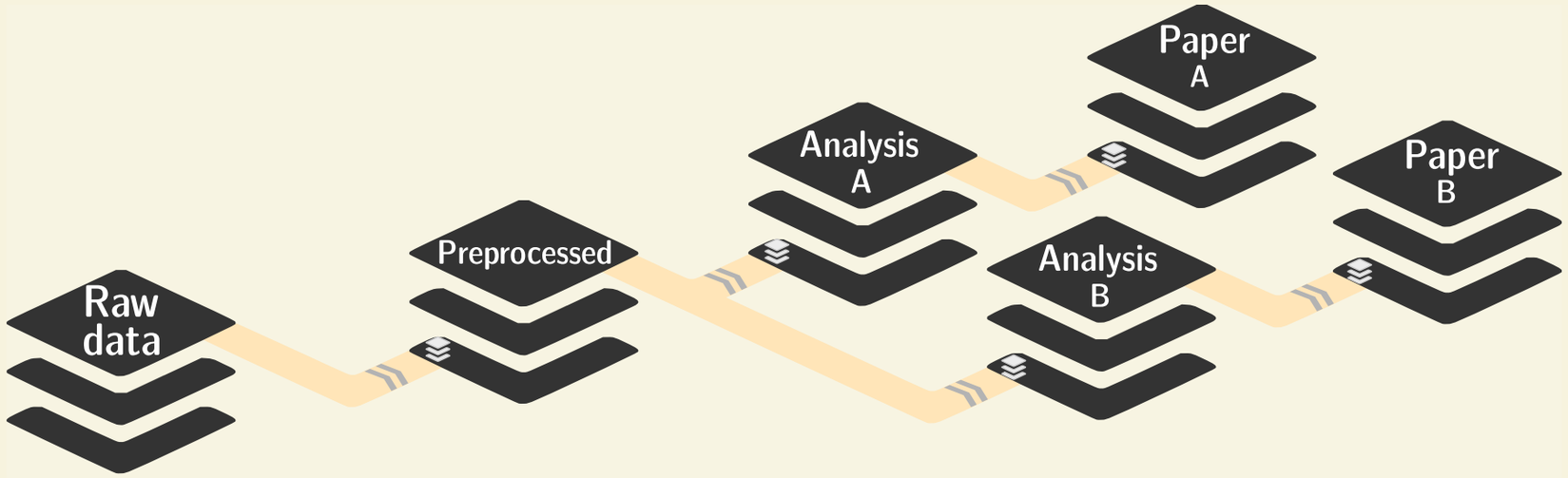

Nest modular datasets to create a linked hierarchy of datasets, and enable recursive operations throughout the hierarchy

- Overcomes scaling issues with large amounts of files

```
adina@bulk1 in /ds/hcp/super on git:master❱ datalad status --annex -r
  15530572 annex'd files (77.9 TB recorded total size)
  nothing to save, working tree clean
```

(github.com/datalad-datasets/human-connectome-project-openaccess)

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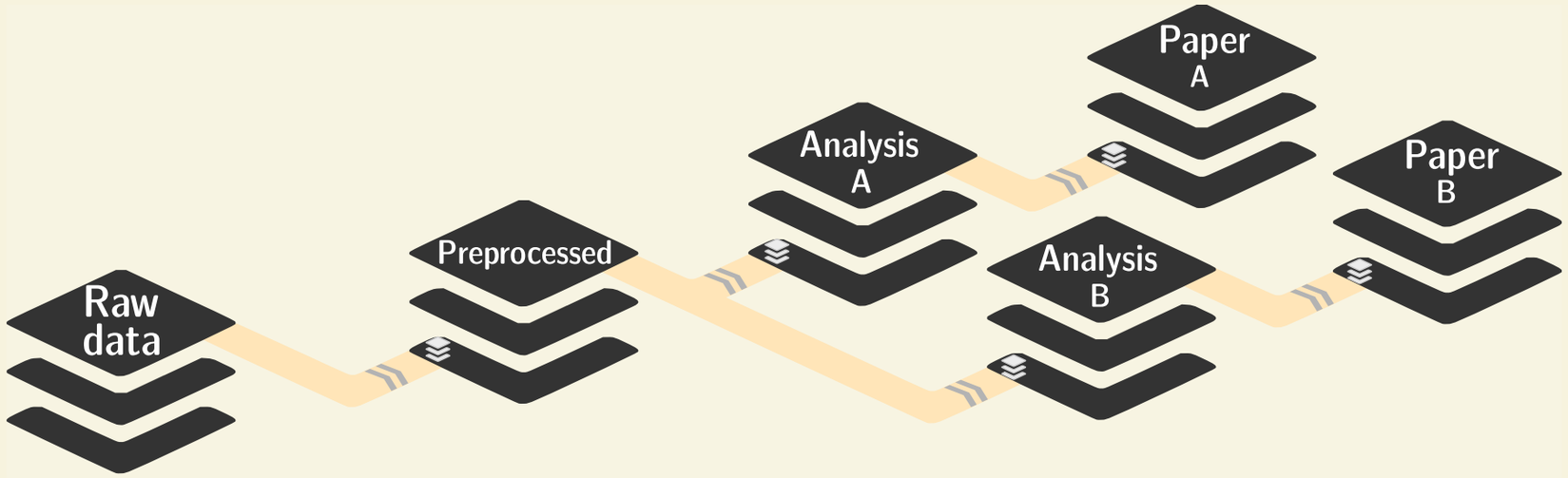

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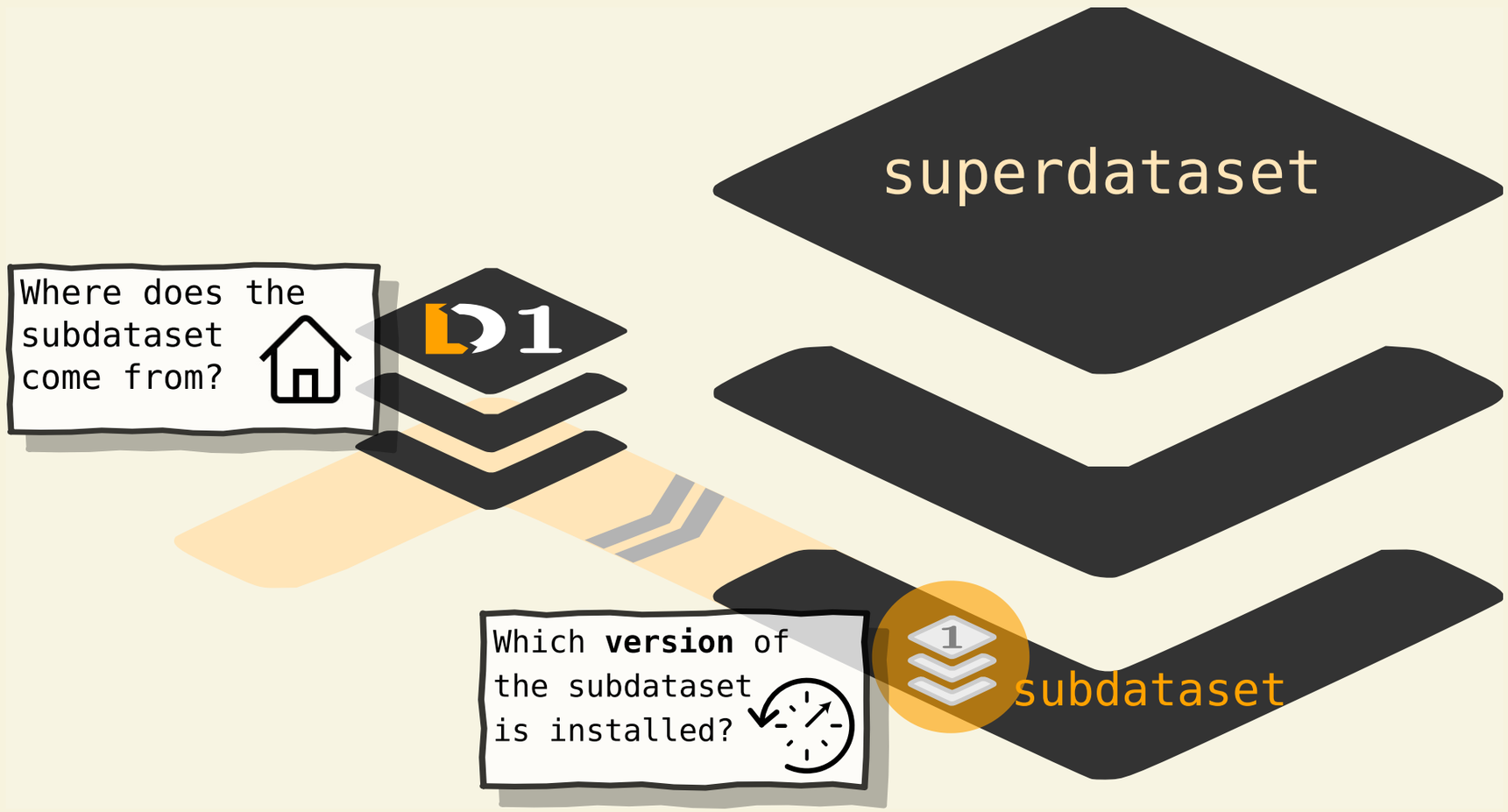
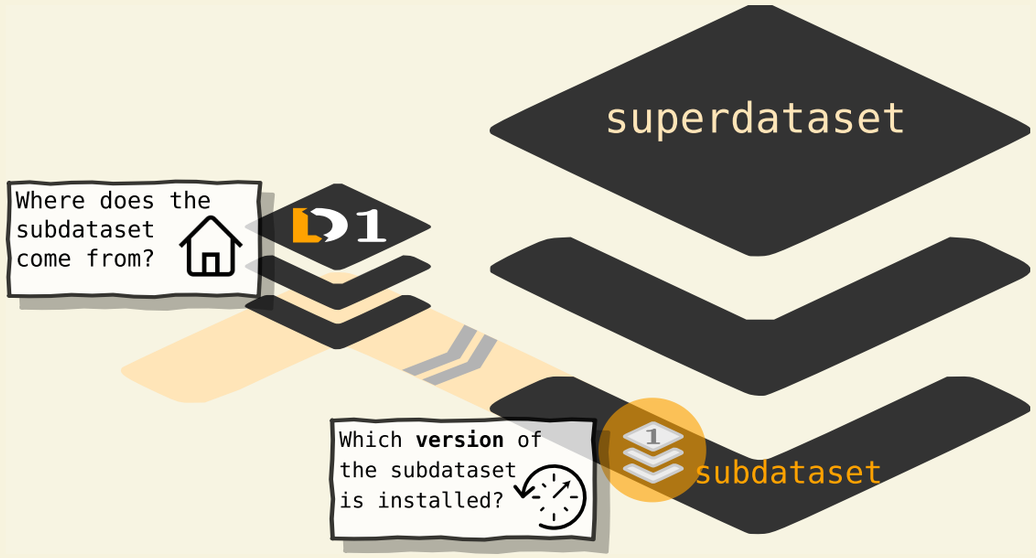
- Modularizes research components for transparency, reuse, and access management (more on this in the **section on reproducible science**)

DATASET NESTING



DATALAD: DATASET LINKAGE




```
$ datalad clone --dataset . http://example.com/ds inputs/rawdata
```

```
$ git diff HEAD~1
diff --git a/.gitmodules b/.gitmodules
new file mode 100644
index 0000000..c3370ba
--- /dev/null
+++ b/.gitmodules
@@ -0,0 +1,3 @@
+[submodule "inputs/rawdata"]
+       path = inputs/rawdata
+       url = http://example.com/importantds
diff --git a/inputs/rawdata b/inputs/rawdata
new file mode 160000
index 0000000..fabf852
--- /dev/null
+++ b/inputs/rawdata
@@ -0,0 +1 @@
+Subproject commit fabf8521130a13986bd6493cb33a70e580ce8572
```

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Datasets preserve their history.

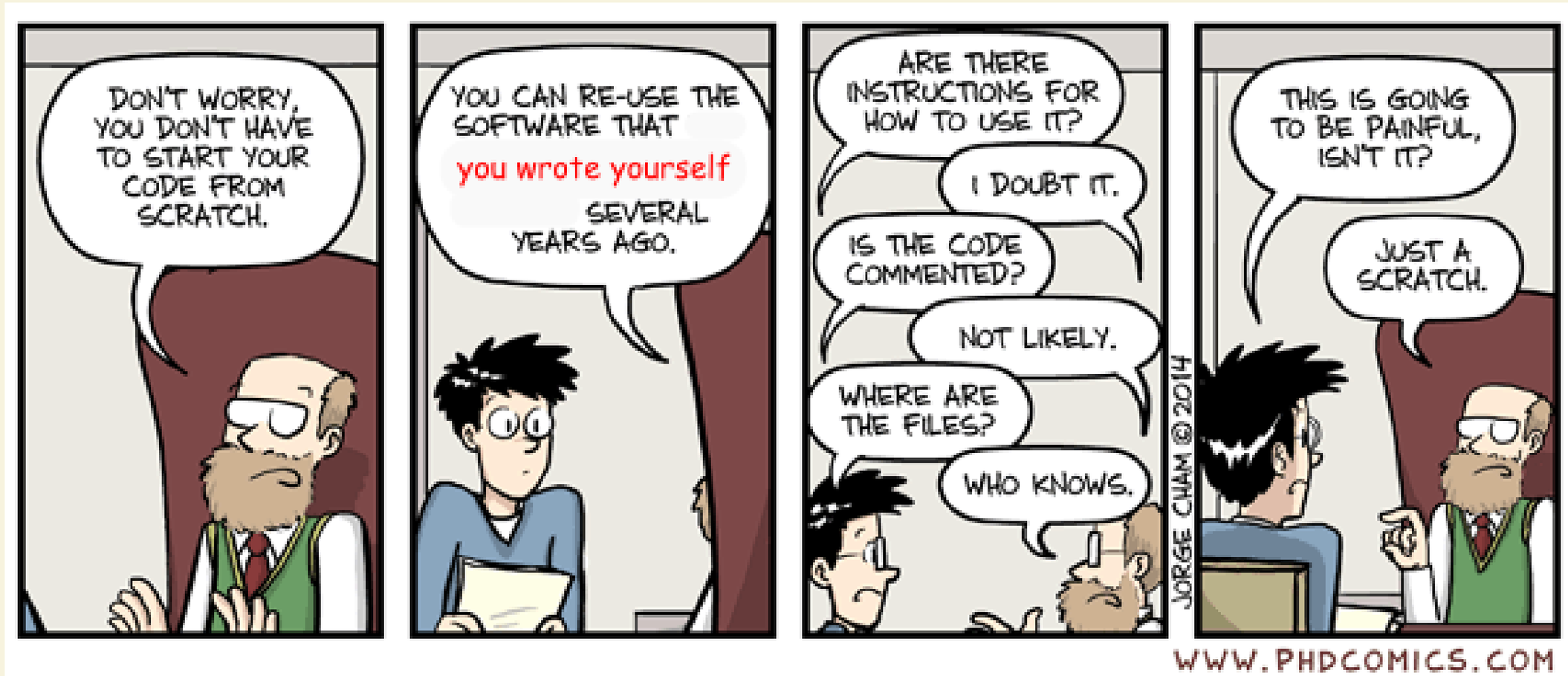
The superdataset records only the *version state* of the subdataset.

QUESTIONS!

http://etc.ch/5xo7

REPRODUCIBLE DATA ANALYSIS

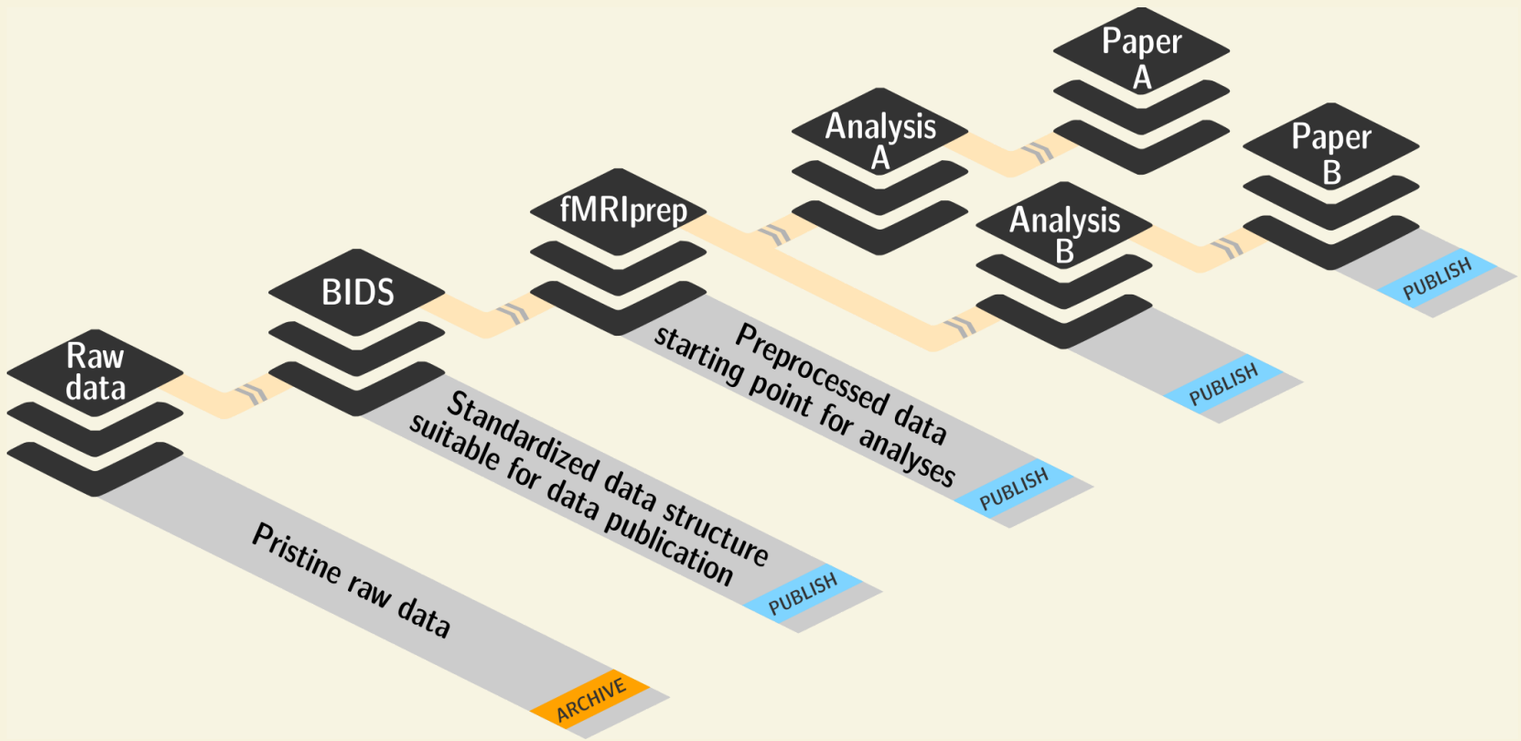
Your past self is the worst collaborator:

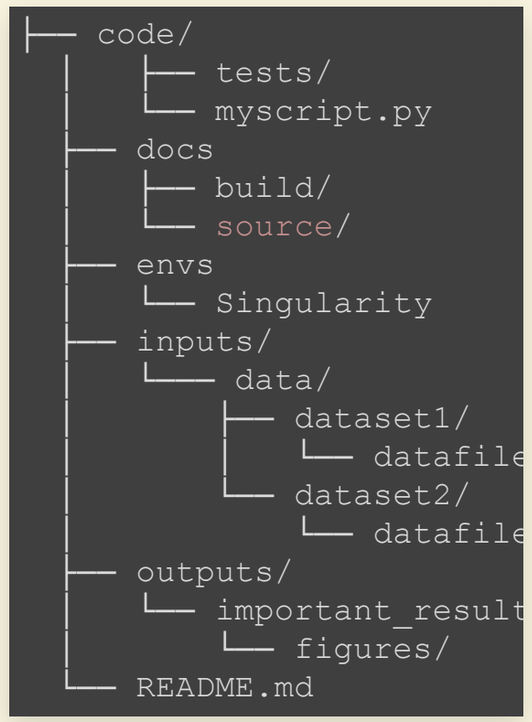


BASIC ORGANIZATIONAL PRINCIPLES FOR DATASETS

Keep everything clean and modular

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



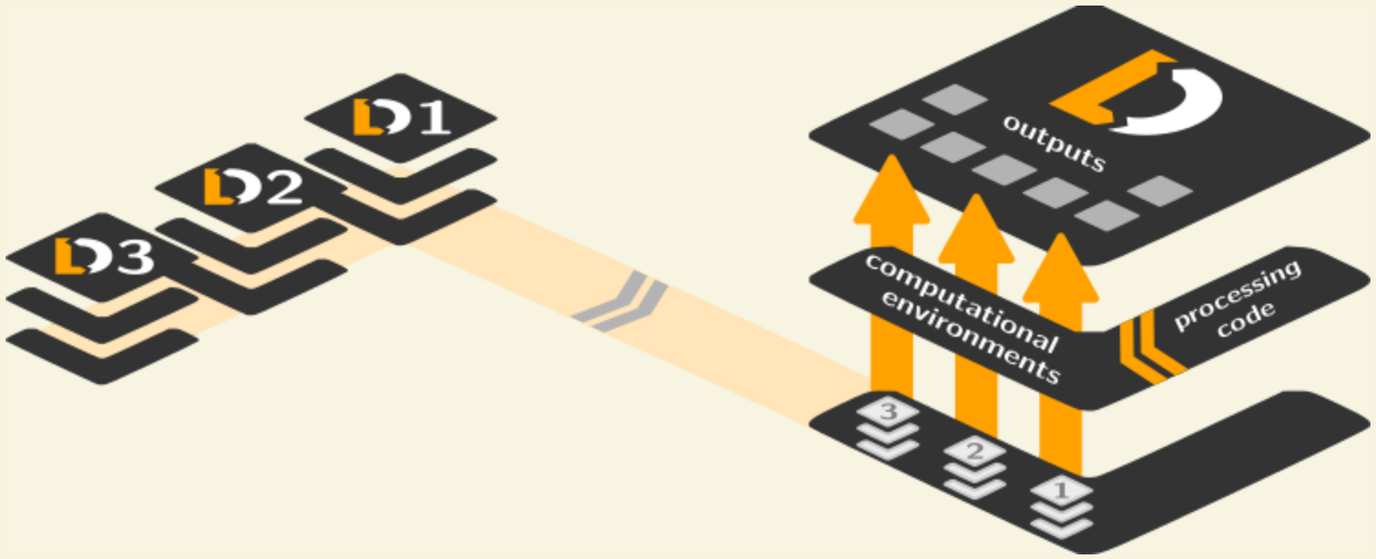


- do not touch/modify raw data: save any results/computations *outside* of input datasets
- Keep a superdataset self-contained: Scripts reference subdatasets or files with *relative paths*

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

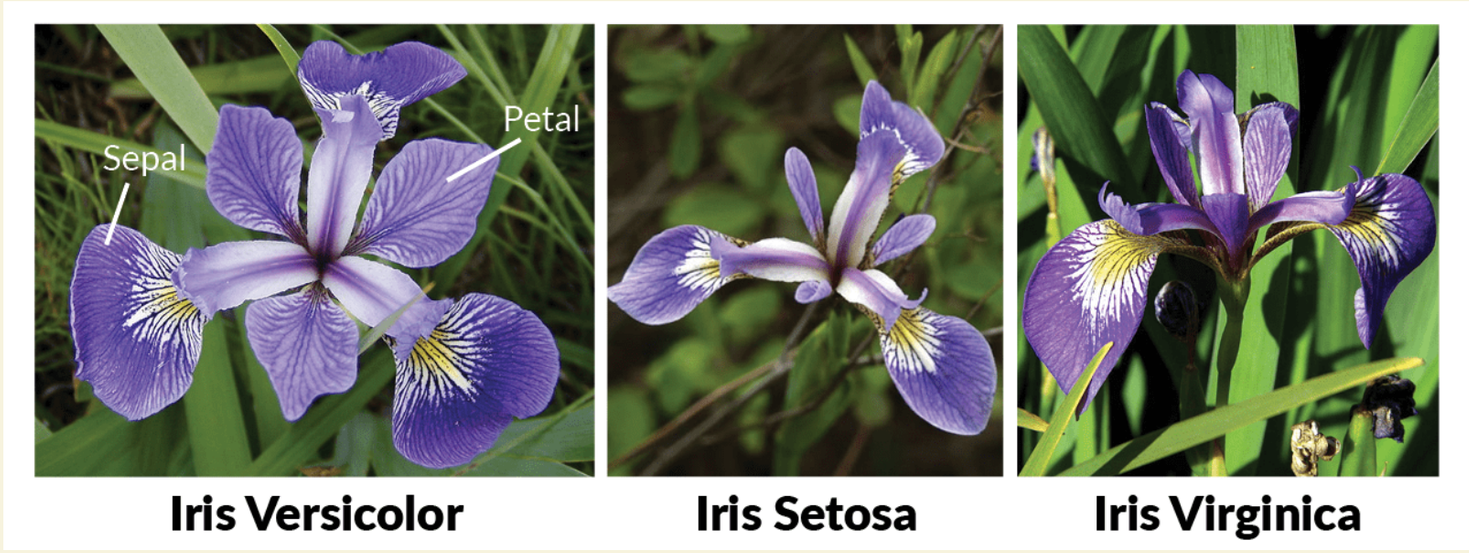


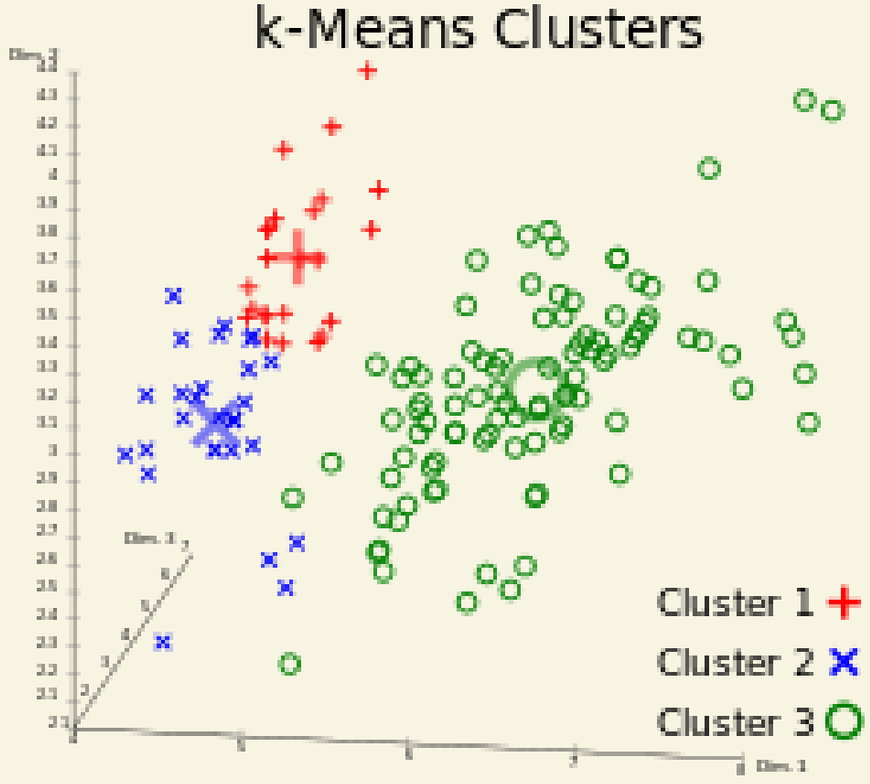
Document everything:

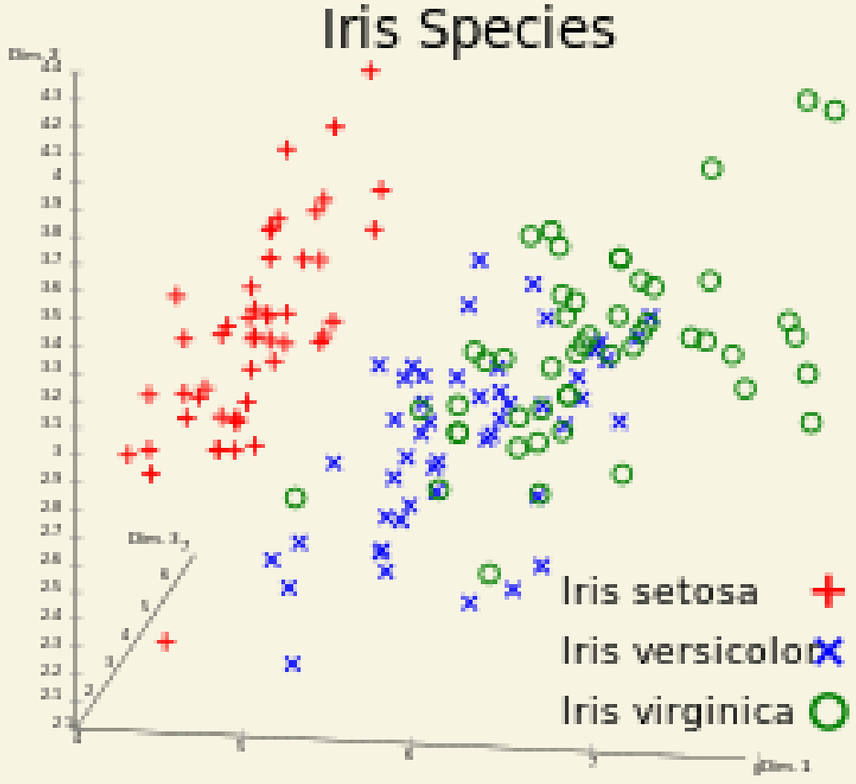
- Which script produced which output? From which data? In which software environment? …

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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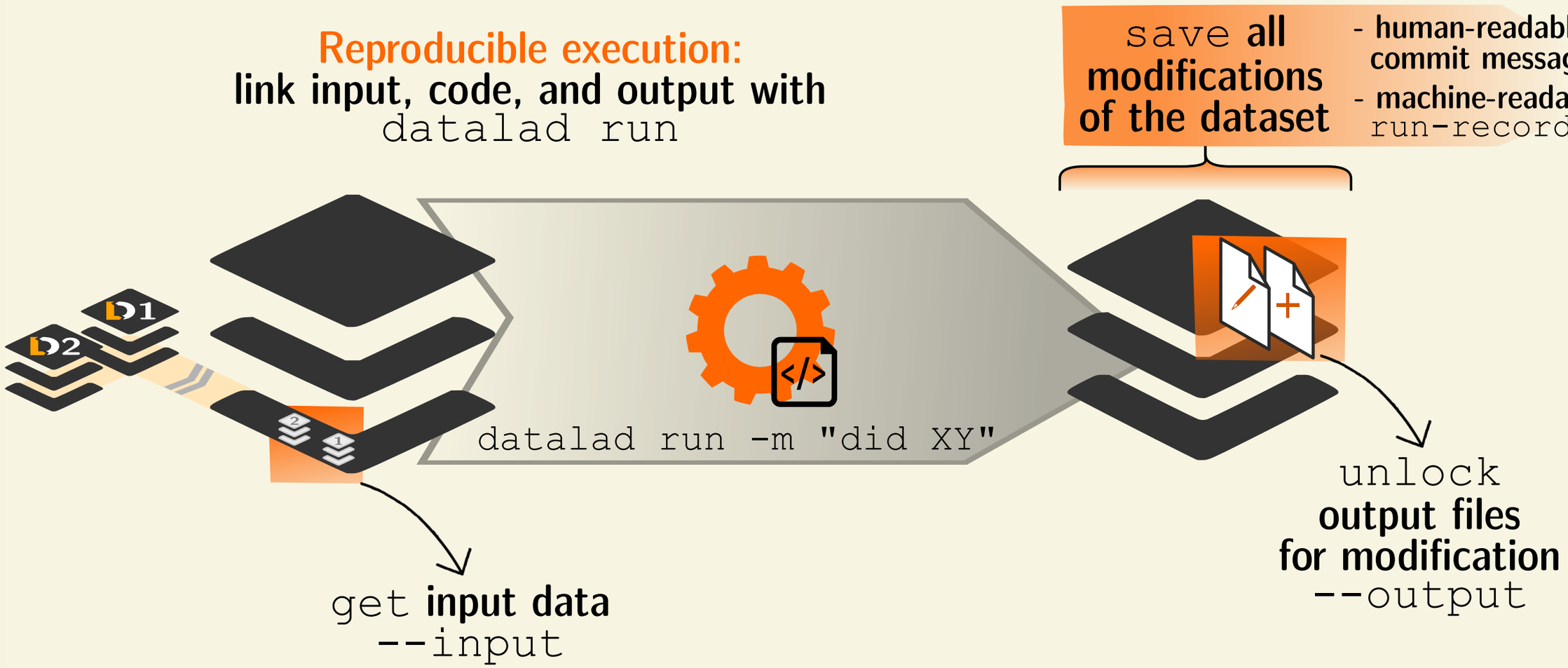

COMPUTATIONAL REPRODUCIBILITY

- Code may fail (to reproduce) if run with different software
- 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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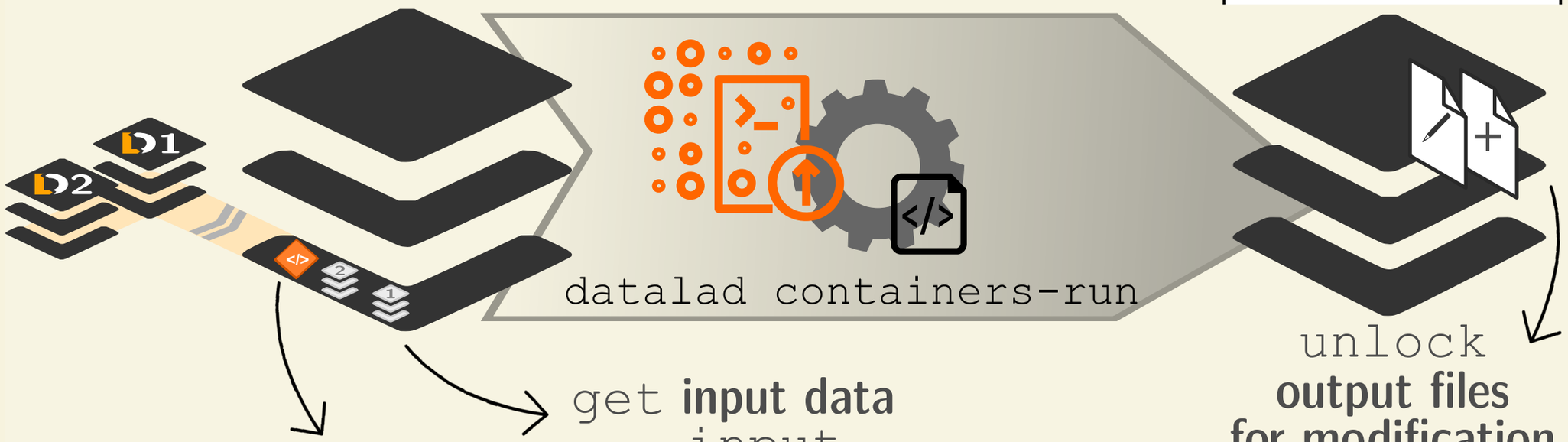
datalad-containers run

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

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

SUMMARY - REPRODUCIBLE EXECUTION

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Its ensures computations are ran in the desired software set up. Supports Docker and Singularity containers

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Data/directories specified as `--output` will be unlocked for modifications prior to a rerun of the command.

Its optional to specify, but helpful for recomputations.

`datalad containers-run` can be used to capture the software environment as provenance.

Its ensures computations are ran in the desired software set up. Supports Docker and Singularity containers

`datalad rerun` can automatically re-execute run-records later.

SUMMARY - REPRODUCIBLE EXECUTION

`datalad run` records a command and its impact on the dataset.

All dataset modifications are saved - use it in a clean dataset.

Data/directories specified as `--input` are retrieved prior to command execution.

Use one flag per input.

Data/directories specified as `--output` will be unlocked for modifications prior to a rerun of the command.

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`datalad rerun` can automatically re-execute run-records later.

They can be identified with any commit-ish (hash, tag, range, ...)

DATALAD RERUN

- `datalad rerun` is helpful to spare others and yourself the short- or long-term memory task, or the forensic skills to figure out how you performed an analysis
- But it is also a digital and machine-reable provenance record
- Important: The better the run command is specified, the better the provenance record
- Note: run and rerun only create an entry in the history if the command execution leads to a change.

QUESTIONS!

http://etc.ch/5xo7

UNLOCKING THINGS

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- Outside of `datalad run`, you can use `datalad unlock`
- This makes annex'ed files *writeable*:

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$ ls -l myfile
lrwxrwxrwx 1 adina adina  108 Nov 17 07:08 myfile -> .git/annex/objects/22/Gw/MD5E-s7--f447b20a7fcbf53a5d5

# unlocking
$ datalad unlock myfile
unlock(ok): myfile (file)
$ ls -l myfile
-rw-r--r-- 1 adina adina    7 Nov 17 07:08 myfile  # not a symlink anymore!
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- `datalad save` "locks" the file again

```
$ datalad save
add(ok): myfile (file)
action summary:
  add (ok: 1)
  save (notneeded: 1)

$ ls -l myfile
lrwxrwxrwx 1 adina adina 108 Nov 17 07:08 myfile -> .git/annex/objects/22/Gw/MD5E-s7--f447b20a7fcbf53a5d5b
```

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```

Some tools (e.g., MatLab) don't like symlinks. Unlocking or running matlab with "datalad run" helps!

REMOVING DATASETS

- As mentioned before, annexed data is write-protected. So when you try to `rm -rf` a dataset, this happens:

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```
$ rm -rf mydataset
rm: cannot remove 'mydataset/.git/annex/objects/70/GM/MD5E-s27246--8b7ea027f6db1cda7af496e97d4eb7c9.png/MD
rm: cannot remove 'mydataset/.git/annex/objects/70/GM/MD5E-s35756--af496e97d4eb7c98b7ea027f6db1cda7.png/MD
[...]
```

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rm: cannot remove 'mydataset/.git/annex/objects/70/GM/MD5E-s35756--af496e97d4eb7c98b7ea027f6db1cda7.png/MD
[...]
```

- (If you accidentally ever do this, you need to apply write permissions recursively to all files)

```
$ chmod -R +w mydataset
$ rm -rf mydataset                # success!
```

REMOVING DATASETS

- The correct way to remove a dataset is using `datalad remove`:

```
$ datalad remove -d ds001241
remove(ok): . (dataset)
action summary:
  drop (notneeded: 1)
  remove (ok: 1)
```

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remove(ok): . (dataset)
action summary:
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- If a dataset contains file for which no other remote copy is known, you'll get a warning:

```
$ datalad remove -d mydataset
[WARNING] Running drop resulted in stderr output: git-annex: drop: 1 failed

[ERROR  ] unsafe; Could only verify the existence of 0 out of 1 necessary copies; Rather than dropping thi
drop(error): interdisciplinary.png (file) [unsafe; Could only verify the existence of 0 out of 1 necessary
[WARNING] could not drop some content in /tmp/mydataset ['/tmp/mydataset/interdisciplinary.png'] [drop(/tm
drop(impossible): . (directory) [could not drop some content in /tmp/mydataset ['/tmp/mydataset/interdisci
action summary:
  drop (error: 1, impossible: 1)
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action summary:
  drop (error: 1, impossible: 1)
```

- In that case, use `--nocheck` to force removal:

```
$ datalad remove -d mydataset --nocheck                                    1 !
remove(ok): . (dataset)
```

REMOVING DATASETS

- If a dataset contains subdatasets, `datalad remove` will also error:

REMOVING DATASETS

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```
$ datalad remove -d myds
drop(ok): README.md (file) [locking gin...]
drop(ok): . (directory)
[ERROR  ] to be uninstalled dataset Dataset(/tmp/myds) has present subdatasets, forgot --recursive? [remov
remove(error): . (dataset) [to be uninstalled dataset Dataset(/tmp/myds) has present subdatasets, forgot -
action summary:
  drop (ok: 3)
  remove (error: 1)
```

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drop(ok): README.md (file) [locking gin...]
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remove(error): . (dataset) [to be uninstalled dataset Dataset(/tmp/myds) has present subdatasets, forgot -
action summary:
  drop (ok: 3)
  remove (error: 1)
```

- In that case, use `--recursive` to remove all subdatasets, too:

```
$ datalad remove -d myds --recursive
uninstall(ok): input (dataset)
remove(ok): . (dataset)
action summary:
  drop (notneeded: 2)
  remove (ok: 1)
  uninstall (ok: 1)
```

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$ datalad remove -d myds
drop(ok): README.md (file) [locking gin...]
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uninstall(ok): input (dataset)
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```
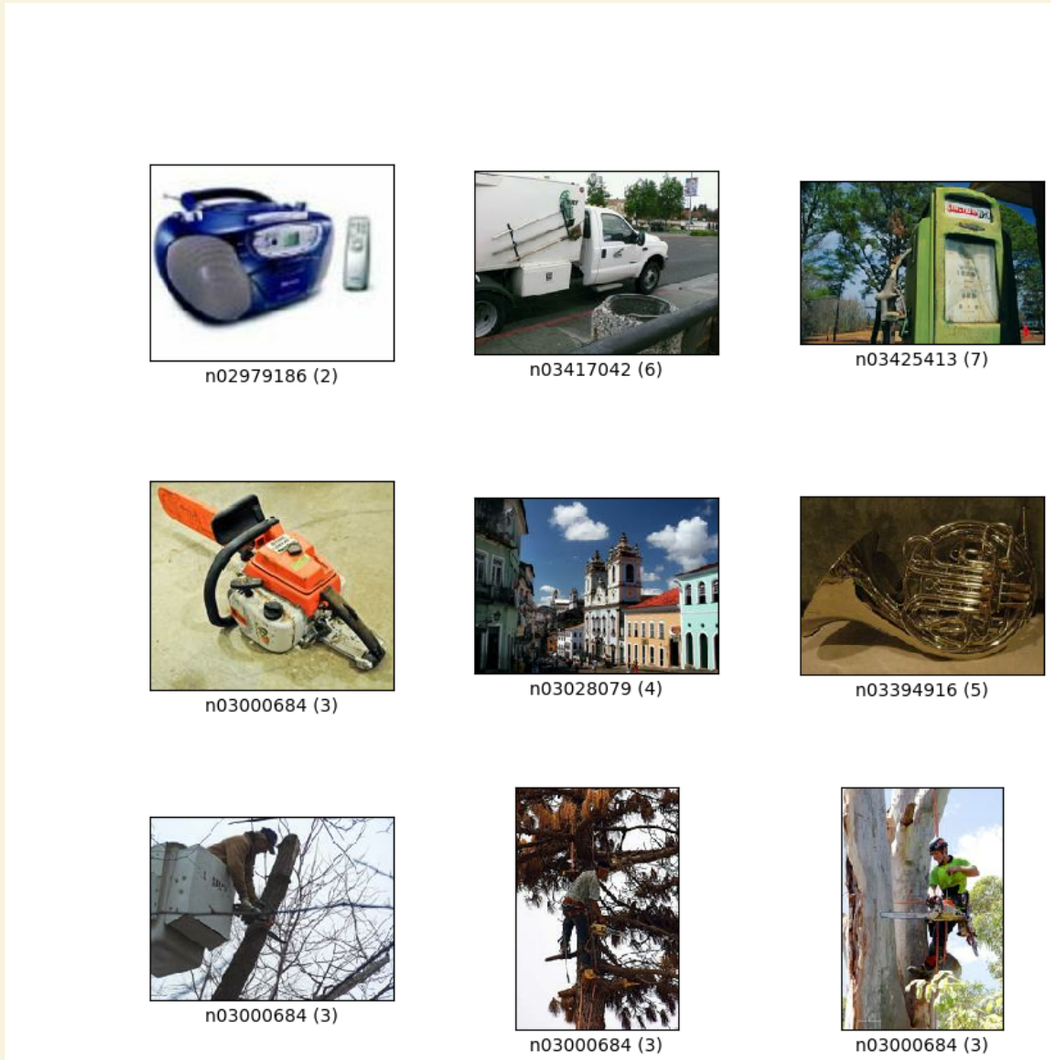

- A complete overview of file system operations is in handbook.datalad.org/en/latest/basics/101-136-filesystem.html

A MACHINE-LEARNING EXAMPLE

ANALYSIS LAYOUT

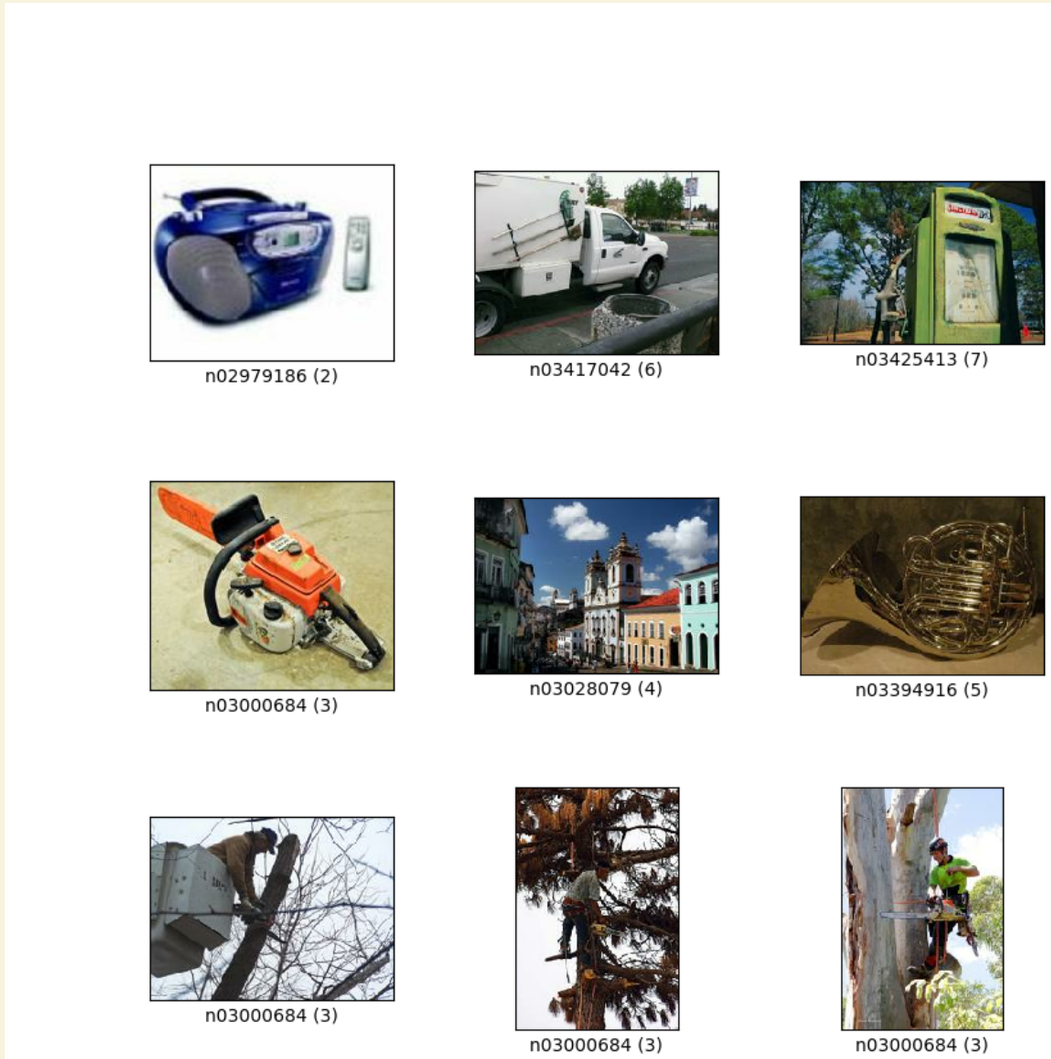
- Prepare an input data set



Imagenette dataset

ANALYSIS LAYOUT

- Prepare an input data set
- Configure and setup an analysis dataset



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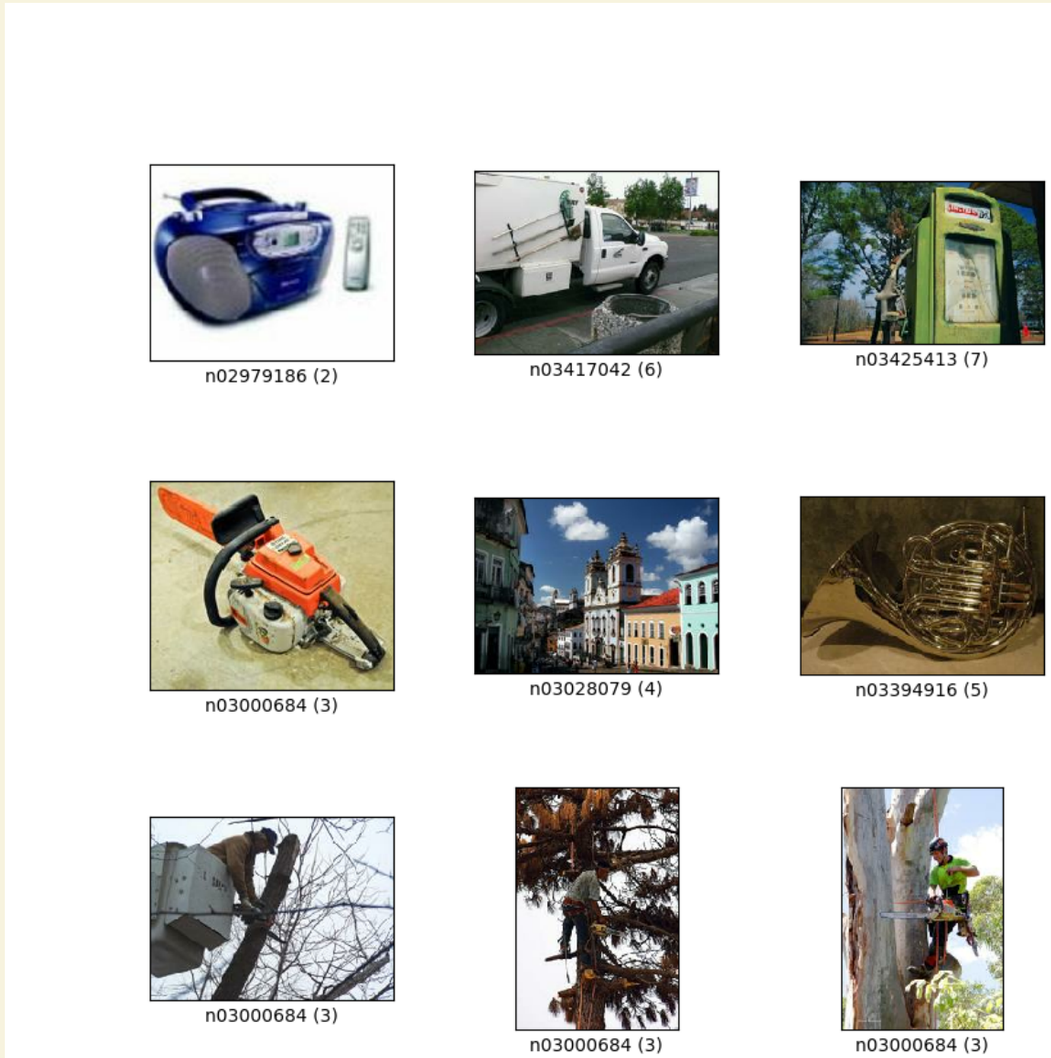

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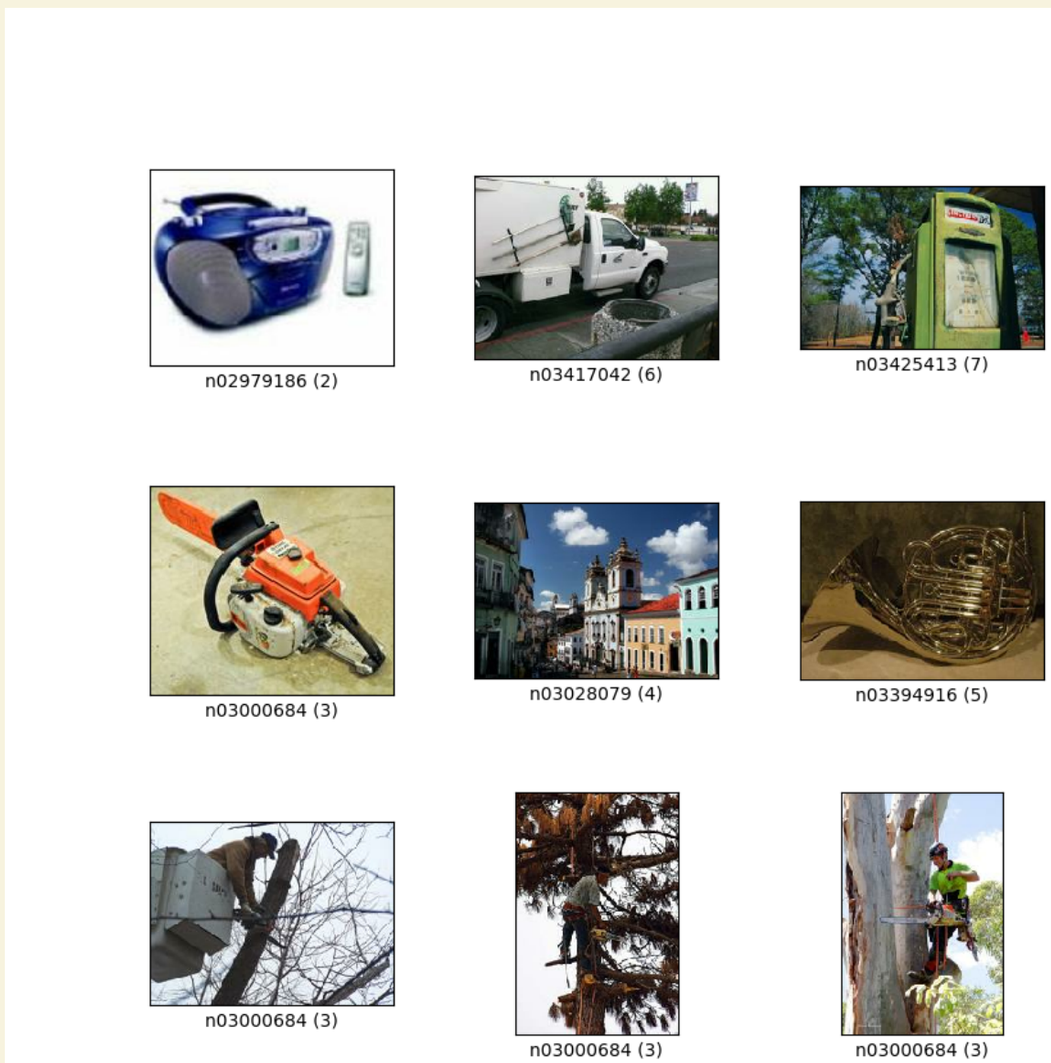
ANALYSIS LAYOUT

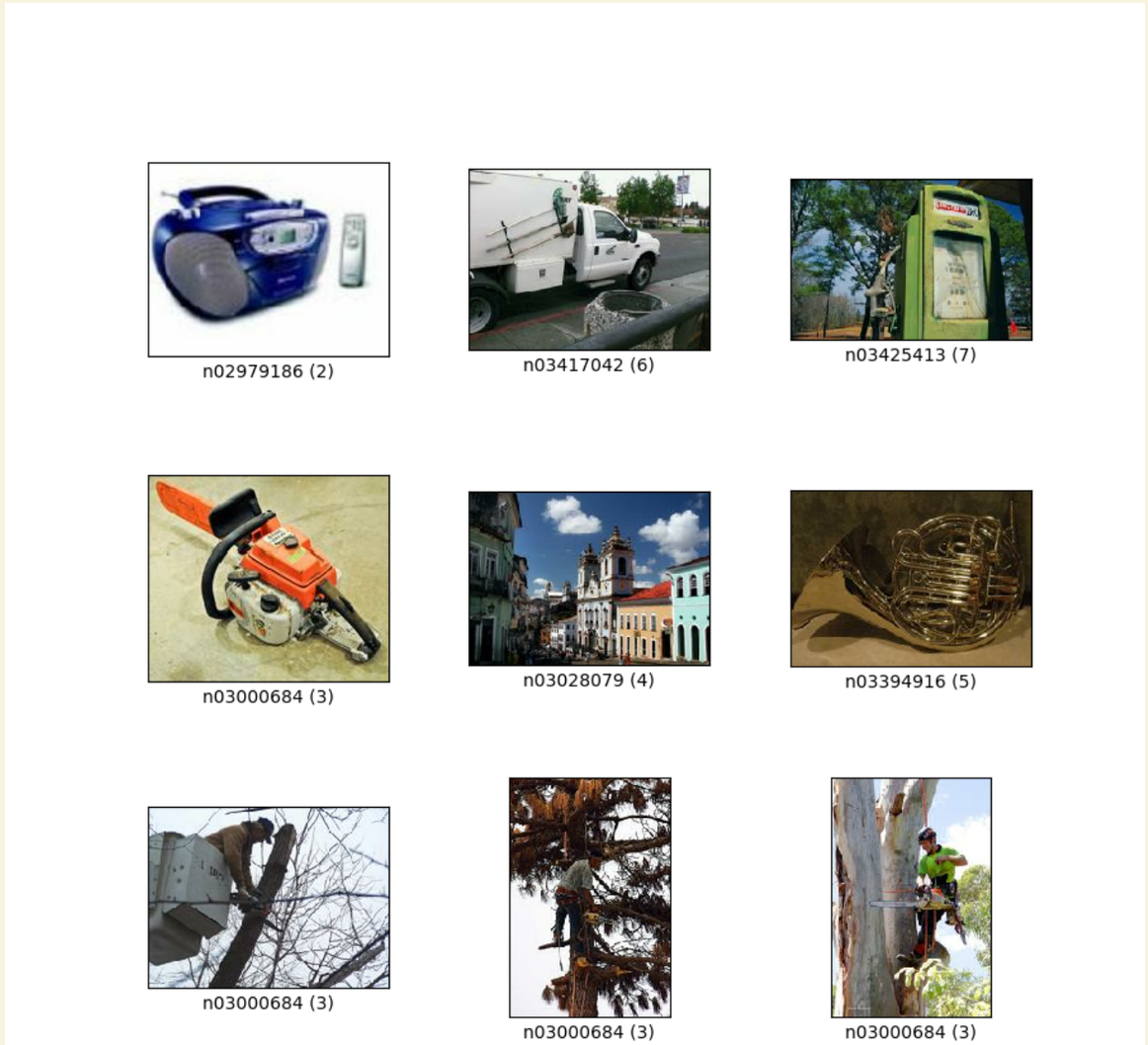
- Prepare an input data set
- Configure and setup an analysis dataset
- Prepare data
- Train models and evaluate them



Imagenette dataset

ANALYSIS LAYOUT

- Prepare an input data set
- Configure and setup an analysis dataset
- Prepare data
- Train models and evaluate them
- Compare different models, repeat with updated data



Imagenette dataset

PREPARE AN INPUT DATASET

- Create a stand-alone input dataset
- Either add data and `datalad save` it, or use commands such as `datalad download-url` or `datalad add-urls` to retrieve it from web-sources

CONFIGURE AND SETUP AN ANALYSIS DATASET

- Given the purpose of an analysis dataset, configurations can make it easier to use:
  - `-c yoda` prepares a useful structure
  - `-c text2git` keeps text files such as scripts in Git
- The input dataset is installed as a subdataset
- Required software is containerized and added to the dataset

PREPARE DATA

- Add a script for data preparation (labels train and validation images)
- Execute it using `datalad containers-run`

TRAIN MODELS AND EVALUATE THEM

- Add scripts for training and evaluation. This dataset state can be tagged to identify it easily at a later point
- Execute the scripts using `datalad containers-run`
- By dumping a trained model as a joblib object the trained classifier stays reusable

TIPS AND TRICKS FOR ML APPLICATIONS

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DataLad is no workflow manager, but by checking out out tags or branches one can switch easy and fast between results of different models

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- Collaboration and updating mechanisms: Alice shares her data with Bob. Alice fixes a mistake and pushes the fix. Bob says "datalad update" and gets her changes. And vice-versa.
- Transparency: Shared datasets keep their history. No need to track down a former student, ask their project what was done.