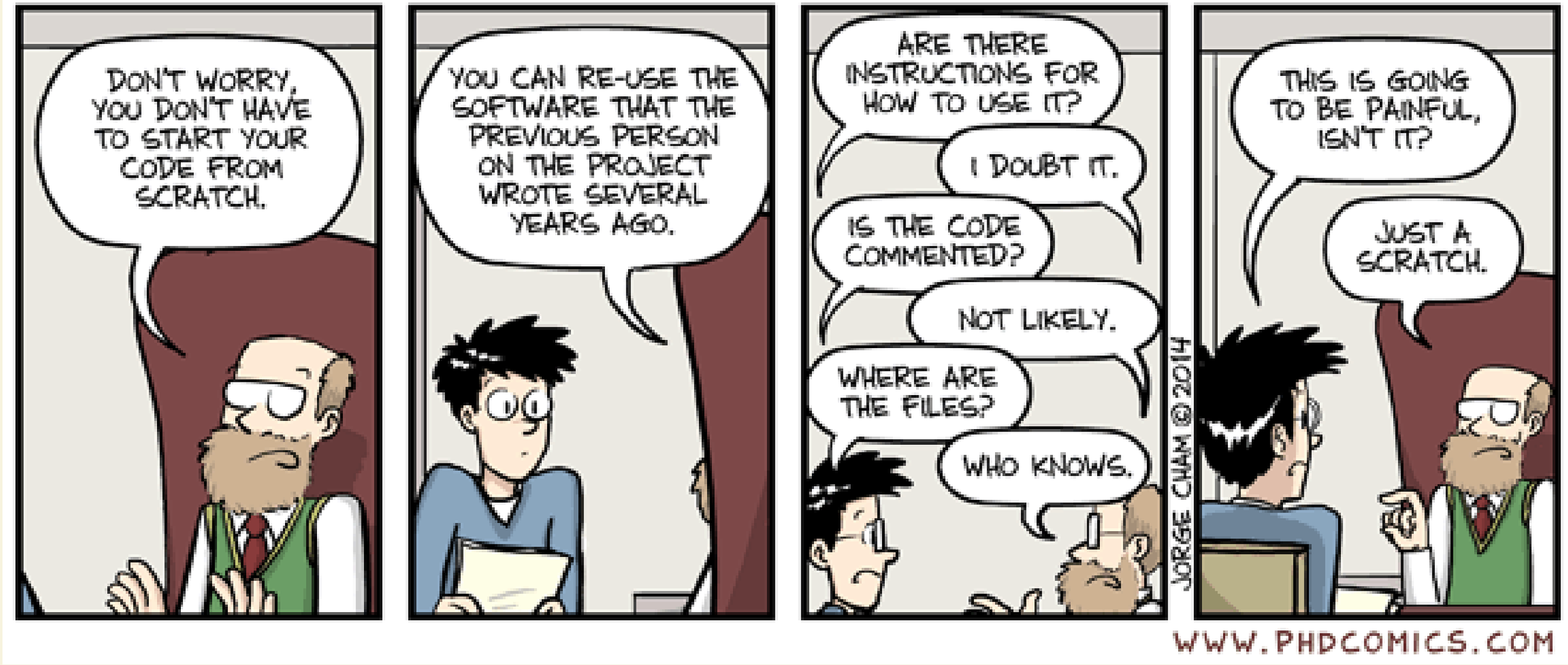
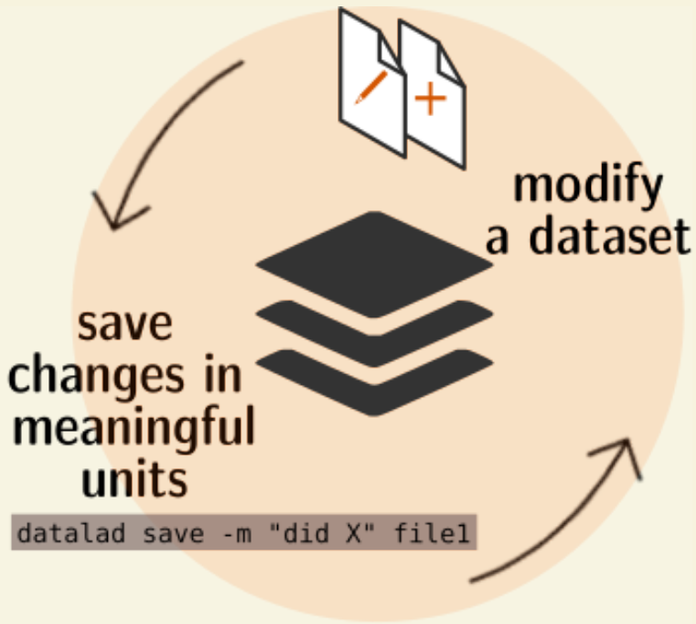
Data management

Reproducible analysis



LAST SESSION...

- **Local version control**: `datalad create`, `datalad save`
- **Datasets**: Exploring & nesting datasets
- **Practice**: Create, structure, and install datasets



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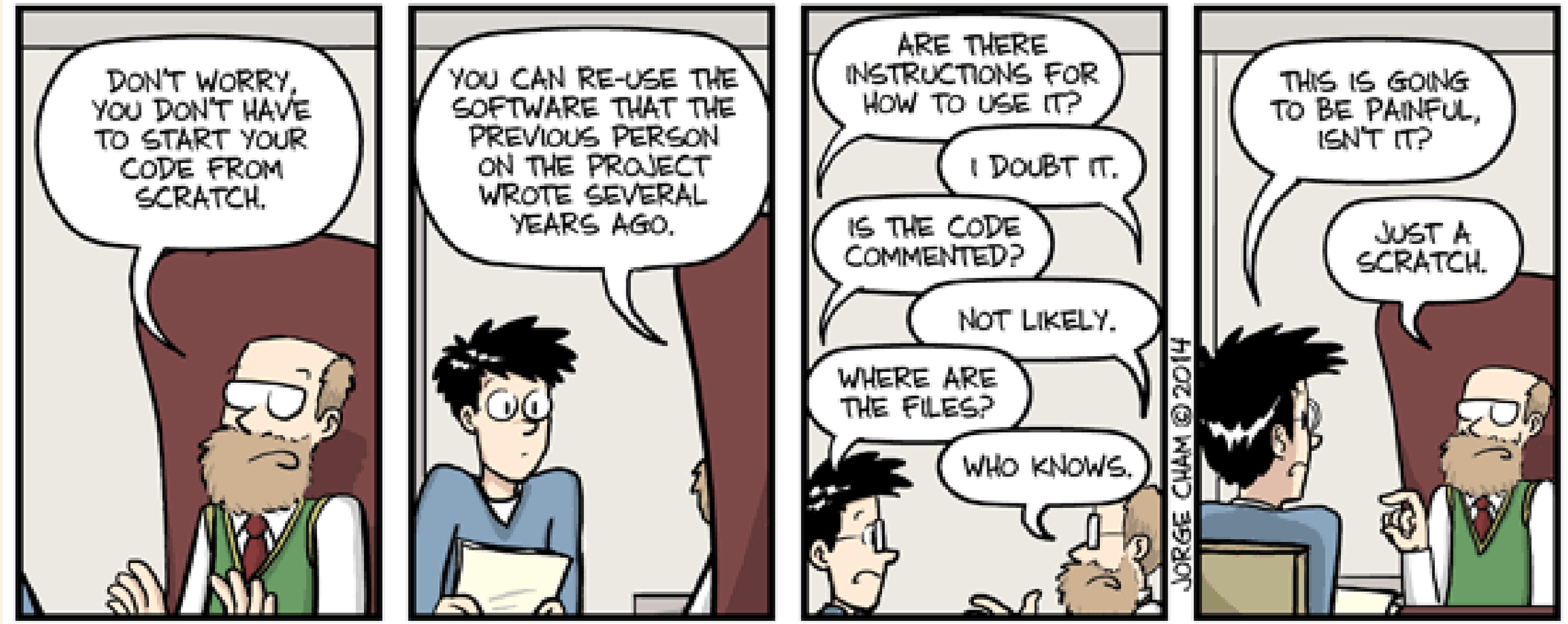
ANY OTHER QUESTIONS?

REPRODUCIBLE ANALYSES ARE HARD...



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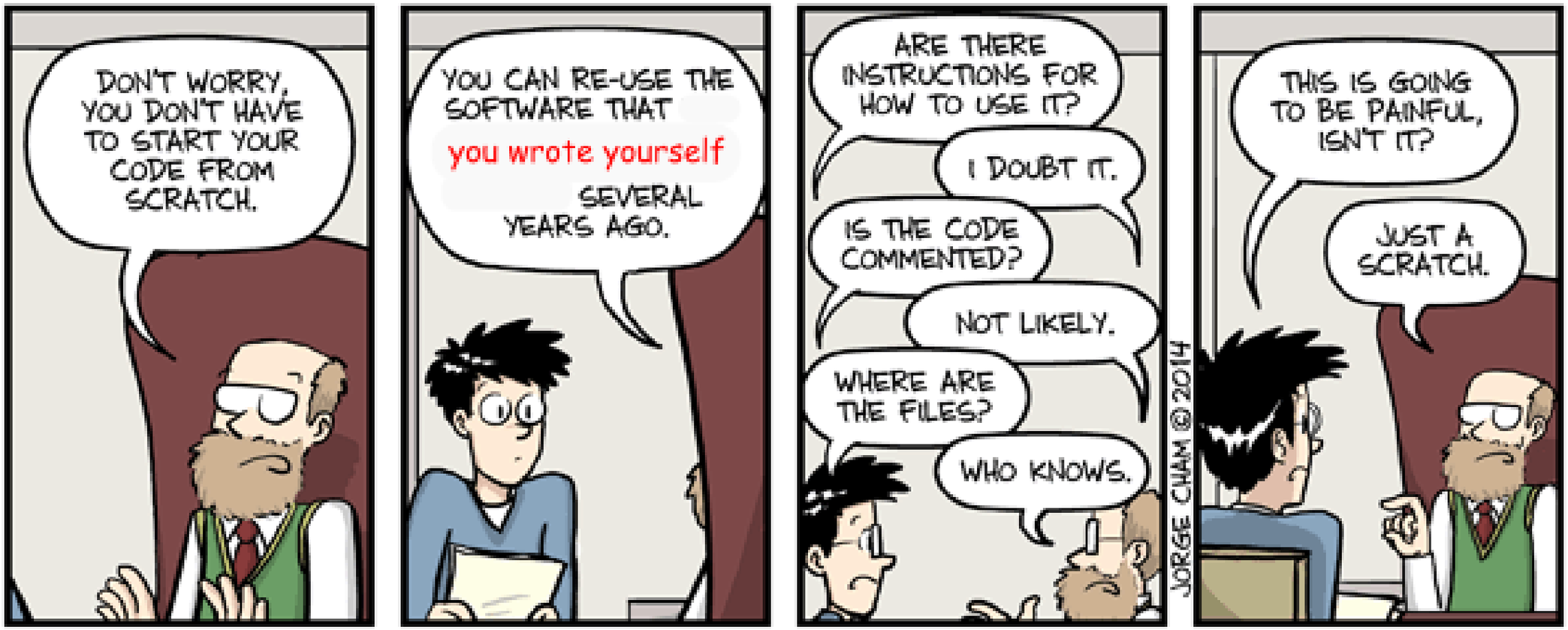

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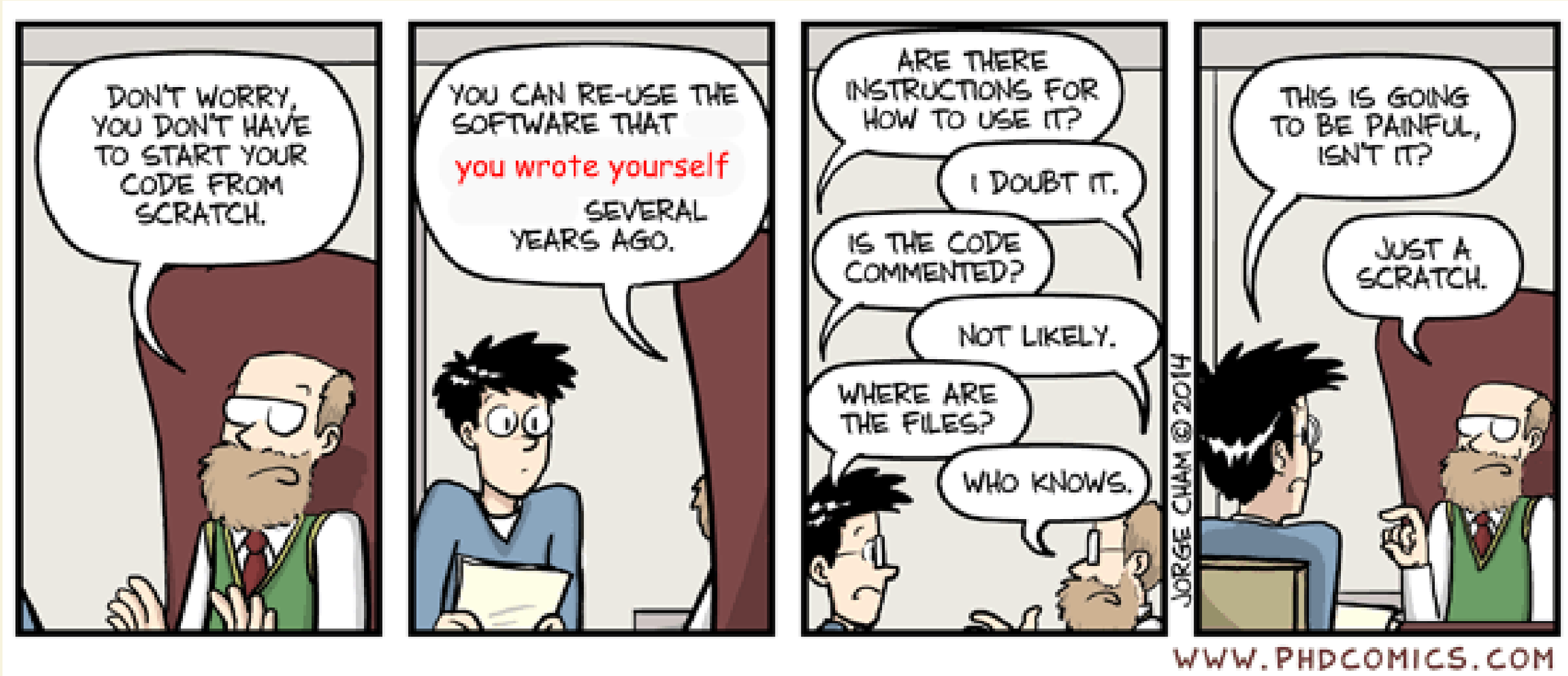

- Which script/unrecorded point-and-click in a GUI produced this figure?

REPRODUCIBLE ANALYSES ARE HARD...

- If I found the correct script, *what version* of this script produced the result?

REPRODUCIBLE ANALYSES ARE HARD...

- If I know the correct code and correct version, *what input data* are all these outputs based on?

REPRODUCIBLE ANALYSES ARE HARD...

- And finally: *How* do I execute the analysis script I want to recompute?

AFTER A WHILE...

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OBJECTIVES

Reproducible analysis

➲ Executing scripts and command line tools reproducibly with `datalad run`

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➲ handbook chapter

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Reproducible analysis

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- ➲ Experience all the ways in which the command can fail

Let's get into a terminal!

➲ handbook chapter

➲ code snippet list

REMINDER: DATALAD-101 NARRATIVE

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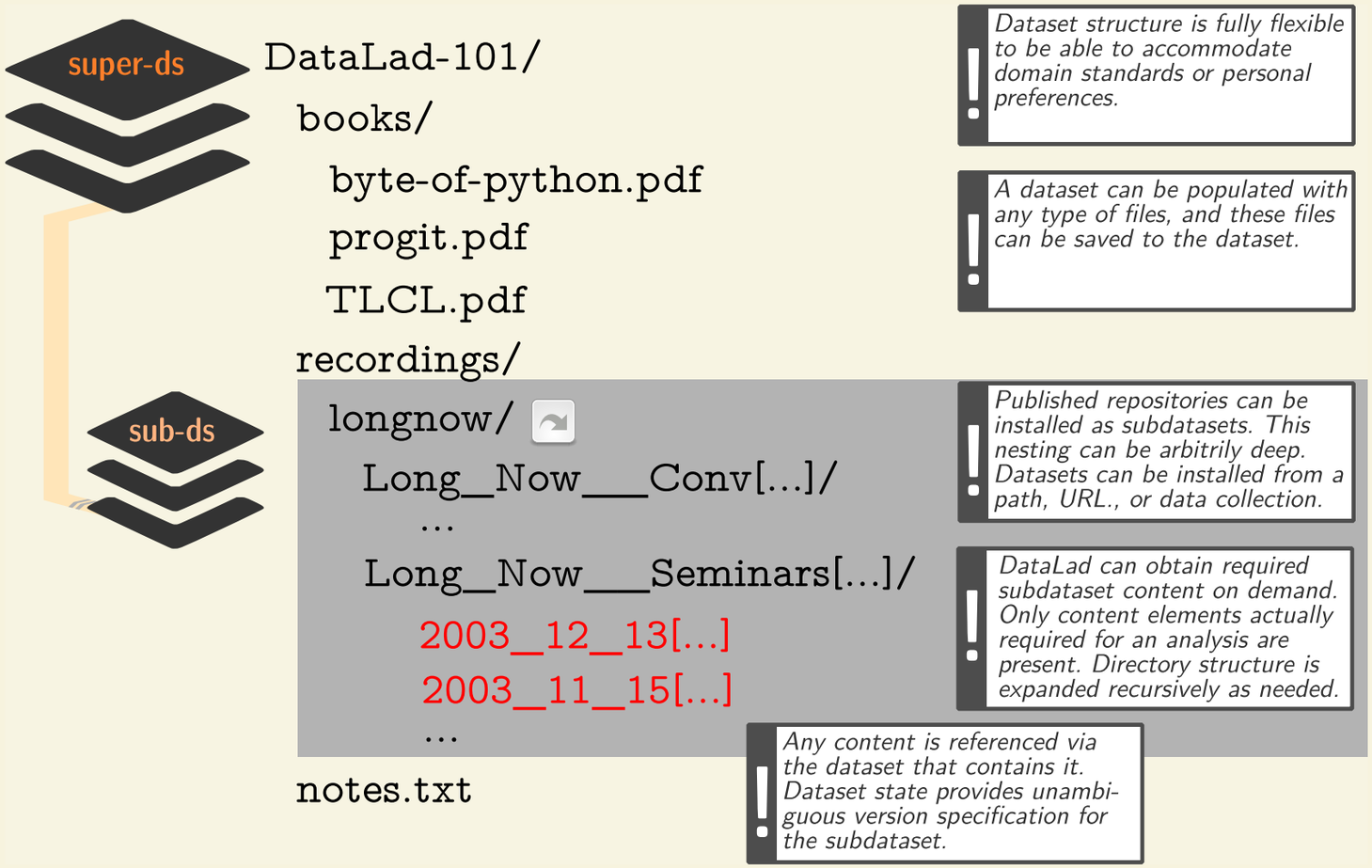

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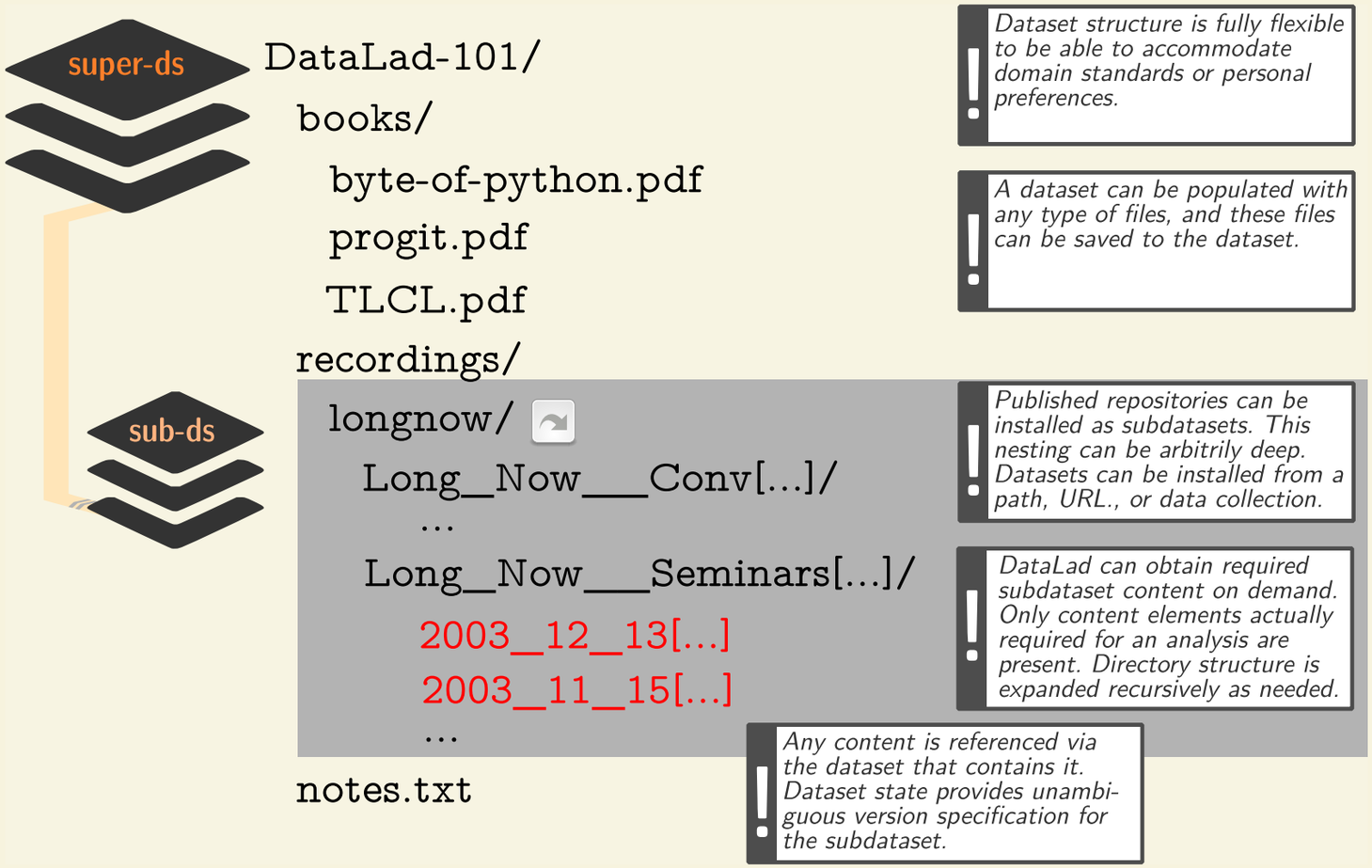

Analysis idea: Write a list of all podcast titles!

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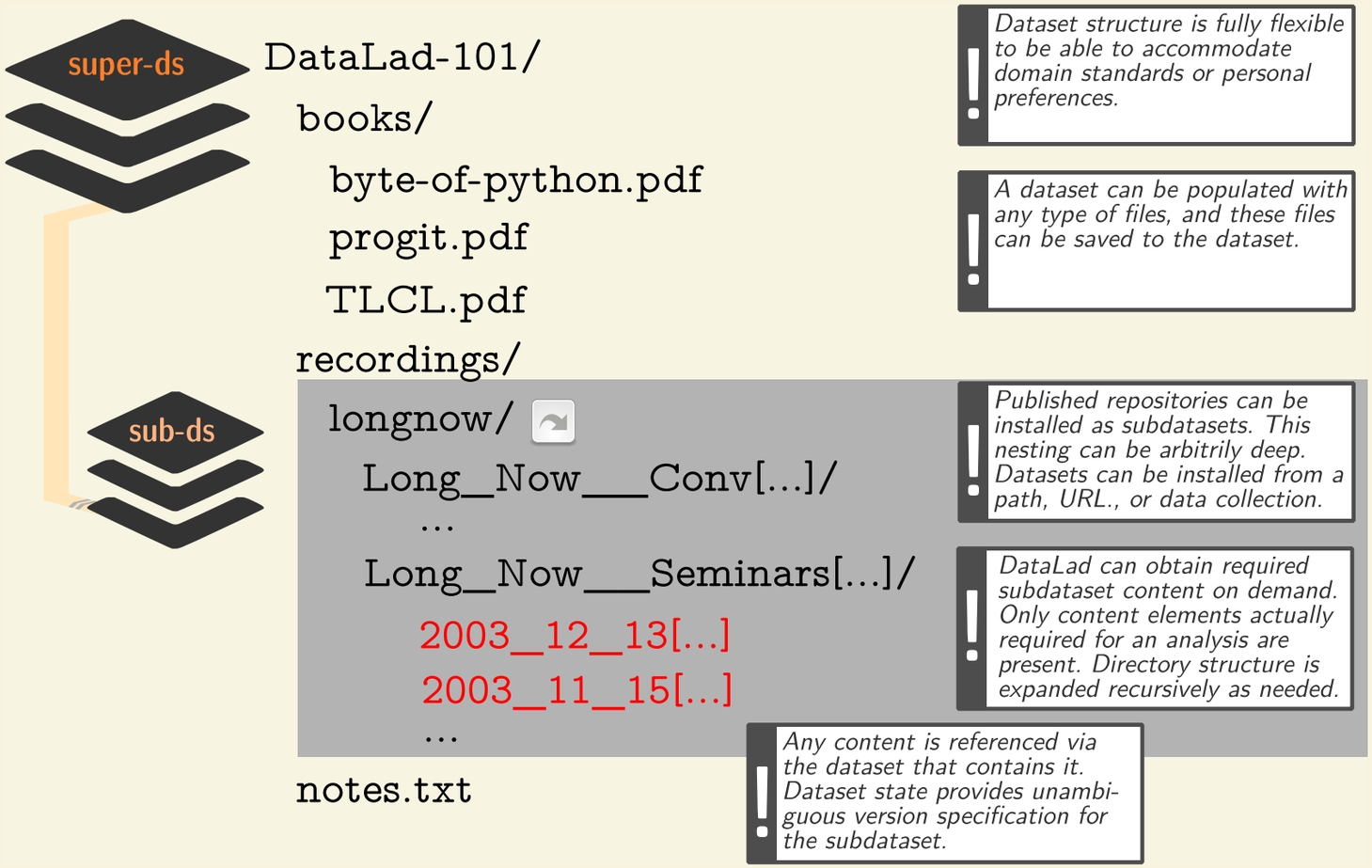

Analysis idea: Write a list of all podcast titles!

If you do not have this directory set up from last time, here is the code that gets you there!

```
for i in recordings/longnow/Long_Now__Seminars*/*.mp3; do
   # get the filename
   base=\$(basename "\$i");
   # strip the extension
   base=\${base%.mp3};
   # date as yyyy-mm-dd
   printf "\${base%%__*}\t" | tr '_' '-';
   # name and title without underscores
   printf "\${base#*__}\n" | tr '_' ' ';
done
```

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➲ A for loop in `shell`, will print each file name as **Date - Speaker - Title** to the terminal.

➲ Redirection to a file with > writes the stream to a file instead of the terminal.

➲ Note: This could be any script or shell command!

A BASIC DATALAD RUN COMMAND

Wrapping any command* in a **datalad run** will record the command's impact on the dataset to the history.

* Running scripts from the command line, using tools from the command line, ...

RUN-RECORDS LINK DATASET MODIFICATIONS TO COMMANDS

```
commit f4a35c8841062eb58f65dbf3cde70ccdc3c9df68 (HEAD -> master)
Author: Adina Wagner adina.wagner@t-online.de
Date:   Mon Nov 11 09:55:02 2019 +0100

    [DATALAD RUNCMD] create a list of podcast titles

    === Do not change lines below ===
    {
     "chain": [],
     "cmd": "bash code/list_titles.sh > recordings/podcasts.tsv",
     "dsid": "02a84dae-faf5-11e9-ba9f-e86a64c8054c",
     "exit": 0,
     "extra_inputs": [],
     "inputs": [],
     "outputs": [],
     "pwd": "."
    }
    ^^^ Do not change lines above ^^^

diff --git a/recordings/podcasts.tsv b/recordings/podcasts.tsv
new file mode 100644
index 0000000..f691b53
--- /dev/null
+++ b/recordings/podcasts.tsv
@@ -0,0 +1,206 @@
+2003-11-15     Brian Eno  The Long Now
+2003-12-13     Peter Schwartz  The Art Of The Really Long View
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[...]
```

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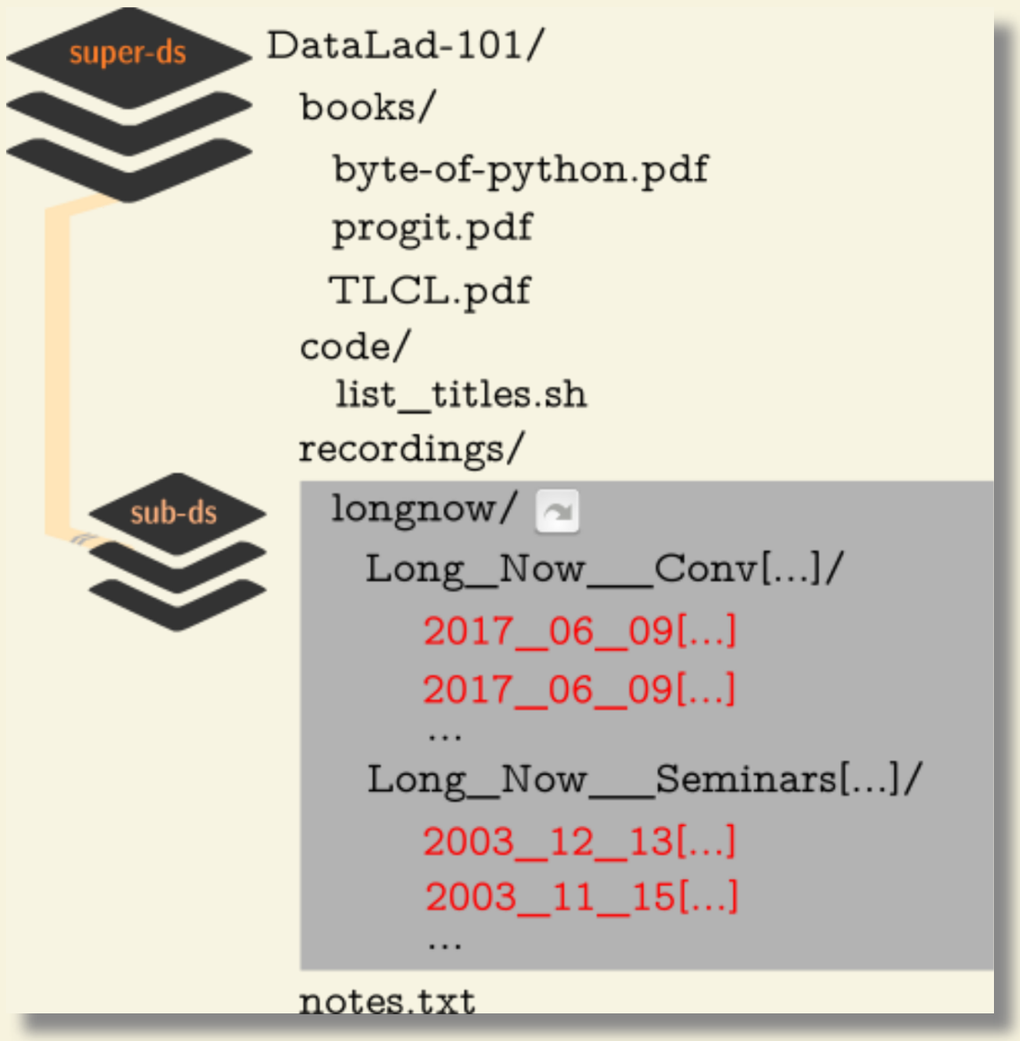
```

It follows logically: If a command does **not** lead to any modification in a dataset, it will not be recorded!

OH! AN ERROR IN THE CODE...

DataLad-101 layout:



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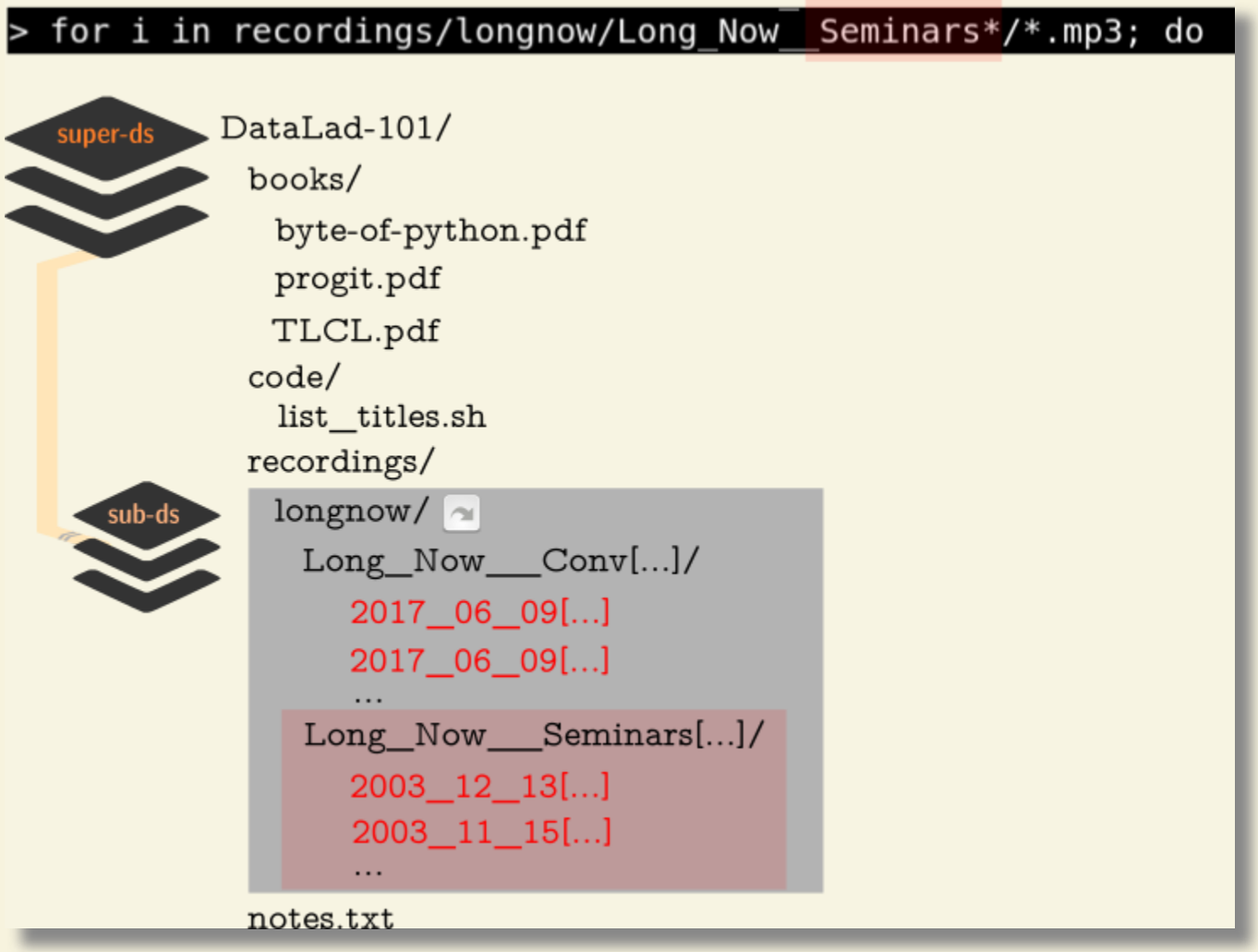
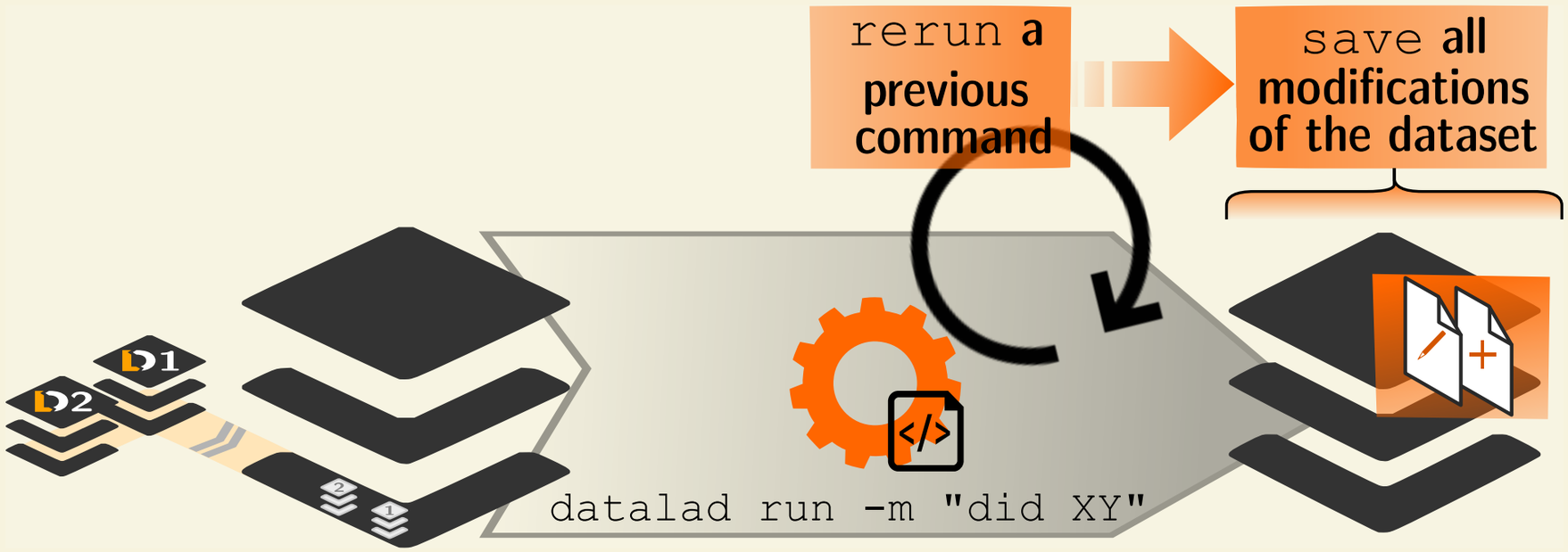


DATALAD RERUN



Re-execute previous datalad run commands

What shall be rerun can be specified via its commit hash:

```
datalad rerun f4a35c884106
```

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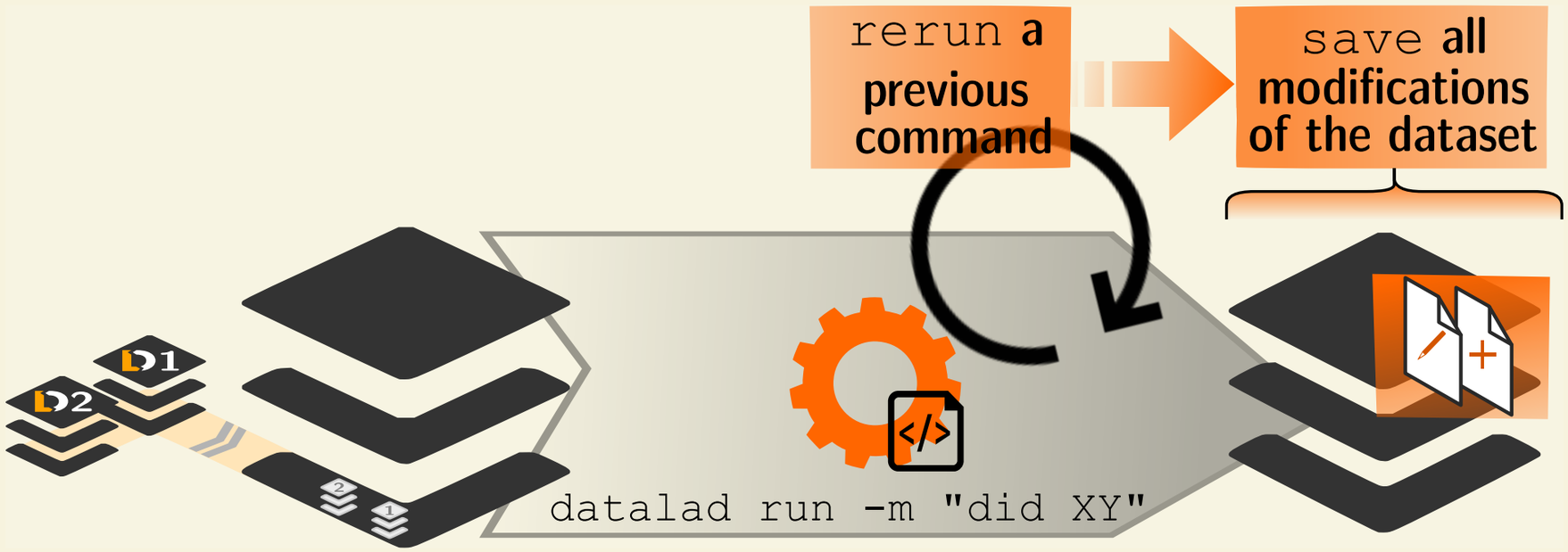

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... but also via tag, revision specifications with HEAD, ..., or by giving a range of commits.

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... but there is more that this command can do for you:

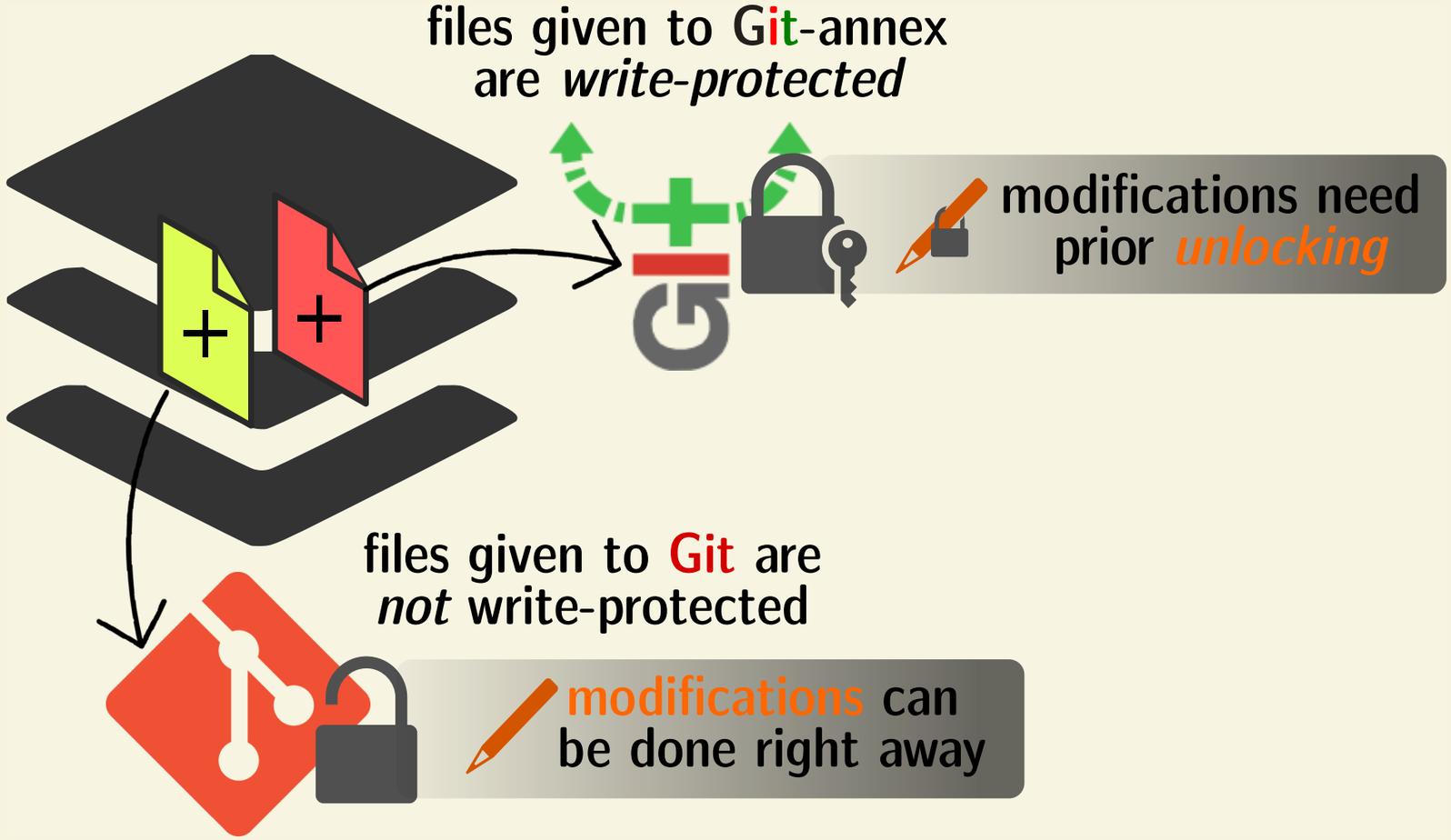
THE ANATOMY OF DATALAD ERROR MESSAGES

```
"convert -resize 400x400 recordings/longnow/.datalad/feed_metadata/logo_salt.jpg recordings/salt_logo_smal
[INFO   ] == Command start (output follows) =====
convert-im6.q16: unable to open image `recordings/longnow/.datalad/feed_metadata/logo_salt.jpg': No such f
convert-im6.q16: no images defined `recordings/salt_logo_small.jpg' @ error/convert.c/ConvertImageCommand/
[INFO   ] == Command exit (modification check follows) =====
[INFO   ] The command had a non-zero exit code. If this is expected, you can save the changes with 'datala
CommandError: command 'convert -resize 400x400 recordings/longnow/.datalad/feed_metadata/logo_salt.jpg rec
Failed to run 'convert -resize 400x400 recordings/longnow/.datalad/feed_metadata/logo_salt.jpg recordings/
```

--INPUT IN DATALAD RUN

Files provided with the --input option are automatically retrieved with **datalad get**, if necessary.

CONTENT-LOCKED FILES (VASTLY SIMPLIFIED)



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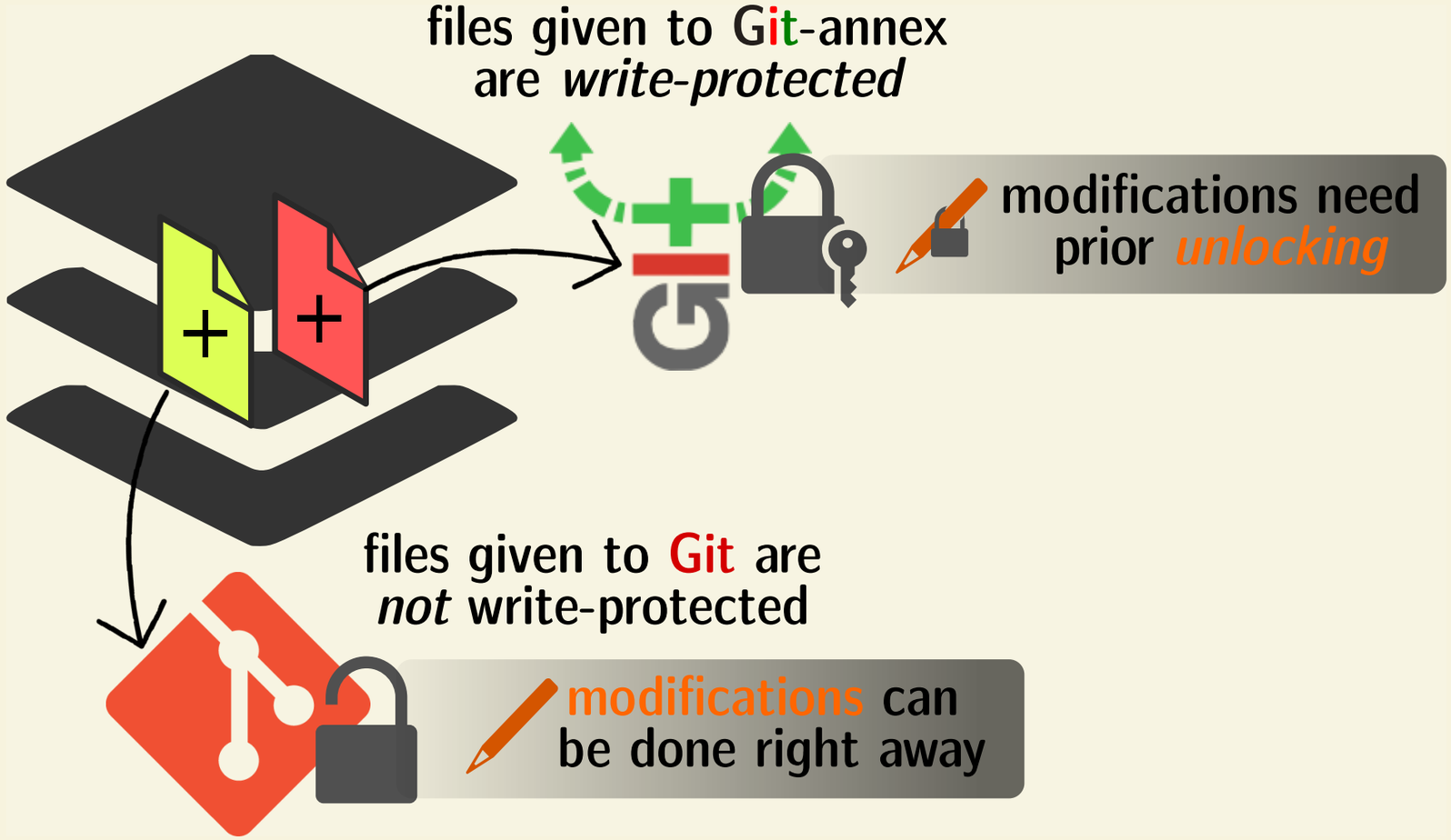

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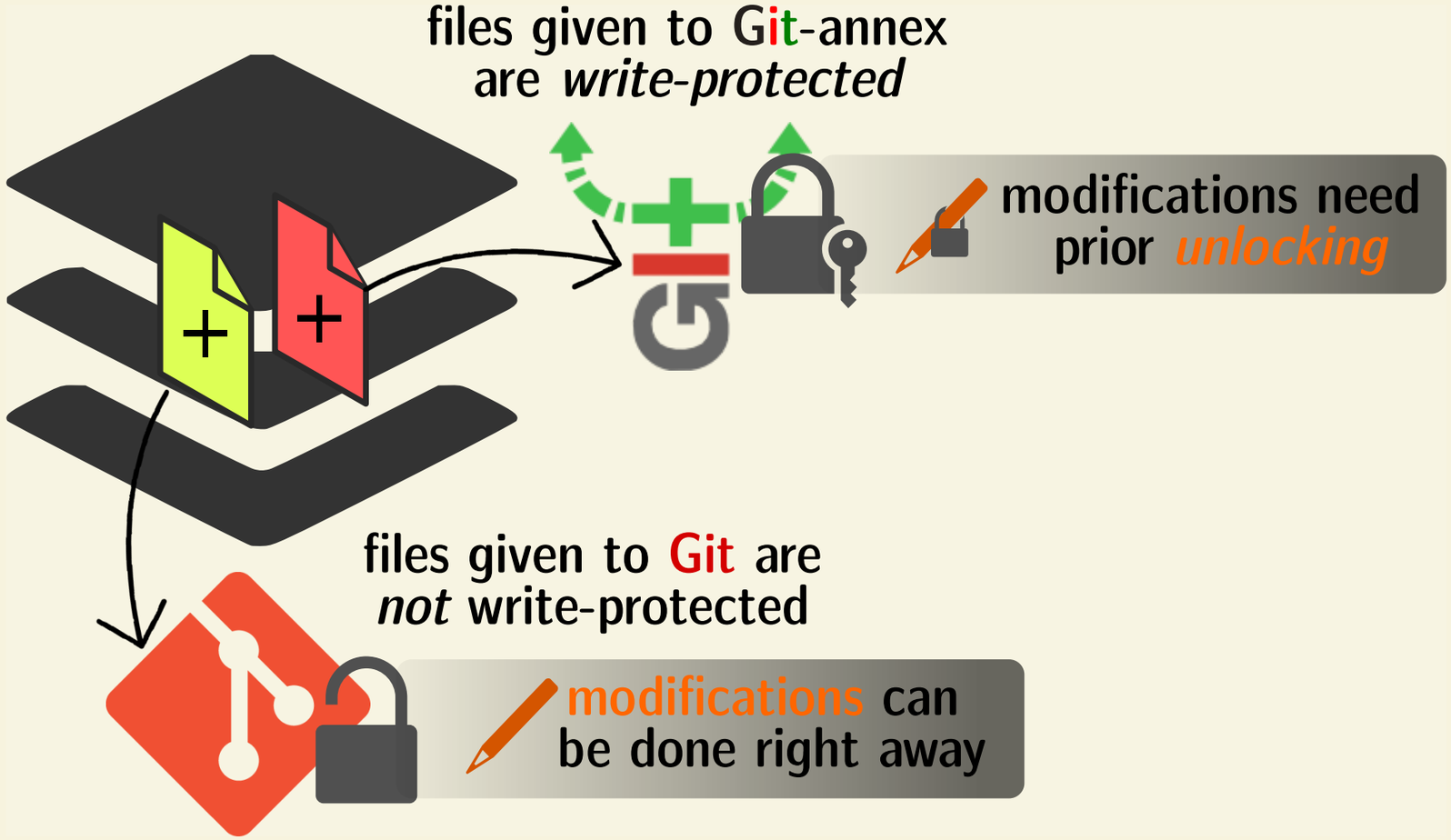

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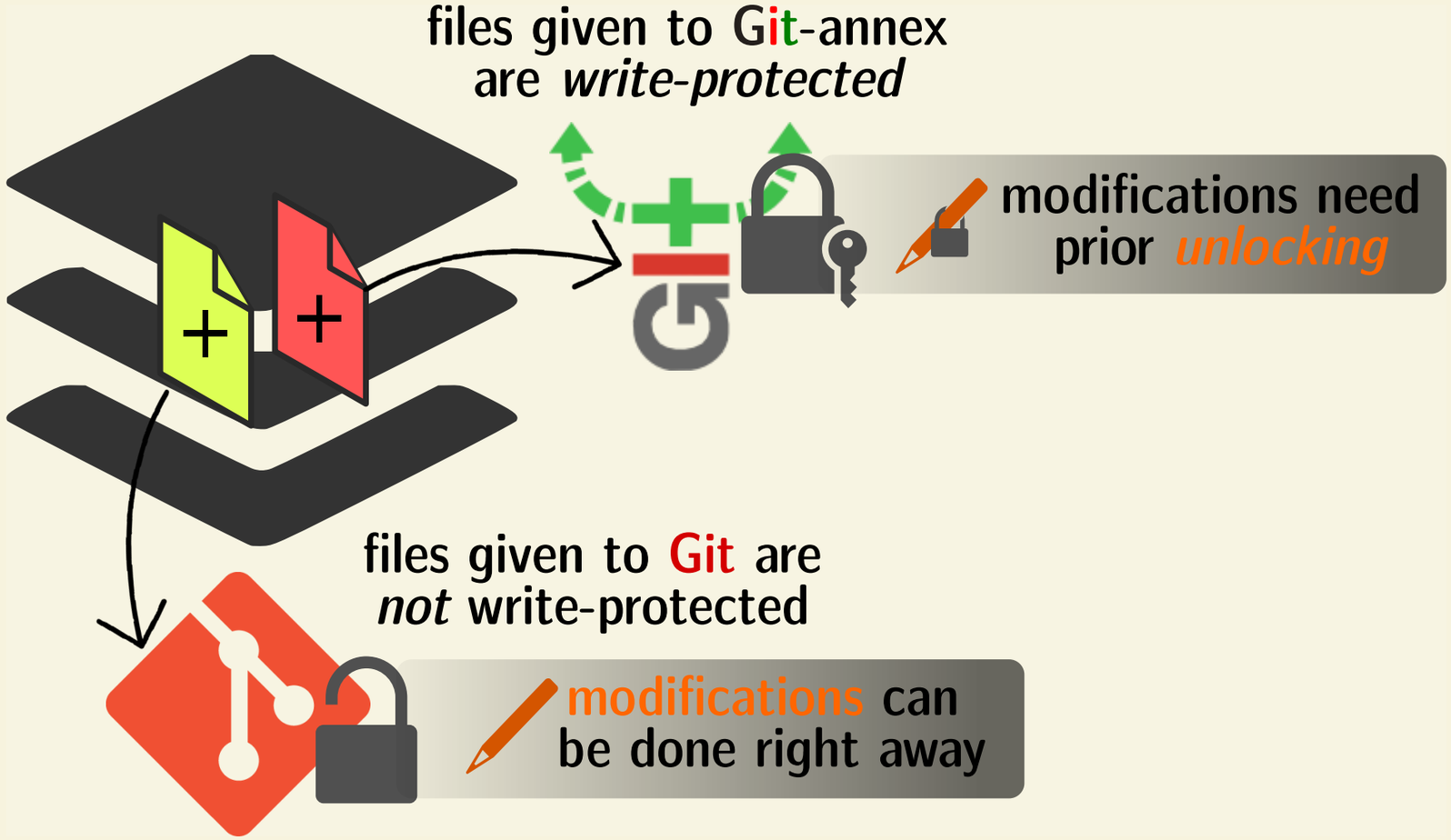

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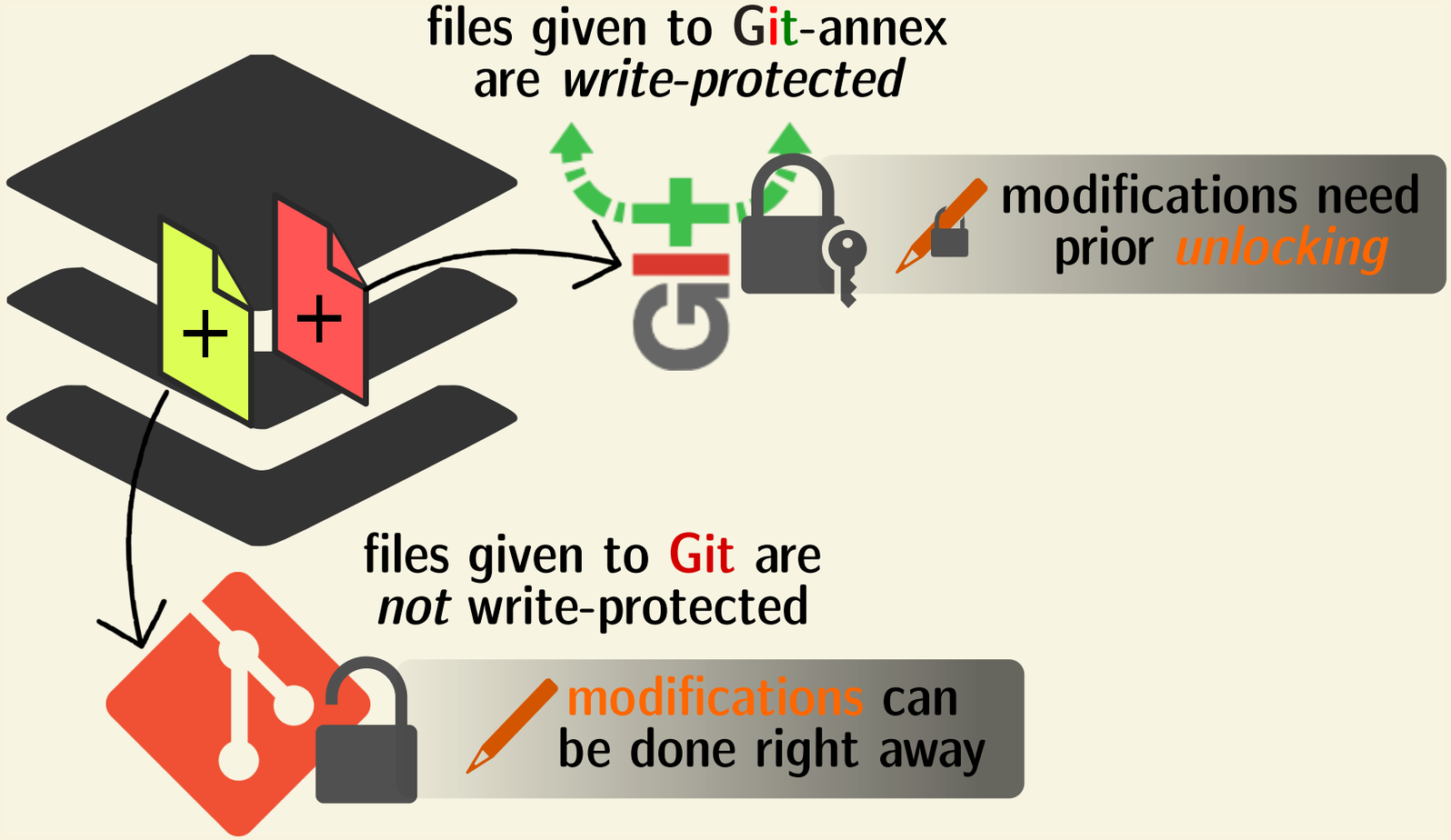

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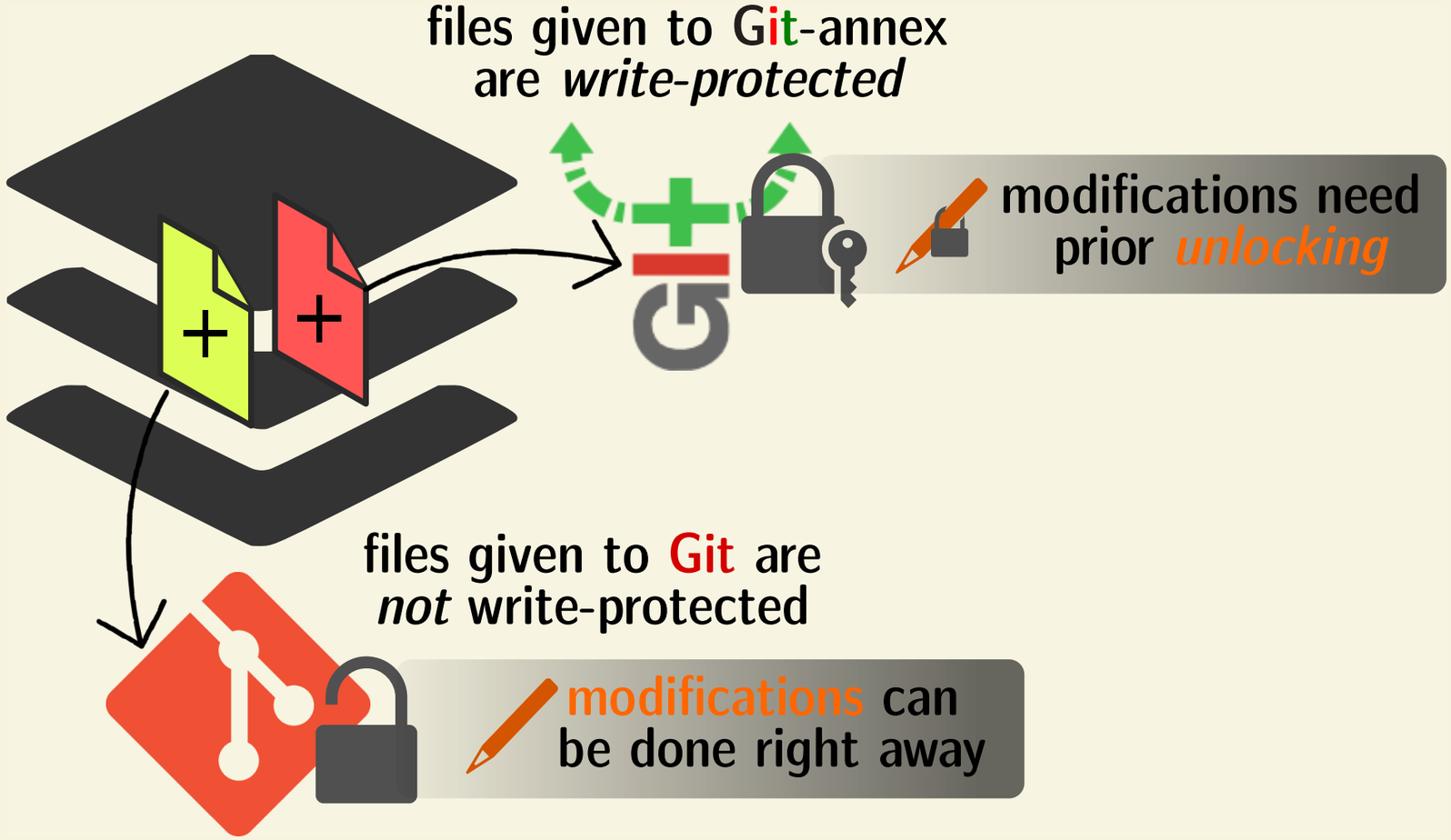

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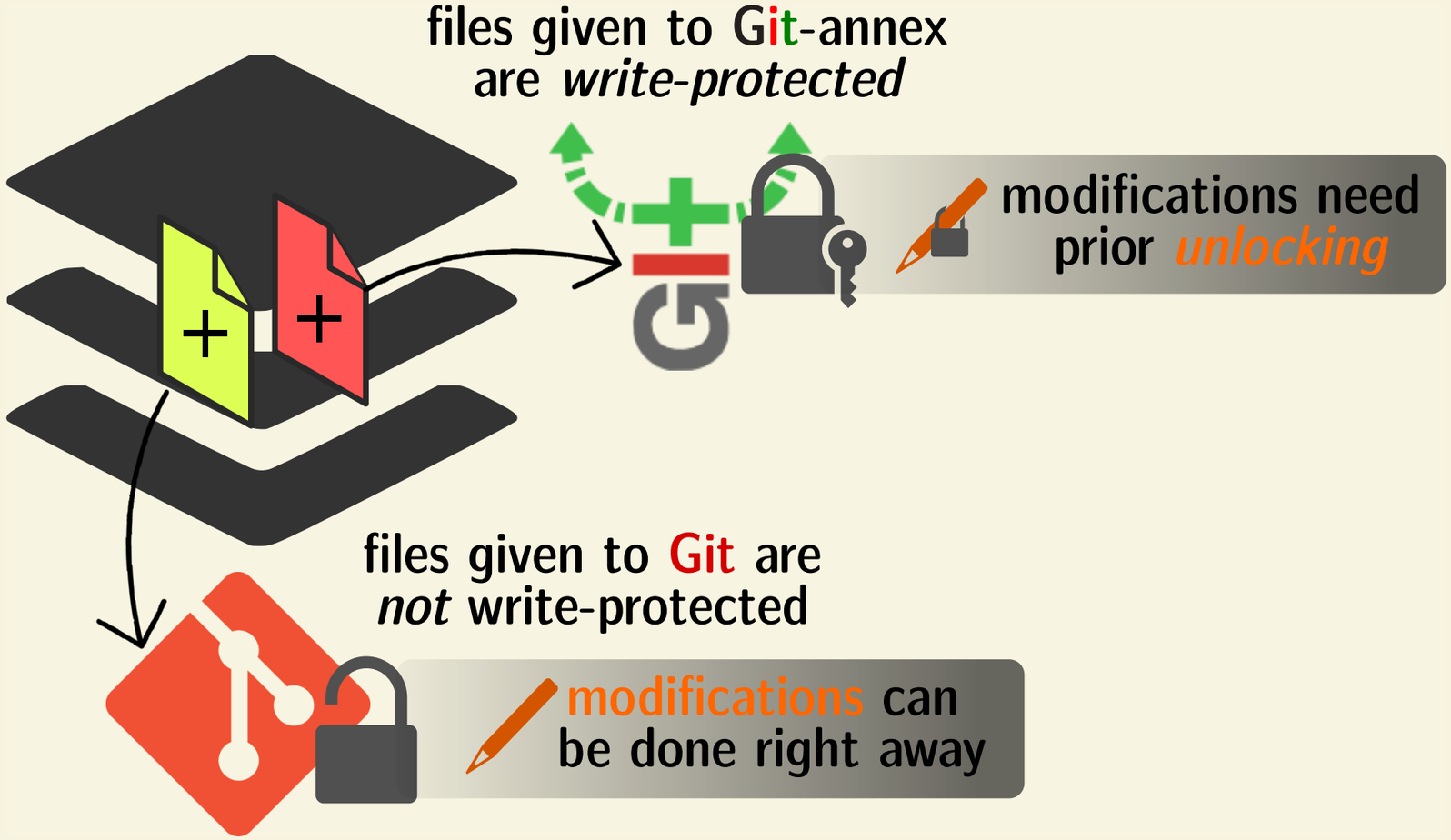

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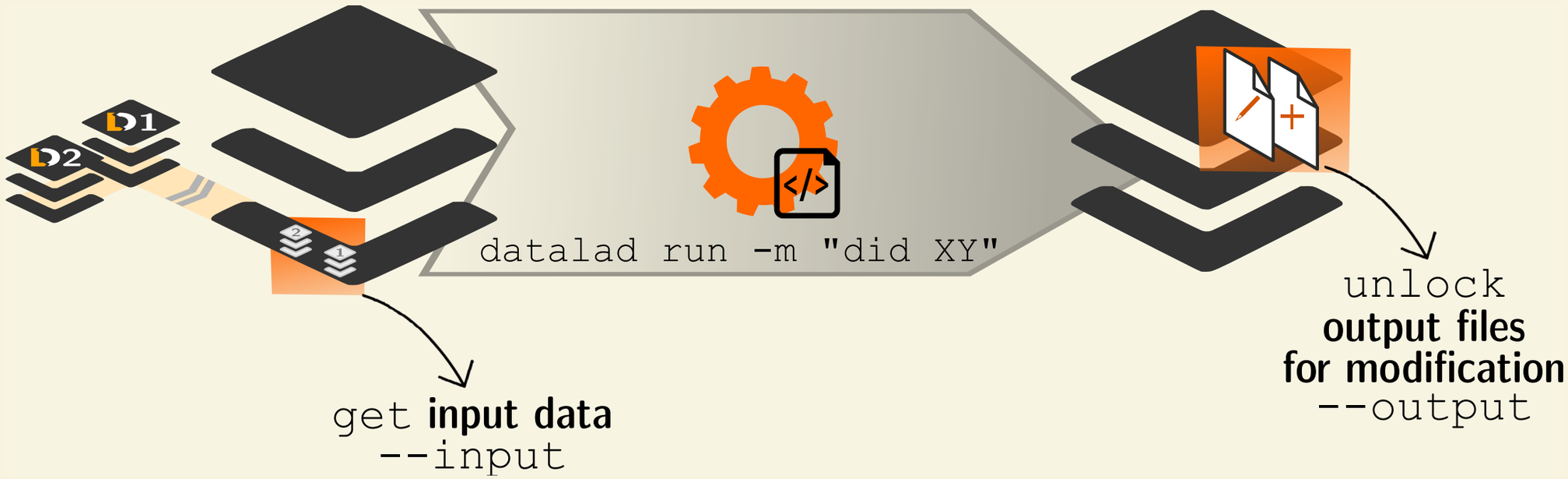
`datalad unlock` can unlock content for modification.

`datalad save` will lock content again.

--OUTPUT IN DATALAD RUN



Files provided with the --output option are automatically unlocked for modification with **datalad unlock**, if necessary.

ANALYSIS PROVENANCE CAPTURE

Easy provanance capture!

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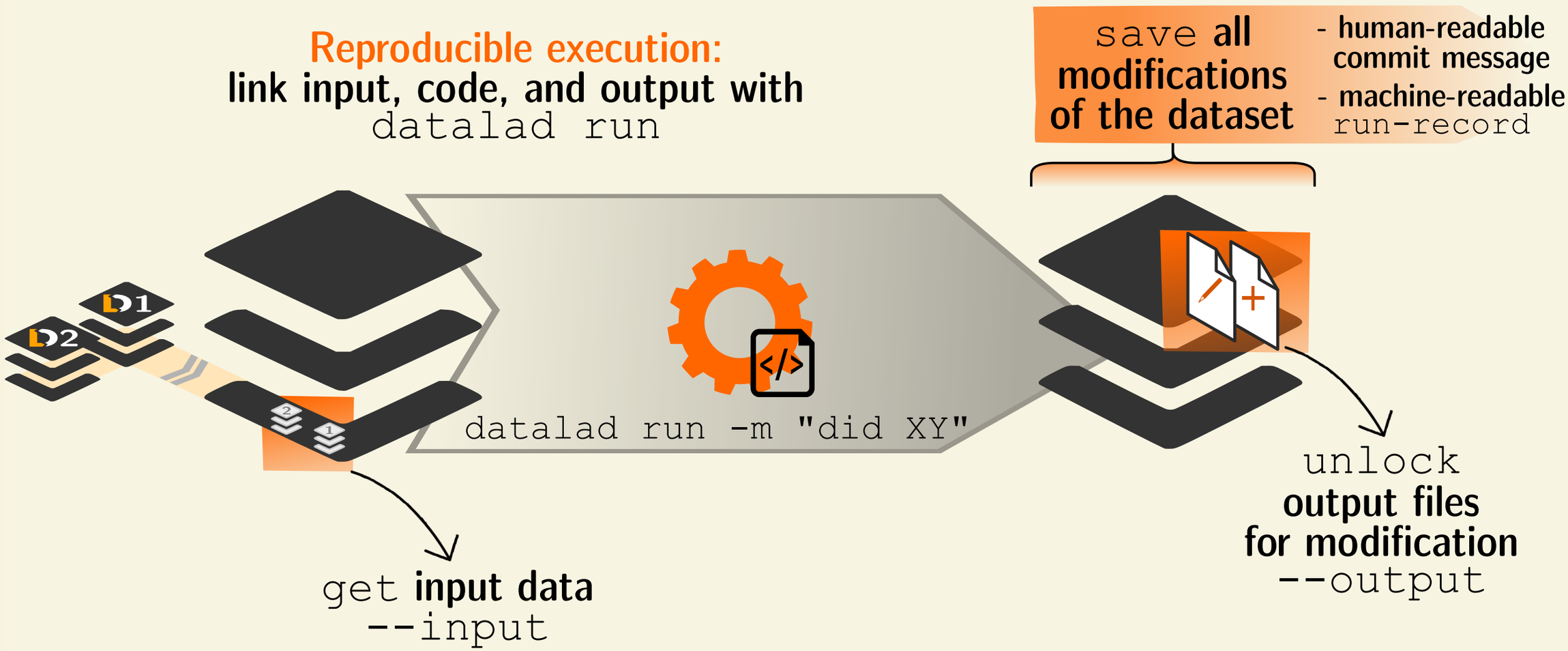
Reproducible execution:
link input, code, and output with
`datalad run`



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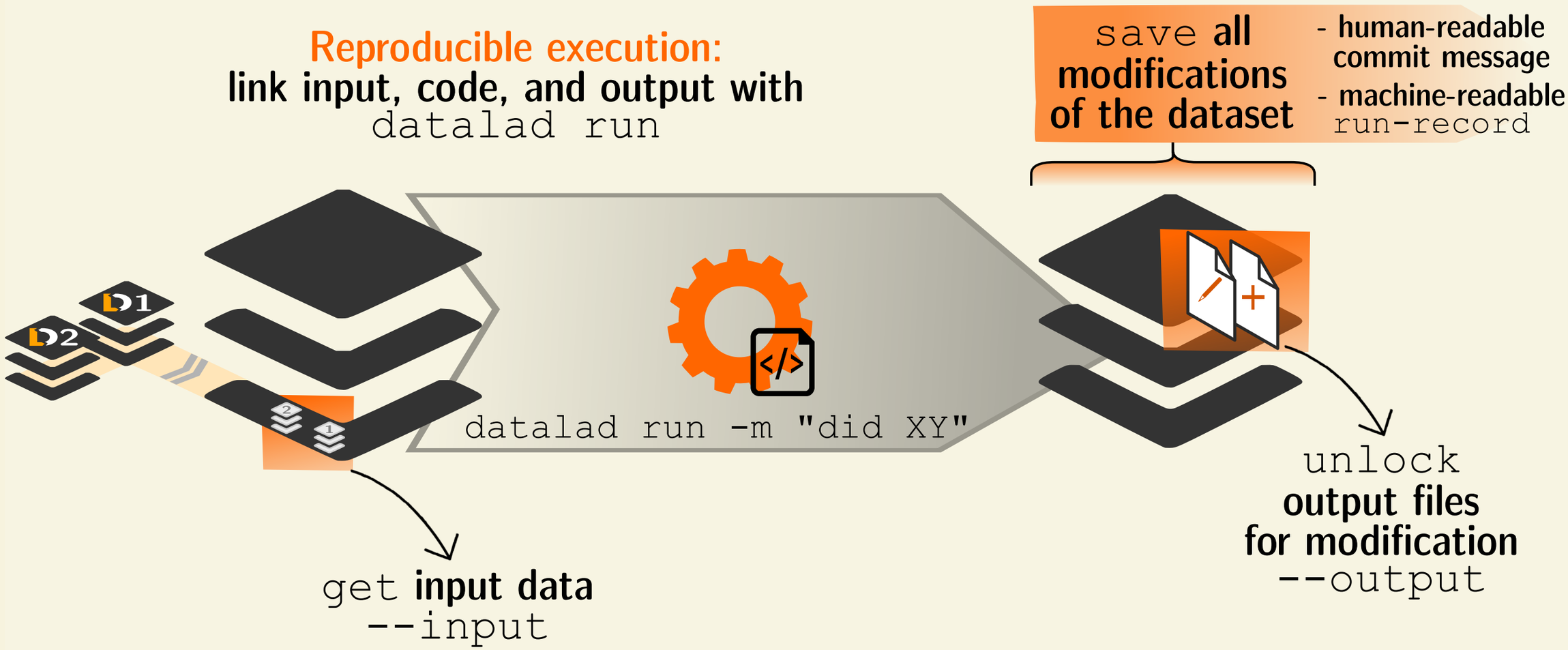

Advice:

ANALYSIS PROVENANCE CAPTURE

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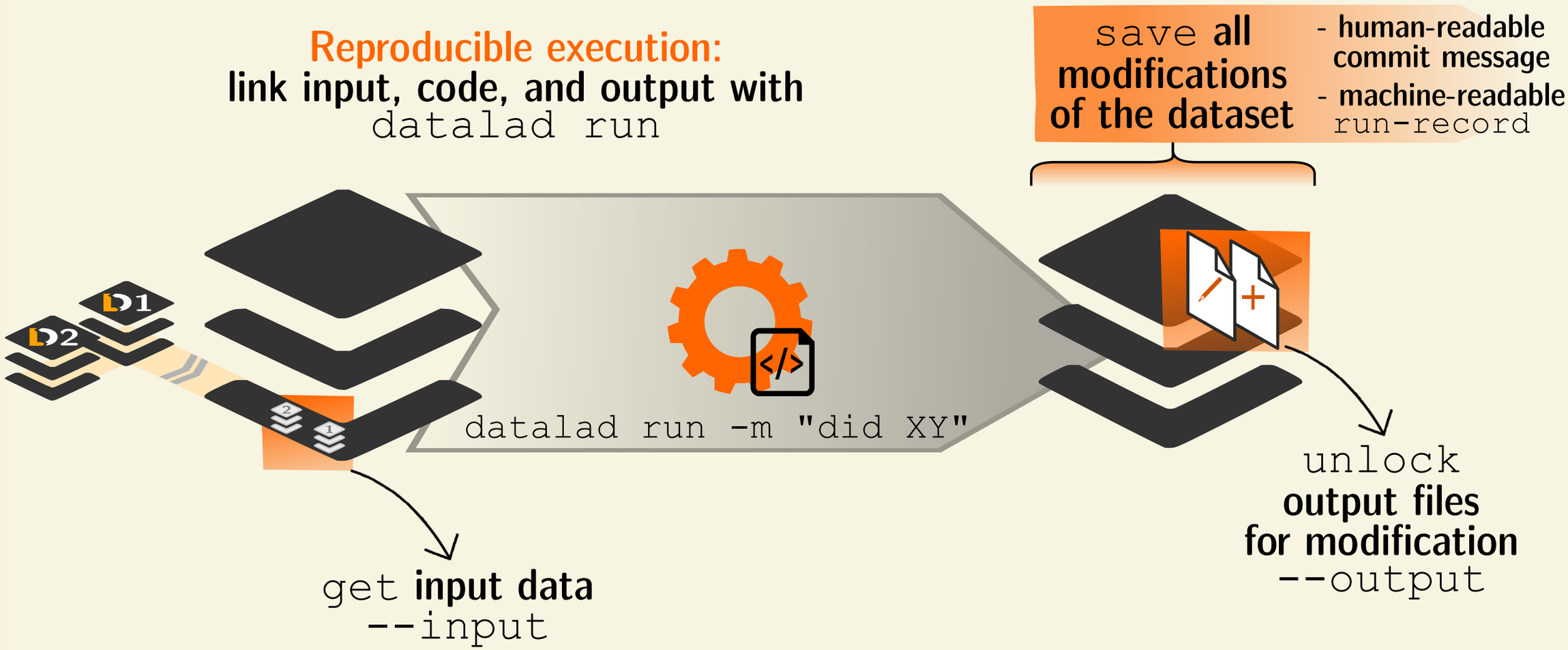

- use `--input` and `--output`

Advice:

ANALYSIS PROVENANCE CAPTURE

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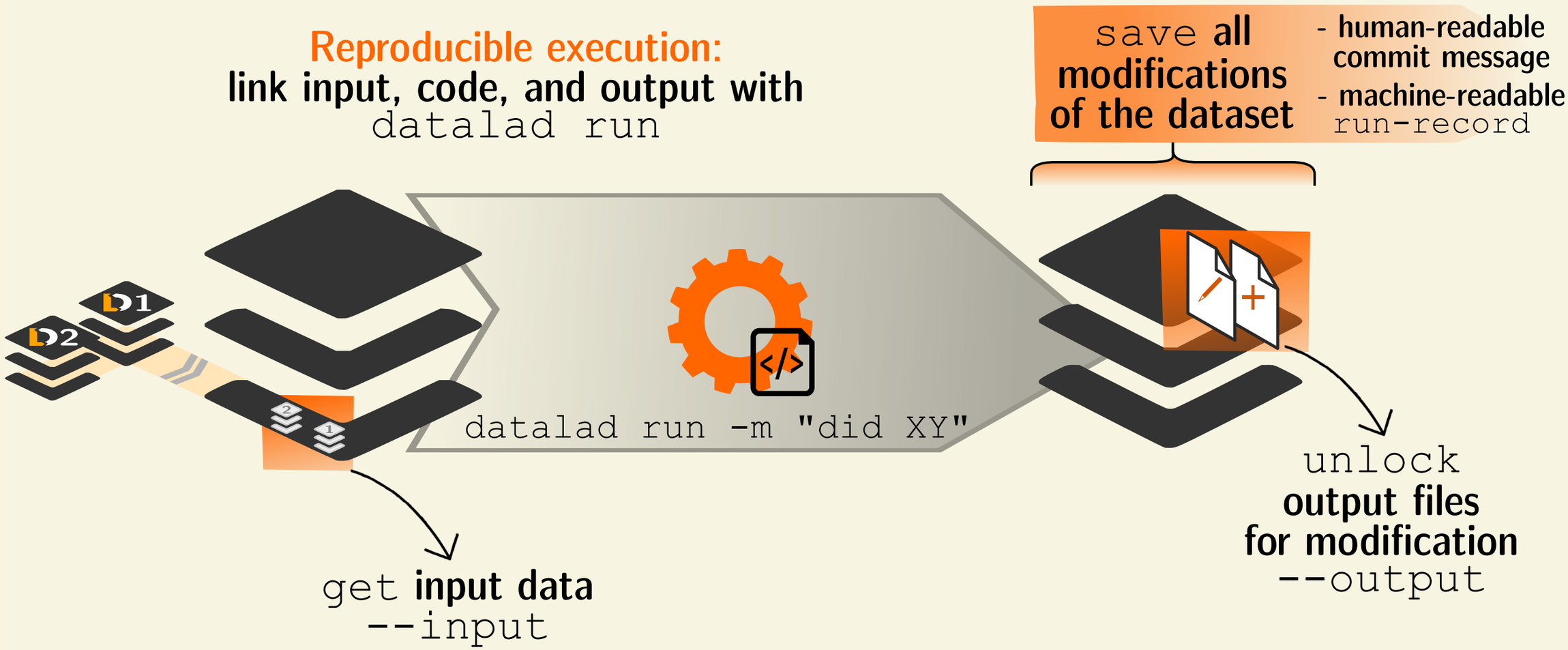
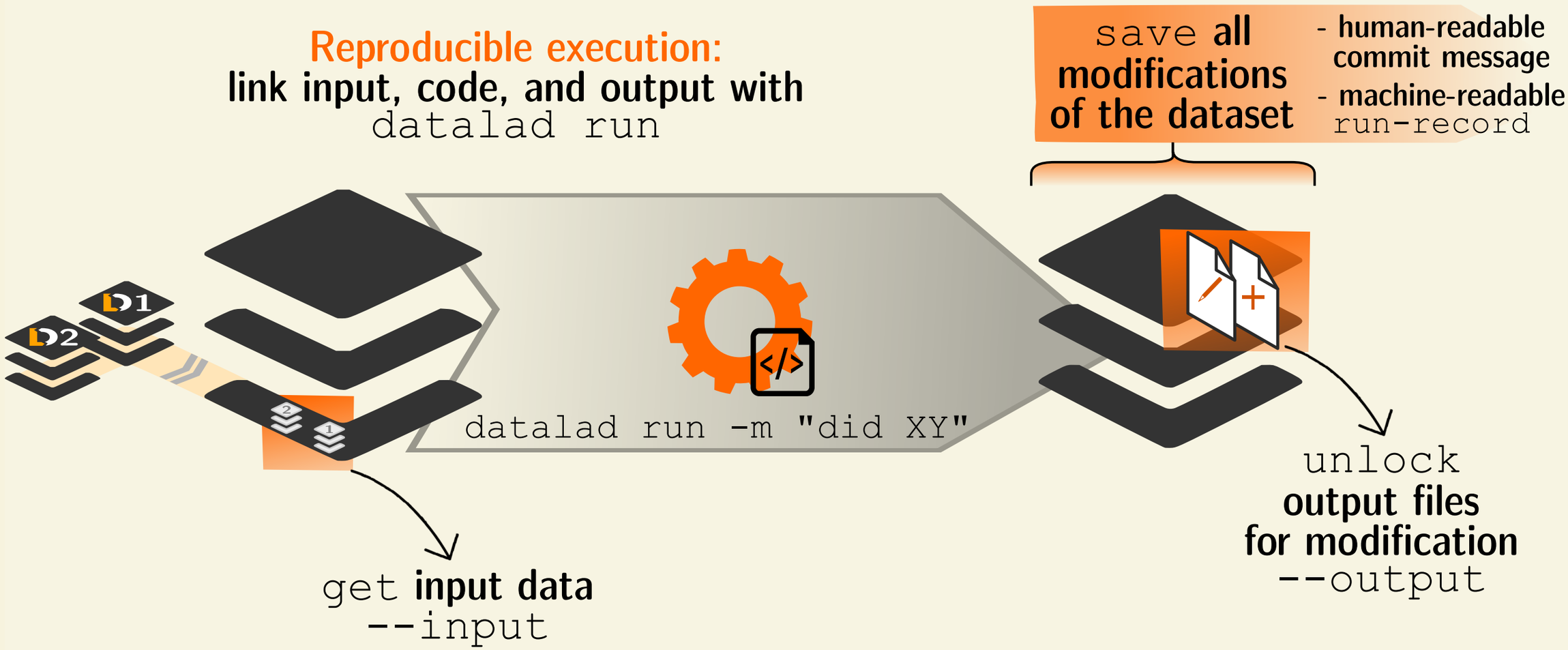


Advice:

- use `--input` and `--output`
- Attach helpful commit messages

ANALYSIS PROVENANCE CAPTURE

Easy provanance capture!



Advice:

- use `--input` and `--output`
- Attach helpful commit messages
- Make sure to have a clean dataset state

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OUTLOOK: COMPUTATIONAL REPRODUCIBILITY

- It may not be enough to record inputs, code, and outputs of an analysis!
- Without sufficient information about **required software (versions)**, analyses may fail to reproduce *or even run*.
- The DataLad extension datalad containers can also capture complete software environments.
- Get a preview soon: chapters on extensions is close to being finished

NOW WHAT I CAN DO WITH THAT?

Reproducible analysis with datalad run

- Record all provenance by wrapping any command in a datalad run
- Link input, output, and code
- Rerun computations with a single command

PRACTICE @HOME

- Wrap any simple shell command (e.g., `cp`) in a datalad run, and (later) also scripts of yours

FURTHER READING

A walk-through on `datalad run`:

- Chapter DataLad, Run! in the handbook.

More on the configurations that determine whether a file is managed by Git or Git-annex:

- Chapter Tuning datasets to your needs in the handbook

How to get help on commands and their options:

- Section How to get help in the handbook

OUTLINE: WHAT COMES NEXT?

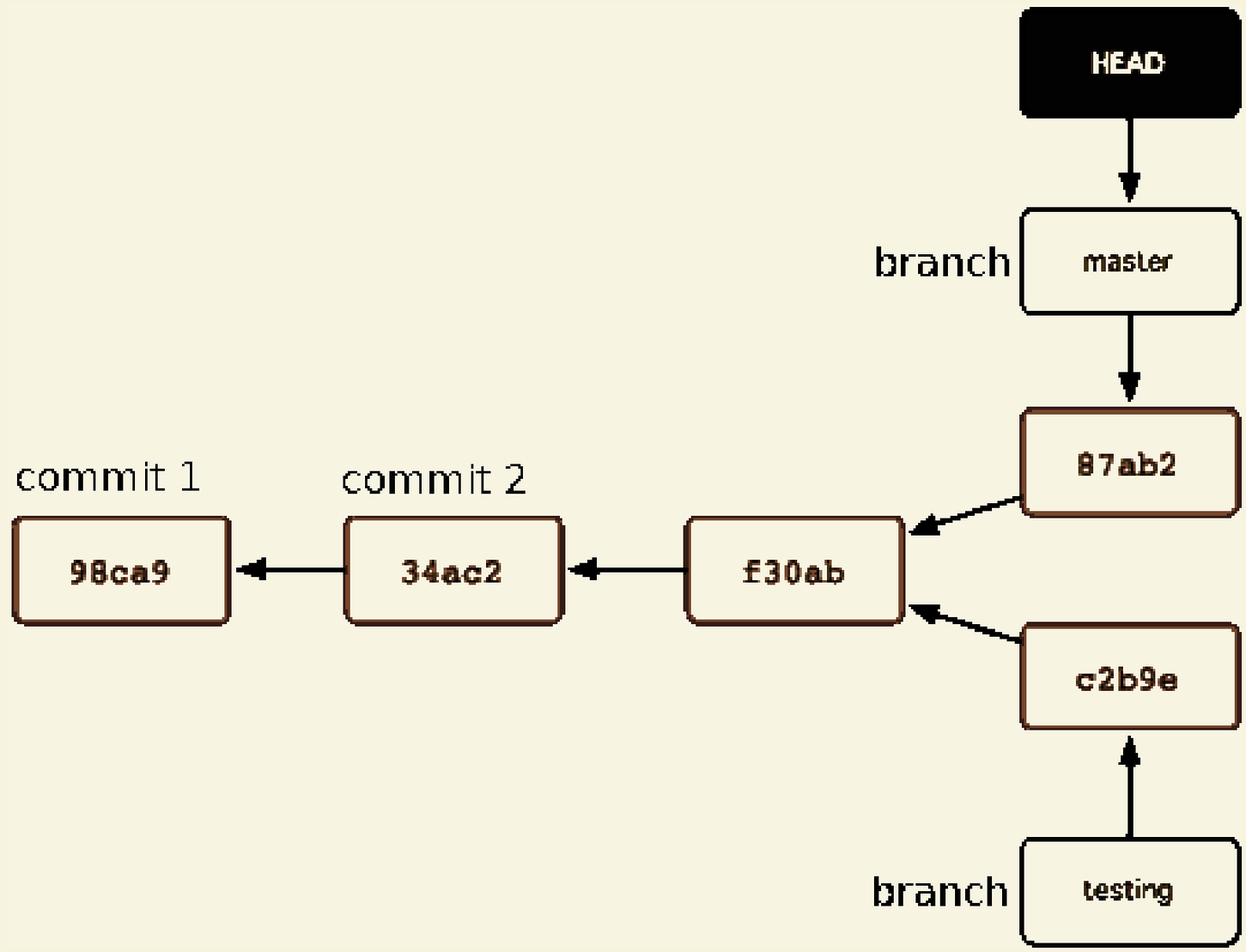
- Symlinks, data integrity, data security (chapter Under the hood: Git-annex in the handbook).
- **Which date is suitable?** > Doodle poll <

OPEN QUESTION SESSION

BACKUP SLIDES FOR ANTICIPATED QUESTIONS

WHAT IS HEAD?

- A git repository is build up as a *tree* of **commits** (history entries).
- A **branch** is a named pointer (reference) to a commit, and allows to isolate developments. The default branch is called `master`.
- HEAD is a pointer to the branch you are on, and thus to the last commit in the given branch.



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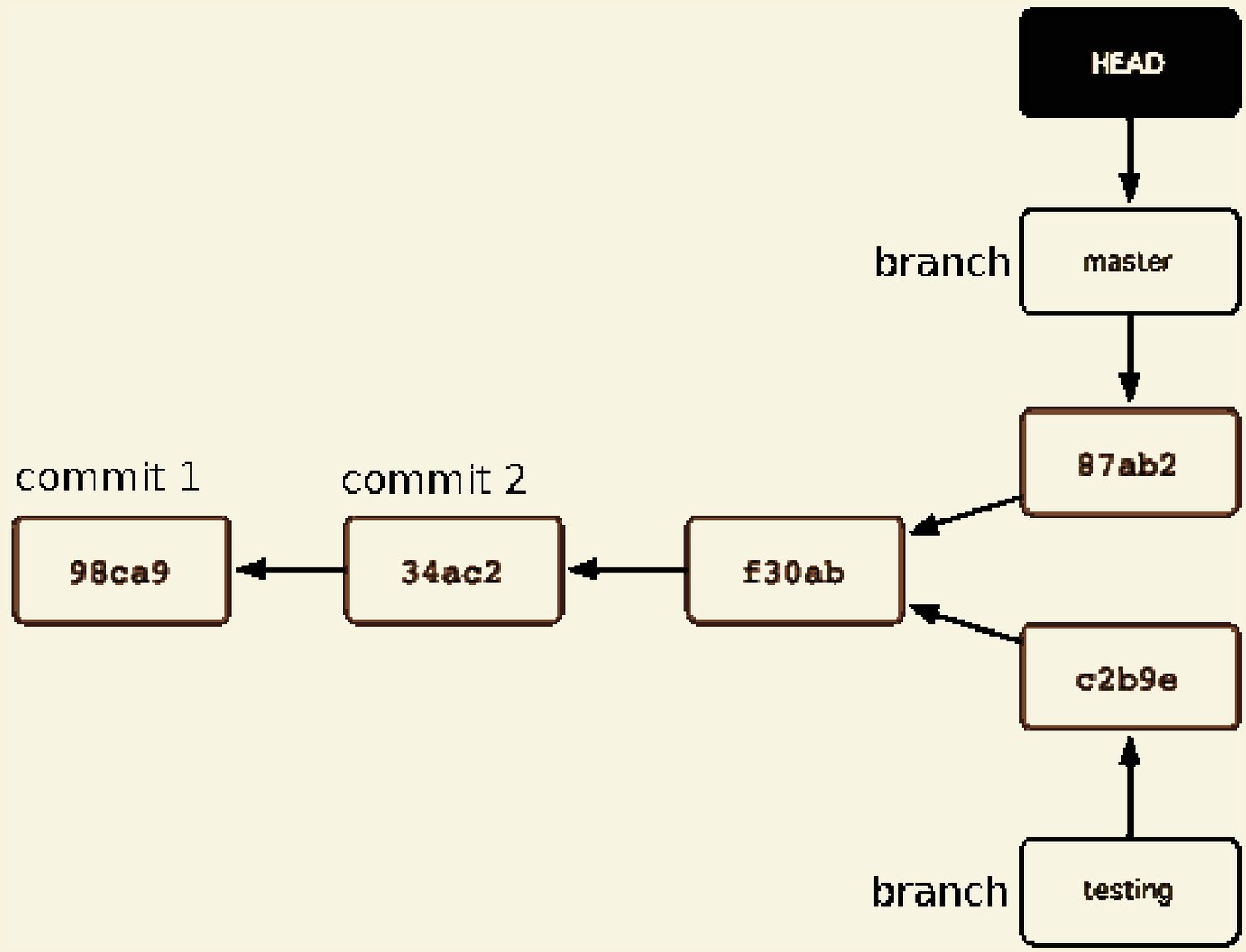

If you'd be on branch "testing", which commit would HEAD point to?

HOW DOES A HERE-DOCUMENT WORK?

```
$ cat << EOT > notes.txt
One can create a new dataset with 'datalad create [--description] PATH'.
The dataset is created empty

EOT
```

- Two *delimiting identifiers* (EOT) wrap any amount of text into a stream
- The << characters *redirect* the stream into *standard input* for the `cat` command
- The > character *redirects* the *standard output* of `cat` and writes it into a new file notes.txt

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Why is it used?

- Allows pretty formating (e.g., line breaks)
- Allows writing documents from the terminal