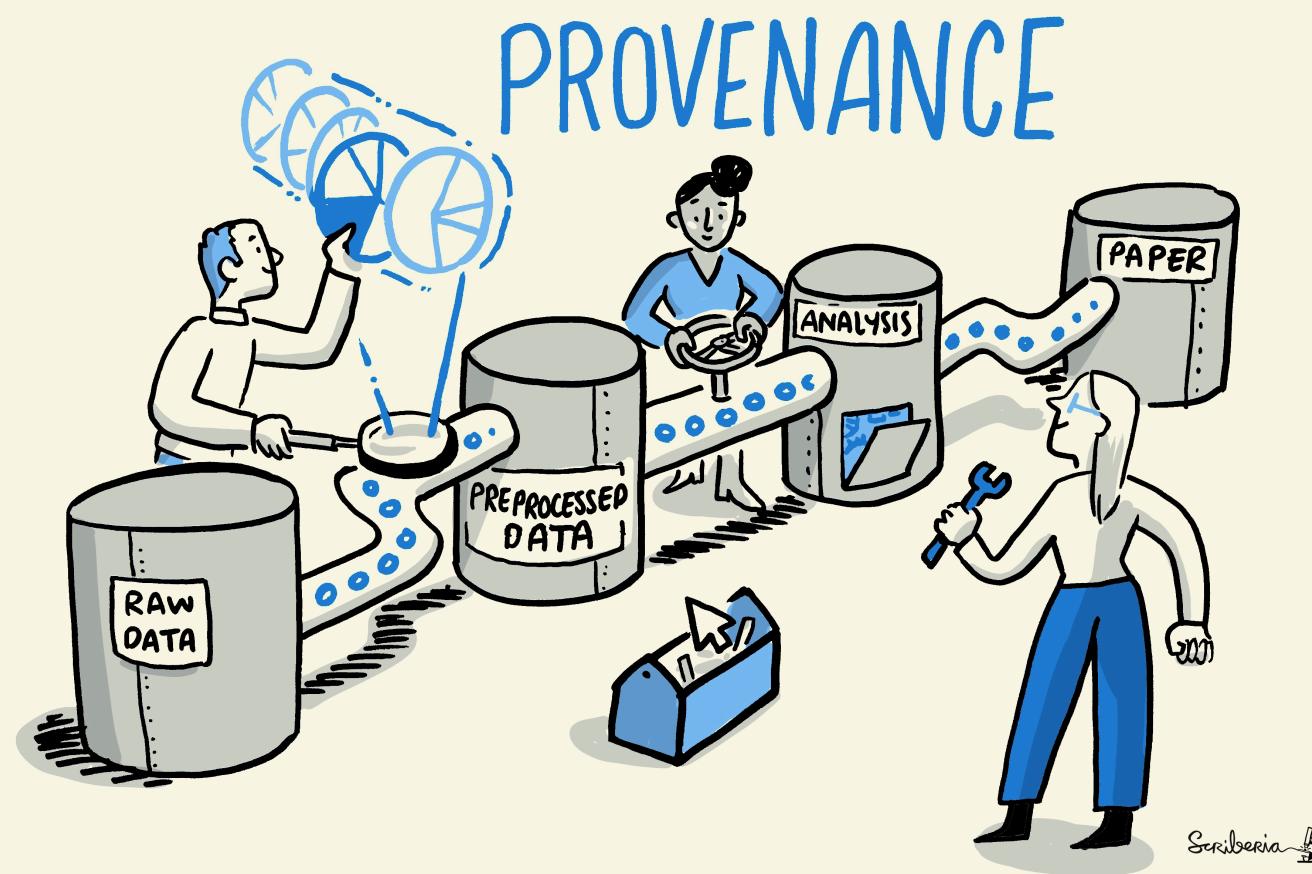


REPRODUCIBLE RESEARCH

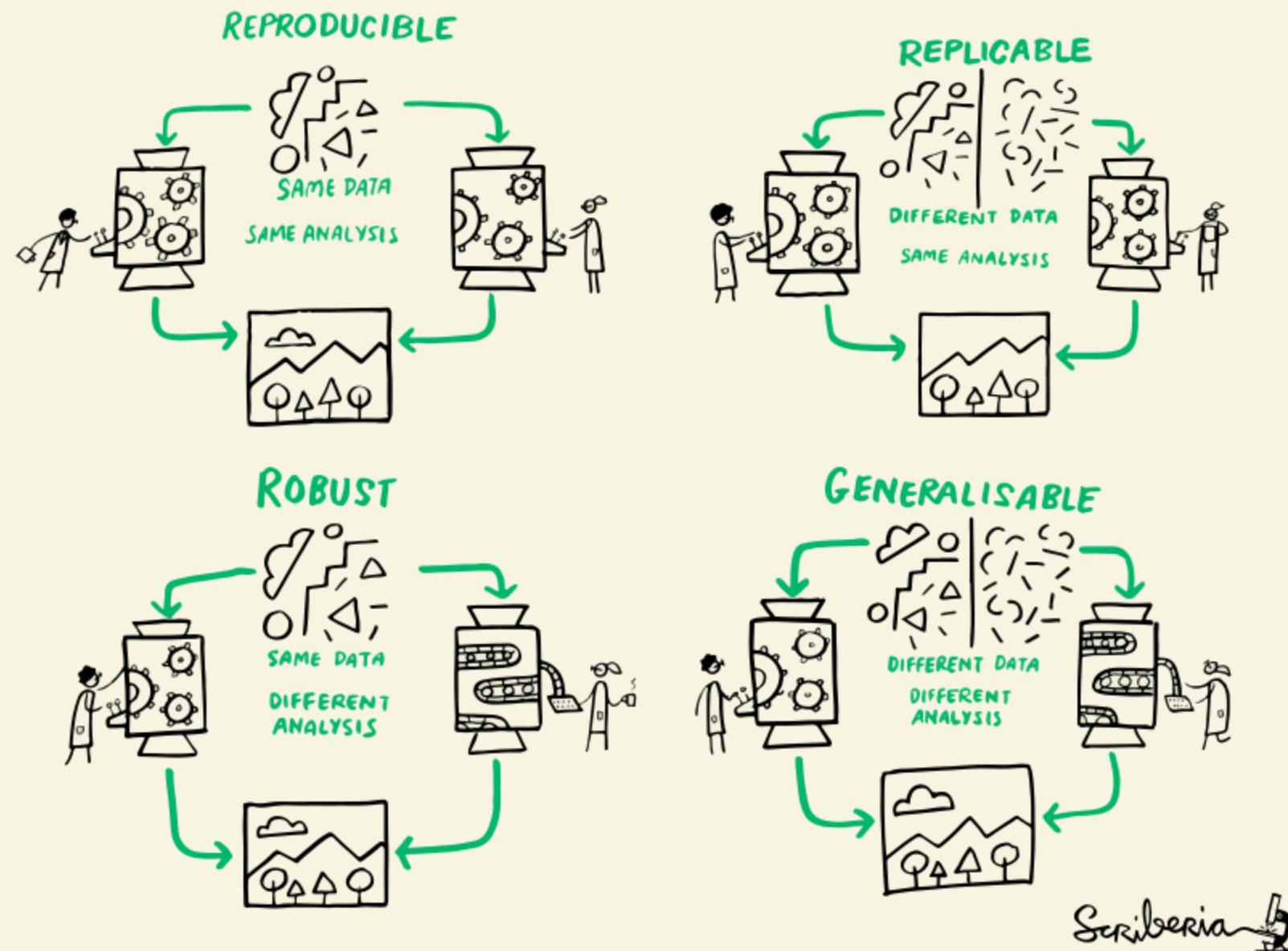




“An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.”

Jon Claerbout (paraphrased)

REMINDER: DEFINITIONS



(The Turing Way)

GENERAL REPRODUCIBILITY CHECKLIST (HINSEN, 2020)

Use code/scripts

Document

Record

Test

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Create a suite of test functions. Use positive and negative control data sets to ensure you get the expected results, and run those tests throughout development to squash bugs as they arise.

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Guide

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GENERAL REPRODUCIBILITY CHECKLIST (HINSEN, 2020)

Automate

Simplify

Verify

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Use continuous-integration services (for example, Travis CI) to automatically test your code over time, and in various computational environments

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Avoid niche or hard-to-install third-party code libraries that can complicate reuse.

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Automate

Use continuous-integration services (for example, Travis CI) to automatically test your code over time, and in various computational environments

Simplify

Avoid niche or hard-to-install third-party code libraries that can complicate reuse.

Verify

Check your code's portability by running it in a range of computing environments.

REPRODUCIBLE RESEARCH

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- DataLad is one tool that can make reproducible research easier

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- Let's take a more detailed look into some ways in which DataLad can help:

REPRODUCIBLE RESEARCH

- DataLad is one tool that can make reproducible research easier
- Let's take a more detailed look into some ways in which DataLad can help:
 - Some miscellaneous facts about DataLad functions
 - Details of the YODA principles for reproducible analyses
 - DataLad as a component in reproducible papers
 - The `datalad-container` extension to add and use software containers

DID YOU KNOW...

Use code/scripts

Workflows based on point-and-click interfaces (e.g. Excel), are not reproducible. Enshrine computations and data manipulation in code.

- First: YES! Very much so!

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- But if your workflow includes interactive code sessions, and you want to at least save the results, you could do

```
datalad run ipython/R/matlab/...
```

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- First: YES! Very much so!
- But if your workflow includes interactive code sessions, and you want to at least save the results, you could do

```
datalad run ipython/R/matlab/...
```

- Once you close the interactive session, every result you created would be saved (although with crappy provenance)

DID YOU KNOW...

Document

Use comments, computational notebooks and README files to explain how your code works, and to define the expected parameters and the computational environment required.

Record

Make a note of key parameters, e.g. 'seed' values used to start a random-number generator.

- Commit messages and run records can do this for you, and are a useful basis to extend upon with "documentation for humans" such as READMEs
- The YODA procedure automatically populated your repository with README files to nudge you into using them.

DID YOU KNOW...

Test

Create a suite of test functions. Use positive and negative control data sets to ensure you get the expected results, and run those tests throughout development to squash bugs as they arise.

- First: YES! Very much so! And there is an excellent [Turing Way](#) chapter about it

DID YOU KNOW...

Test

Create a suite of test functions. Use positive and negative control data sets to ensure you get the expected results, and run those tests throughout development to squash bugs as they arise.

- First: YES! Very much so! And there is an excellent [Turing Way chapter about it](#)
- Because annexed files are stored by their content identity hash, if any change in your pipeline/workflow produces a changed results, the version control software will be able to tell you

DID YOU KNOW...

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- First: YES! Very much so!
- A well-made run record can do this, or at least help
- Makefiles (shown later in this section) are also great

DID YOU KNOW...

Archive

Archiving services such as Zenodo, Figshare and Software Heritage promise long-term stability.

You can archive a dataset to figshare?
If you have a Figshare account, you can do the following:

```
$ datalad export-to-figshare
[INFO    ] Exporting current tree as an archive under /tmp/comics since figshare does not support directories
[INFO    ] Uploading /tmp/comics/datalad_ce82ff1f-e2b3-4a84-9e56-87d8eb6e5b27.zip to figshare
Article
Would you like to create a new article to upload to? If not - we will list existing articles (choices: yes, no)
New article
Please enter the title (must be at least 3 characters long). [comics#ce82ff1f-e2b3-4a84-9e56-87d8eb6e5b27]

[INFO    ] Created a new (private) article 13247186 at https://figshare.com/account/articles/13247186. Please
[INFO    ] 'Registering' /tmp/comics/datalad_ce82ff1f-e2b3-4a84-9e56-87d8eb6e5b27.zip within annex
[INFO    ] Adding URL https://ndownloader.figshare.com/files/25509824 for it
[INFO    ] Registering links back for the content of the archive
[INFO    ] Adding content of the archive /tmp/comics/datalad_ce82ff1f-e2b3-4a84-9e56-87d8eb6e5b27.zip into .
[INFO    ] Initiating special remote datalad-archives
[INFO    ] Finished adding /tmp/comics/datalad_ce82ff1f-e2b3-4a84-9e56-87d8eb6e5b27.zip: Files processed: 4
[INFO    ] Removing generated and now registered in annex archive
export_to_figshare(ok): Dataset(/tmp/comics) [Published archive https://ndownloader.figshare.com/files/25509824]
```

DID YOU KNOW ...

This screenshot shows the figshare account home page at <https://figshare.com/account/home>. The page features a cookie consent banner at the top, followed by the figshare logo, navigation links (Browse, Search, Upload, My data), and user profile information. Below this is a main content area with tabs for My data, Projects, Collections, and Activity. A 'Create a new item' button is visible. The 'Projects' tab is selected, displaying a list of items. One item, 'acomictest', is shown in detail, with its status as 'DATASET', creation date as '17.11.2020 16:01', and size as '27.59 kB'. There is also a 20 GB storage indicator.

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figshare

Browse

Search on figshare...

Upload My data

AW

My data Projects Collections Activity

+ Create a new item

27.59 kB 20 GB

search my data...

Actions STATUS TYPE CREATION ... SIZE

acomictest DATASET 17.11.2020 16:01 27.59 kB

DID YOU KNOW...

Package

Create ready-to-use computational environments using containerization tools (for example, Docker, Singularity), web services (Code Ocean, Gigantum, Binder) or virtual-environment managers (Conda).

- The `datalad - container` extension can help to share software environments in your dataset (more later in this section)

DATALAD DATASETS FOR DATA ANALYSIS

- A DataLad dataset can have *any* structure, and use as many or few features of a dataset as required.
- However, for **data analyses** it is beneficial to make use of DataLad features and structure datasets according to the **YODA principles**:

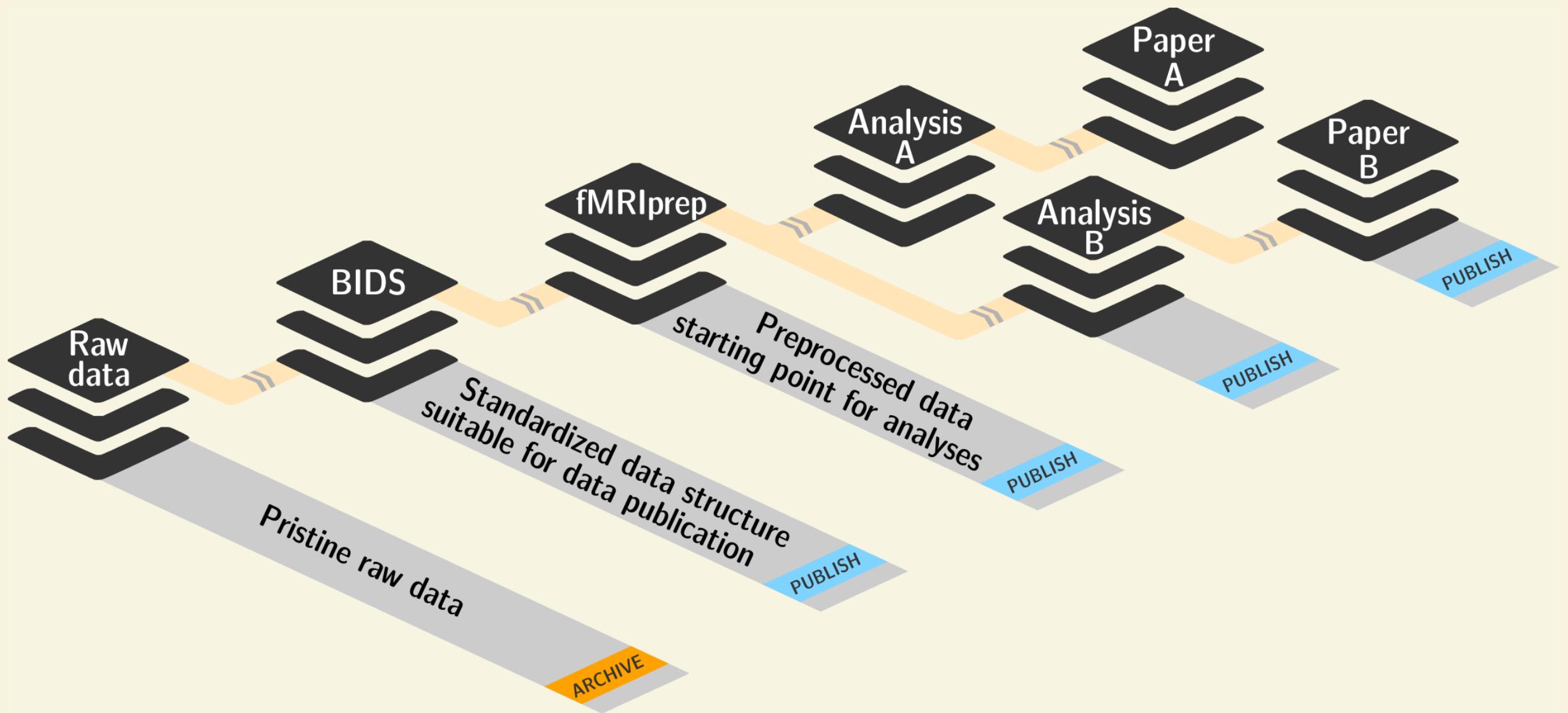


P1: One thing, one dataset

P2: Record where you got it from, and where it is now

P3: Record what you did to it, and with what

P1: ONE THING, ONE DATASET



- Bundle all components of one analysis into one superdataset.
- Whenever a particular collection of files could anyhow be useful in more than one context (e.g. data), put them in their own dataset, and install it as a subdataset.
- Keep everything clean and modular: Within an analysis, separate code, data, output, execution environments.

MODULARITY

Need for meaningful units of data that are clearly recognizable for anyone.

WHY?

Original

```
/dataset
  └── sample1
      └── a001.dat
  └── sample2
      └── a001.dat
...
...
```

WHY?

Original

```
/dataset
├── sample1
│   └── a001.dat
├── sample2
│   └── a001.dat
...
...
```

After applied transform (preprocessing, analysis, ...)

```
/dataset
├── sample1
│   └── ps34t.dat
│       └── a001.dat
├── sample2
│   └── ps34t.dat
│       └── a001.dat
...
...
```

Without expert/domain knowledge no distinction between original and derived data possible anymore.

PRESERVED MODULARITY

Original

```
/raw_dataset
  └── sample1
      └── a001.dat
  └── sample2
      └── a001.dat
...
...
```

PRESERVED MODULARITY

Original

```
/raw_dataset
├── sample1
│   └── a001.dat
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│   └── a001.dat
...
...
```

After applied transform (preprocessing, analysis, ...)

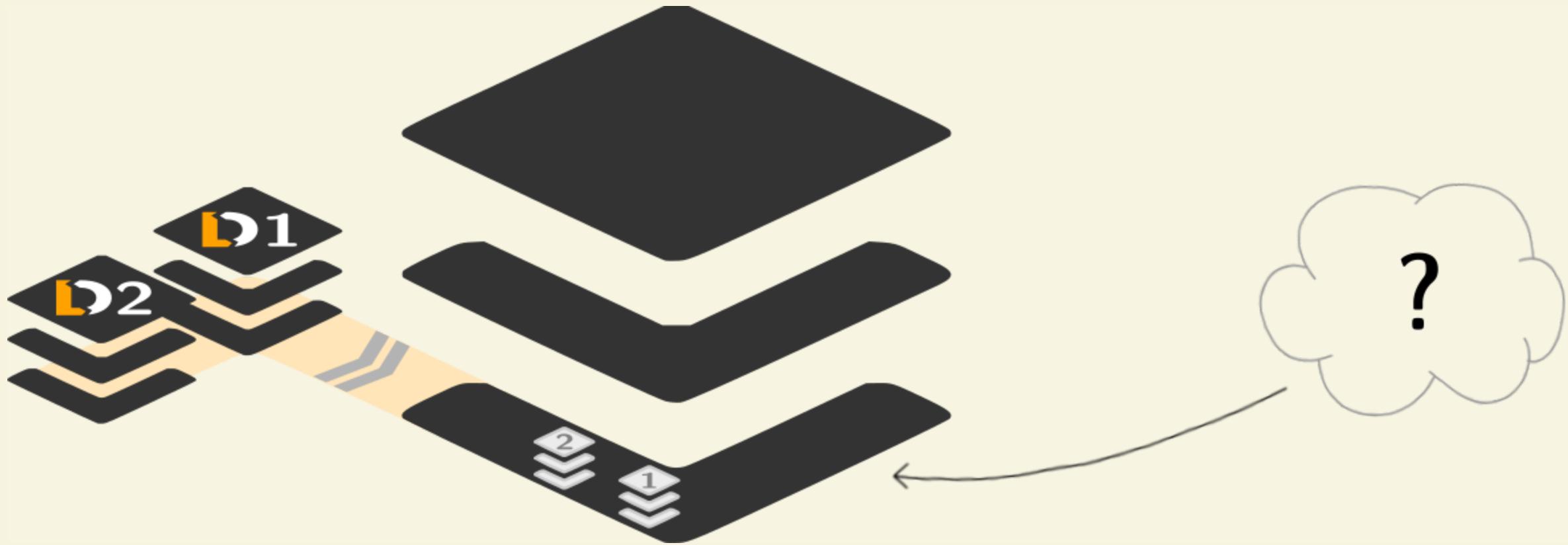
```
/derived_dataset
├── sample1
│   └── ps34t.dat
├── sample2
│   └── ps34t.dat
...
└── inputs
    └── raw
        ├── sample1
        │   └── a001.dat
        ├── sample2
        │   └── a001.dat
...
...
```

Clearer separation of semantics, through use of pristine version of original dataset within a *new, additional* dataset holding the outputs.

WHEN TO MODULARIZE?

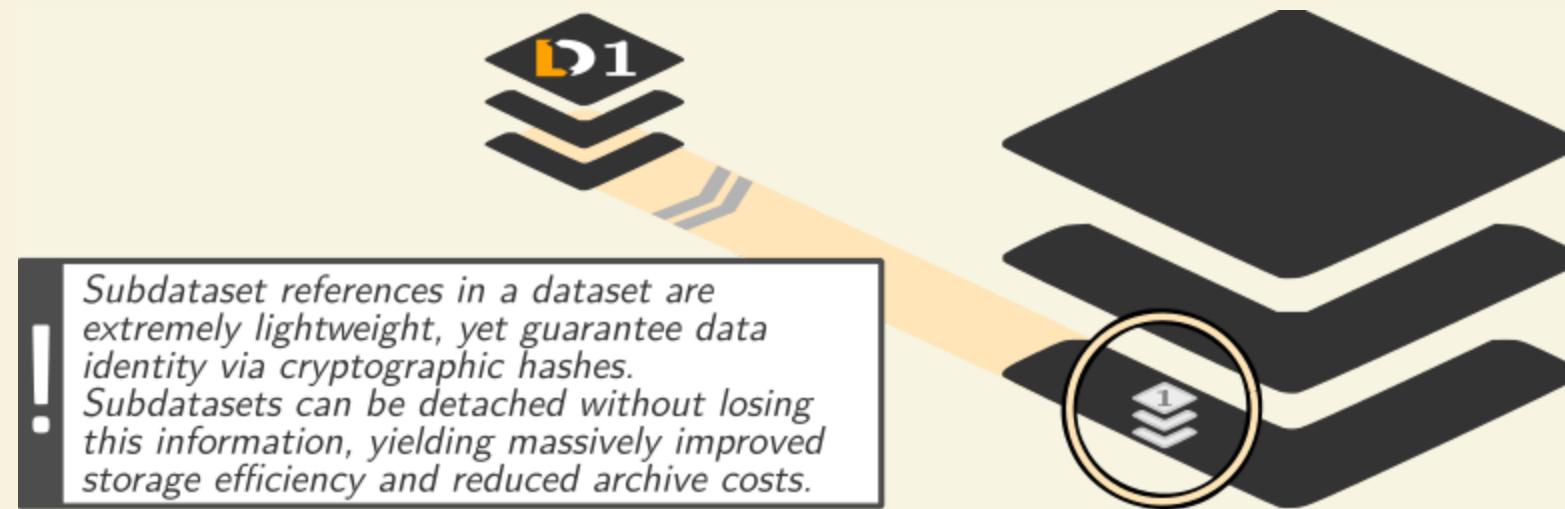
- Target audience is different
 - public vs. private
 - domain specific vs. domain general
- Pace of evolution is different
 - "factual" raw data vs. choices of (pre-)processing
 - completed acquisition vs. ongoing study
- Size impacts I/O and logistics
 - Git can struggle with 1M+ files
 - filesystems (licensing) can struggle with large numbers of inodes
 - More infos: Go Big or Go Home chapter
- Legal/Access constraints
 - personal vs. anonymized data

P2: RECORD WHERE YOU GOT IT FROM, AND WHERE IT IS NOW



- Link individual datasets to declare data-dependencies (e.g. as subdatasets).
- Record data's origin with appropriate commands, for example to record access URLs for individual files obtained from (unstructured) sources "in the cloud".
- Keep a dataset self-contained with relative paths in scripts to subdatasets or files.
- Share and publish datasets to collaborate.

DATALAD: DATASET LINKAGE

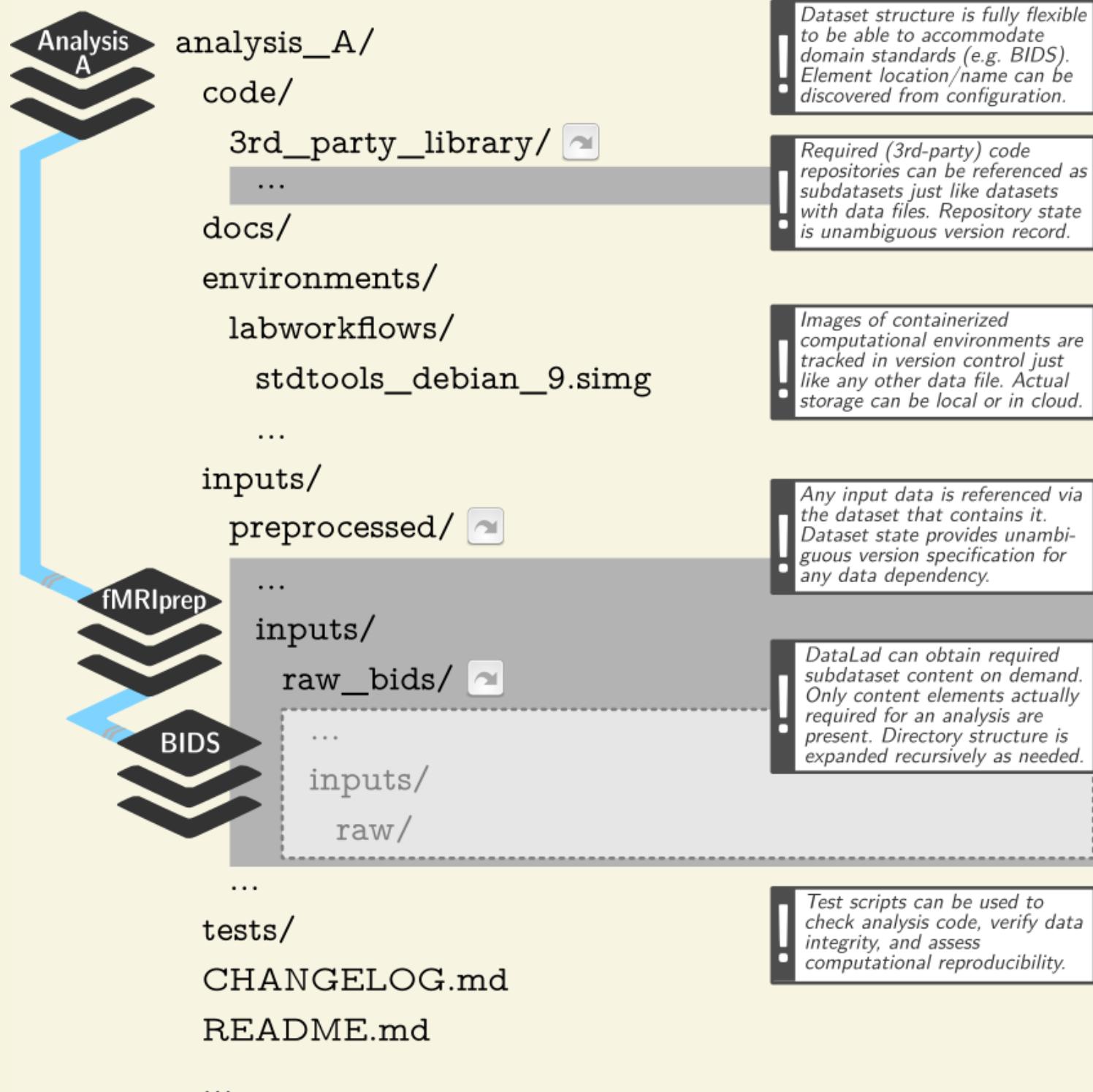


```
$ datalad clone --dataset . http://example.com/ds inputs/rawdata
```

```
$ 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
```

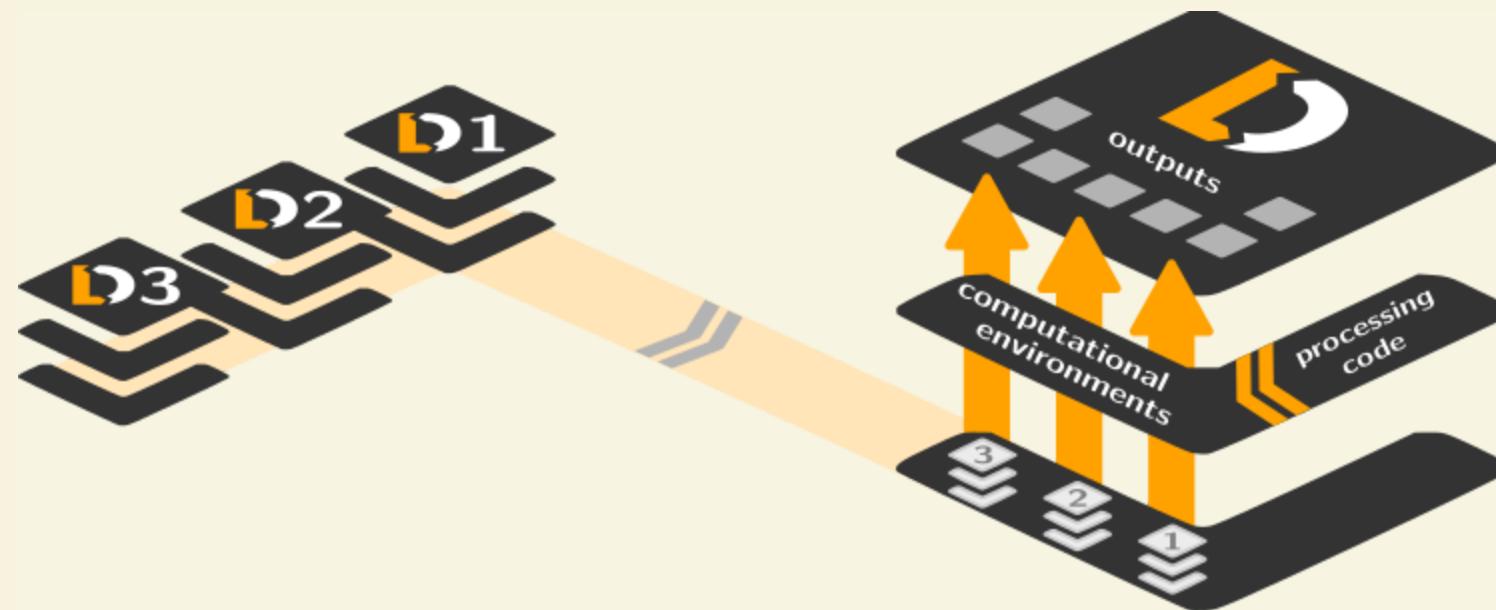
Each (sub)dataset is a separately, but jointly version-controlled entity.

EXAMPLE MODULAR DATA STRUCTURE



Link precisely versioned inputs to version-controlled outputs

P3: RECORD WHAT YOU DID TO IT, AND WITH WHAT



- Collect and store provenance of all contents of a dataset that you create.

A PDF IS NOT ENOUGH

... neither for others, nor for your future self.

What do we need apart from a PDF?

- code
- data
- software

GOING BEYOND A PDF: A REPRODUCIBLE PAPER

Let's take a look into a reproducible paper: github.com/psychoinformatics-de/paper-remodnav/

- This is not the only way to create a reproducible paper
- This is certainly not the easiest way to do it
- But it is *one* way of connecting established tools into a functional solution
- You could redo this with the tools that you are familiar with
- A hands-on explanation and a demo of an alternative approach will follow

Disclaimer

A REPRODUCIBLE PAPER SKETCH

- We have created a template to recreate this analysis at github.com/datalad-handbook/repro-paper-sketch
- Team up in break-out rooms, and follow the instructions in the README to make a paper, adjust the code, and re-make an updated paper (Hands-on 1 on the website).

AN ALTERNATIVE WITH RMARKDOWN

demo by Lennart (at the end of the workshop)

SUMMARY: REPRODUCIBLE PAPERS

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- There are many tools that allow you to create a reproducible paper

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- The setup has a number of advantages

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- There are many tools that allow you to create a reproducible paper
- The setup has a number of advantages
 - Save time
 - Have a framework for collaboration
 - Gain confidence in the validity of your results
 - Make a more convincing case with your research
 - Make your research accessible and adaptable for everyone

SHARING SOFTWARE ENVIRONMENTS

WHY SHARE SOFTWARE?

- difficult or impossible to install (e.g. conflicts with existing software, or on HPC)
- different software versions/operating systems can produce different results

The screenshot shows a research article page from the journal "Frontiers in Neuroinformatics". The top navigation bar includes links for LOGIN, REGISTER, and ABOUT. The main title of the article is "Reproducibility of". Below the title, there are sections for TABLE OF CONTENTS, ORIGINAL RESEARCH ARTICLE, and Download Article / Export citation. A sidebar on the left provides links to Materials and Methods, and a note about cookie usage. The page has a light blue background with white text and some dark blue highlights.

LOGIN (HTTPS://WWW.FRONTIERSIN.ORG/PEOPLE/LOGIN) / REGISTER (HTTPS://WWW.FRONTIERSIN.ORG/REGISTER) ABOUT(HTTPS://WWW.FRONTIERSIN.ORG/ABOUT/ABOUT-FRONTIERS) JC
(https://www.frontiersin.org)
(https://www.frontiersin.org/about/impact?utm_source=fweb&utm_medium=fjour&utm_campaign=impact-2020-jour-hp-top) Impact Factor 2.649 | CiteScore 4.8
More on impact >

in Neuroinformatics (<https://www.frontiersin.org>)

< Articles (<https://www.frontiersin.org/journals/12#articles>)

TABLE OF CONTENTS ORIGINAL RESEARCH ARTICLE

Abstract Front. Neuroinform., 24 April 2015 | <https://doi.org/10.3389/fninf.2015.00012>
(<https://doi.org/10.3389/fninf.2015.00012>)

1. Introduction

We use cookies on this website to improve your user experience. Learn more (<https://www.frontiersin.org/legal/list-of-cookies>)

2. Materials and Methods

Reproducibility of

Download Article Export citation

CLOSE 15,593

SOFTWARE CONTAINERS

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- Software containers encapsulate a software environment and isolate it from a surrounding operating system. Common solutions: Docker, Singularity

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- How familiar are you with software containers?

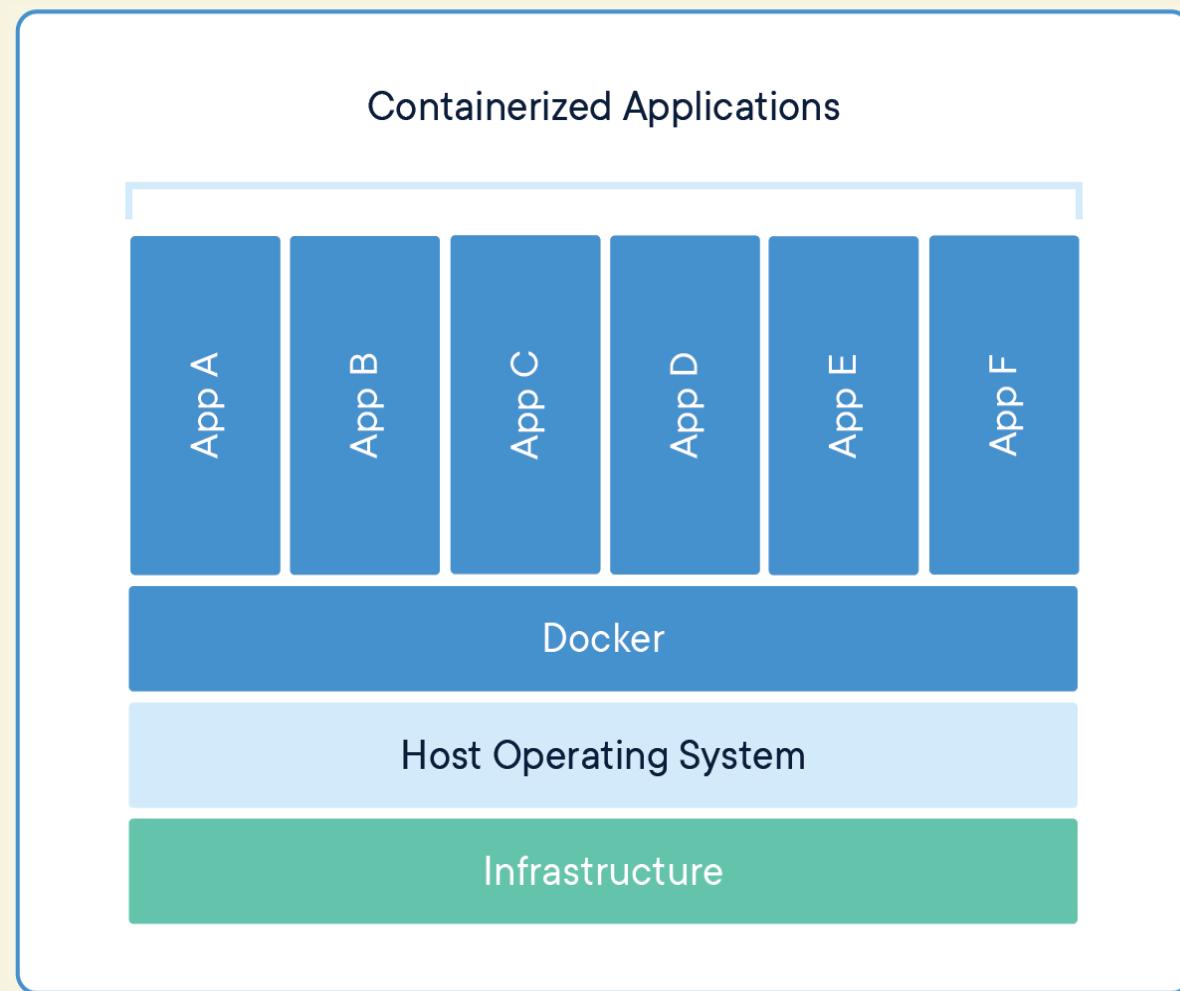
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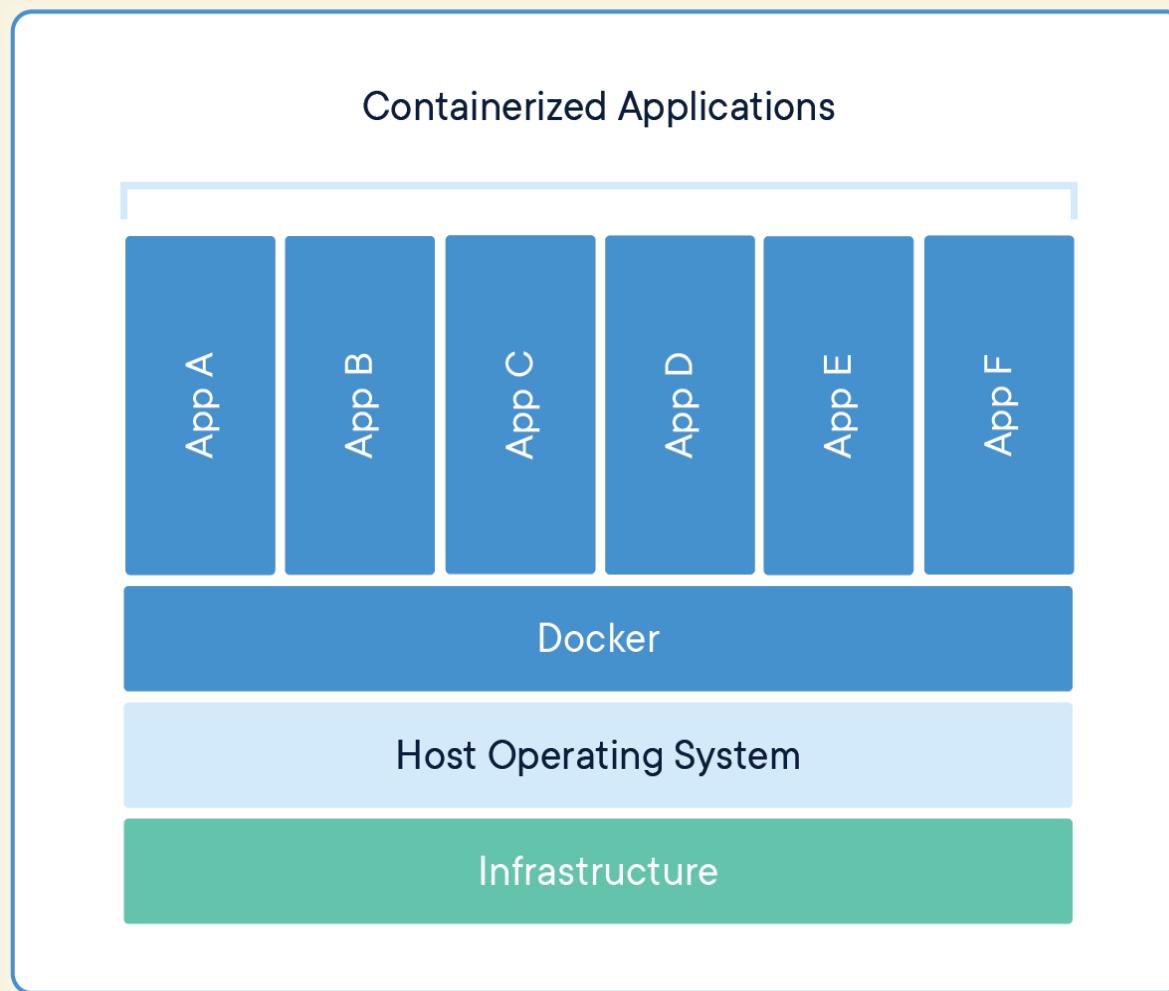
<http://etc.ch/5xo7>



SOFTWARE CONTAINERS

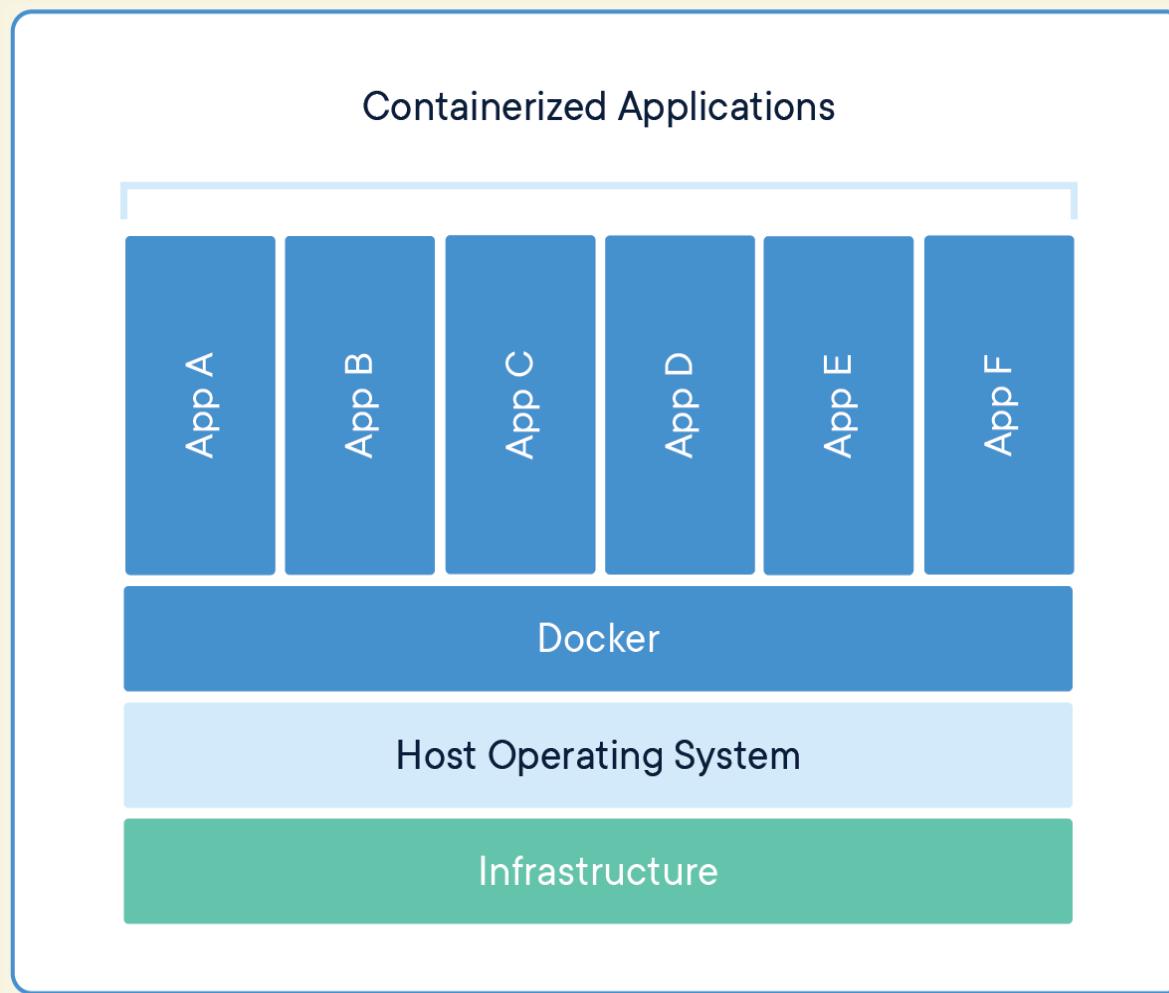


SOFTWARE CONTAINERS



- Put simple, a cut-down virtual machine that is a portable and shareable bundle of software libraries and their dependencies

SOFTWARE CONTAINERS



- Put simple, a cut-down virtual machine that is a portable and shareable bundle of software libraries and their dependencies
- Includes: Code, runtime, system tools, system libraries, settings
Does not include: Resource management

GLOSSARY

recipe

A text file template that lists all required components of the computational environment, e.g. a *Dockerfile* or *.def* file.

image

A static file system inside a file, populated with software specified in the recipe.
"Describes everything we run"

container

A running instance of an Image

Hub

A storage resource to share and consume images, e.g. Docker-Hub or Singularity-Hub

DOCKER VERSUS SINGULARITY

- Main disadvantage of Docker: requires "sudo" (i.e., admin) privileges
- "Scientific alternative": Singularity
 - built to run on computational clusters
 - same user inside image than outside (no root)
 - easier to access GPUs and run graphical applications
- Singularity can use and build Docker Images
- DataLad can register Docker and Singularity Images to a dataset

THE DATALAD-CONTAINER EXTENSION

- DataLad extensions are Python packages that equip DataLad with additional functionality
- Examples: `datalad - osf` for publishing and cloning dataset to and from the Open Science Framework, `datalad - hirni` for transforming neuroimaging datasets to BIDS, ... Full overview at [the DataLad handbook](#)
- `datalad - container` gives DataLad commands to add, track, retrieve, and execute Docker or Singularity containers.

```
pip install datalad-container
```

ADDING SOFTWARE TO DATASETS

- DataLad can register software containers as "just another file" to your dataset
- This allows you to include software in your analyses!
- Containers can be added from a local path or a URL. **Advice:** Put your image on a Hub, and register it from a public URL

ADDING A SINGULARITY IMAGE FROM A PATH

- You can get Singularity images by "pulling" them from Singularity or Dockerhub:

```
$ singularity pull docker://nipy/heudiconv:0.5.4
```

```
$ singularity pull shub://adswa/python-ml:1
INFO:    Downloading shub image
265.56 MiB / 265.56 MiB [=====] 100.00% 10.23 MiB/s 25
```

- You can also take/write a recipe file and build a container on your computer:

```
$ sudo singularity build myimage Singularity.2
INFO:    Starting build...
Getting image source signatures
Copying blob 831751213a61 done
[...]
INFO:    Creating SIF file...
INFO:    Build complete: myimage
```

- pulled or build images lie around as `.sif` or `.simg` files:

```
$ ls
heudiconv_0.5.4.sif
python-ml_1.sif
```

ADDING A SINGULARITY IMAGE FROM A PATH

- Adding a container from a local path (inside of a dataset):

```
$ datalad containers-add software --url /home/me/singularity/myimage
[INFO    ] Copying local file myimage to /home/adina/repos/resources/.datalad/environments/software/image
add(ok): .datalad/environments/software/image (file)
add(ok): .datalad/config (file)
save(ok): . (dataset)
containers_add(ok): /home/adina/repos/resources/.datalad/environments/software/image (file)
action summary:
  add (ok: 2)
  containers_add (ok: 1)
  save (ok: 1)
```

```
$ datalad containers-list
software -> .datalad/environments/software/image
```

- Note: Singularity Images are a single file

ADDING A SINGULARITY IMAGE FROM A URL

- Tip: If you add Images from public URLs (e.g., Dockerhub or Singularity Hub), others can retrieve your Image easily

```
$ datalad containers-add software --url shub://adswa/python-ml:1
add(ok): .datalad/config (file)
save(ok): . (dataset)
containers_add(ok): /tmp/bla/.datalad/environments/software/image (file)
action summary:
  add (ok: 1)
  containers_add (ok: 1)
  save (ok: 1)
```

ADDING A SINGULARITY IMAGE FROM A URL

- Tip: If you add Images from public URLs (e.g., Dockerhub or Singularity Hub), others can retrieve your Image easily

```
$ datalad containers-add software --url shub://adswa/python-ml:1
add(ok): .datalad/config (file)
save(ok): . (dataset)
containers_add(ok): /tmp/bla/.datalad/environments/software/image (file)
action summary:
  add (ok: 1)
  containers_add (ok: 1)
  save (ok: 1)
```

- My workflow: Create a repository/dataset. Use **Neurodocker** with **datalad run** to create a Singularity recipe and link the repository to Singularity hub. Singularity-hub takes care of building the Image, and I can add from its URL: **demo**

ADDING A DOCKER IMAGE FROM A PATH

- You can get Docker images by "pulling" them from Dockerhub:

```
$ docker pull repronim/neurodocker:latest
latest: Pulling from repronim/neurodocker
```

1 !

- You can also take/write a Dockerfile and build a container on your computer:

```
$ sudo docker build -t adwagner/somedockercontainer .
Sending build context to Docker daemon 6.656kB
Step 1/4 : FROM python:3.6
[...]
Successfully built 31d6acc37184
Successfully tagged adwagner/somedockercontainer:latest
```

- Show docker images:

REPOSITORY	TAG	IMAGE ID	CREATED
repronim/neurodocker	latest	84b9023f0019	7 months ago
adwagner/min_prepoc	latest	fca4a144b61f	8 months ago
[...]			

ADDING A DOCKER IMAGE FROM A URL

```
● $ datalad containers-add --url dhub://busybox:1.30 bb
[INFO] Saved busybox:1.30 to C:\Users\datalad\testing\blablabla\.datalad\environments\bb\image
add(ok): .datalad\environments\bb\image\64f5d945efcc0f39ab11b3cd4ba403cc9fefef1fa3613123ca016cf3708e8caf.json
add(ok): .datalad\environments\bb\image\ a57c26390d4b78fd575fac72ed31f16a7a2fa3ebdccae4598513e8964dace9b2\VERS.json
add(ok): .datalad\environments\bb\image\ a57c26390d4b78fd575fac72ed31f16a7a2fa3ebdccae4598513e8964dace9b2\json
add(ok): .datalad\environments\bb\image\ a57c26390d4b78fd575fac72ed31f16a7a2fa3ebdccae4598513e8964dace9b2\layer.json
add(ok): .datalad\environments\bb\image\manifest.json (file)
add(ok): .datalad\environments\bb\image\repositories (file)
add(ok): .datalad\config (file)
save(ok): . (dataset)
containers_add(ok): C:\Users\datalad\testing\blablabla\.datalad\environments\bb\image (file)
action summary:
 add (ok: 7)
 containers_add (ok: 1)
 save (ok: 1)
```

CONFIGURE CONTAINERS

- `datalad containers` - run executes any command inside of the specified container. How does it work?

```
$ cat .datalad/config
[datalad "containers.midterm-software"]
    updateurl = shub://adswa/resources:1
    image = .datalad/environments/midterm-software/image
    cmdexec = singularity exec {img} {cmd}
```

CONFIGURE CONTAINERS

- `datalad containers` - run executes any command inside of the specified container. How does it work?

```
$ cat .datalad/config
[datalad "containers.midterm-software"]
    updateurl = shub://adswa/resources:1
    image = .datalad/environments/midterm-software/image
    cmdexec = singularity exec {img} {cmd}
```

- You can configure the command execution however you like:

```
$ datalad containers-add fmriprep \
--url shub://ReproNim/containers:bids-fmriprep--20.1.1 \
--call-fmt 'singularity run --cleanenv -B $PWD,$PWD/.tools/license.txt {img} {cmd}'
```

workflow demonstration fMRIprep: OHBM 2020 Open Science Room presentation

SOFTWARE CONTAINERS

Helpful resources for working with software containers:

- **repo2docker** can fetch a Git repository/DataLad dataset and builds a container image from configuration files
- **neurodocker** can generate custom Dockerfiles and Singularity recipes for neuroimaging.
- The **ReproNim container collection**, a DataLad dataset that includes common neuroimaging software as configured singularity containers.
- **rocker** - Docker container for R users

SUMMARY

Where can DataLad help?

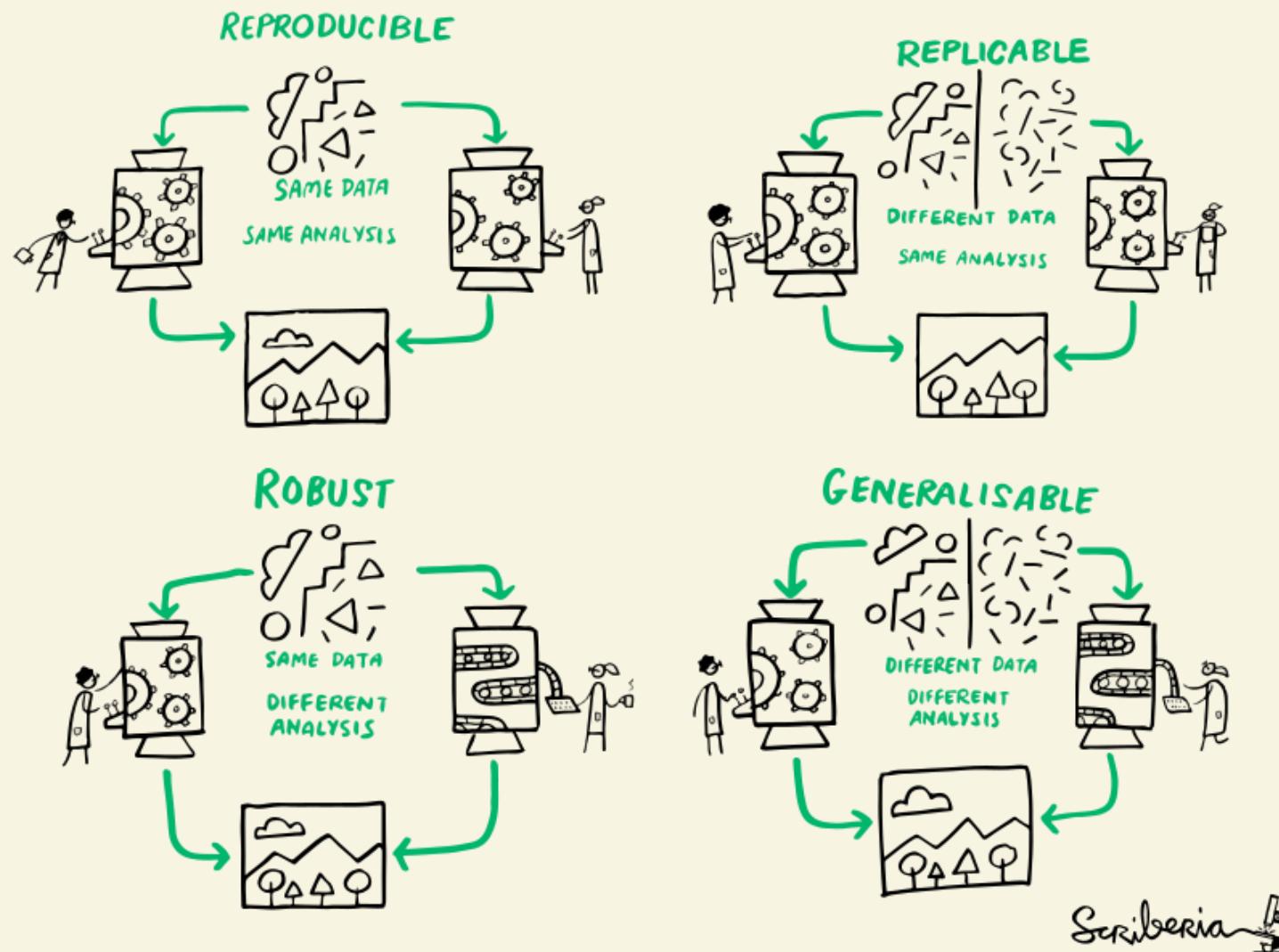


Image credit: Illustration by Scriberia and The Turing Way

Reproducible
automatic recompute
and identity checks

Replicable
Easily exchange
input data

Robust
Reuse data & change
code, update paper

Generalisable
Share analysis in an
easily reusable and
adaptable framework