



DECENTRALIZED MANAGEMENT OF DIGITAL OBJECTS FOR OPEN SCIENCE

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Research Center Jülich



Debian in Arts & Science

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

ACKNOWLEDGEMENTS

Software

- Michael Hanke
- Yaroslav Halchenko
- Joey Hess (git-annex)
- Kyle Meyer
- Benjamin Poldrack
- *26 additional contributors*

Documentation project

- Michael Hanke
- Laura Waite
- *28 additional contributors*



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Funders

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BMBF 01GQ1411



EUROPEAN UNION
European Regional Development Fund



Collaborators



Human Brain Project



VirtualBrainCloud



OpenNEURO



brainlife.io

PERKS OF BEING A (NEURO)SCIENTIST...

PERKS OF BEING A (NEURO)SCIENTIST...

A growing culture of open data

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The Free Encyclopedia 

List of neuroscience databases

From Wikipedia, the free encyclopedia

A number of online neuroscience databases are available which provide information regarding [gene expression](#), [neurons](#), [macroscopic](#) brain structure, and [neurological](#) or [psychiatric](#) disorders. Some databases contain descriptive and numerical data, some to brain function, others offer access to 'raw' imaging data, such as [postmortem](#) brain sections or 3D [MRI](#) and [fMRI](#) images. Some focus on the human brain, others on non-human.

As the number of databases that seek to disseminate information about the structure, development and function of the brain has grown, so has the need to collate these resources themselves. As a result, there now exist databases of neuroscience databases, some of which reach over 3000 entries.^[1]

Contents [hide]

- [1 Neuroscience databases](#)
- [2 Databases of neuroscience databases](#)
- [3 Neuroscience article aggregators](#)
- [4 See also](#)
- [5 References](#)

Neuroscience databases [edit]

Name	Description	Organism	Level (gene, neuron, macroscopic)	Data (MRI, fMRI, images, descriptive, numerical)	Disorder	Register to view data?	Ref.
Allen Brain Atlas	Atlas, stained sections from brains showing development and gene expression	Mouse, Human	Macroscopic, Gene	Images	Healthy	No	[2]
Alzheimer's Disease Neuroimaging Initiative (ADNI)	Structural MRI images	Human	Macroscopic	MRI datasets	Healthy and Alzheimer's Disease	Yes	[3]
Big Brain	3D reconstruction of complete brain from cell-body stained histology sections at 20 micron isotropic resolution	Human	Microscopic	Images	Healthy	No	[4]
BIRN fMRI and MRI data	fMRI, MRI scans and atlases for human and mouse brains	Mouse, Human	Multilevel: brain regions, connections, neurons, gene expression patterns	MRI datasets, fMRI datasets	Healthy, Elderly	No	
Bipolar Disorder Neuroimaging Database	Meta-analysis and database of MRI studies	Human	Macroscopic	Descriptive, numerical	Bipolar Disorder	No	[5]
Brain Architecture Management System	Online resource for information about neural circuitry	Rat, mouse, human	Multilevel: brain regions, connections, neurons, gene expression patterns	Descriptive, numerical	Healthy	No	
Brain Cloud	Gene expression in the human prefrontal cortex	Human	Gene expression patterns	Descriptive, numerical	Healthy	No	
Brain-Development.org	Structural MRI images and Atlases	Human	Macroscopic	MRI datasets	Fetuses, healthy and prematurely born neonates	Yes	[6]
Braingraph.org	Braingraphs computed from the Human Connectome Project data	Human	Macroscopic, up to 1015 nodes	directed and undirected graphs in anatomically annotated GraphML format	Healthy	No	[7]

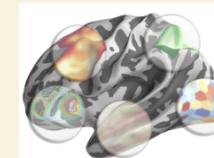
Image credit: https://en.wikipedia.org/wiki/List_of_neuroscience_databases

PERKS OF BEING A (NEURO)SCIENTIST...

A large and growing amount of open source software



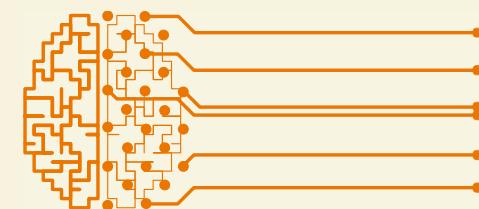
FreeSurfer



PySurfer



ni
learn



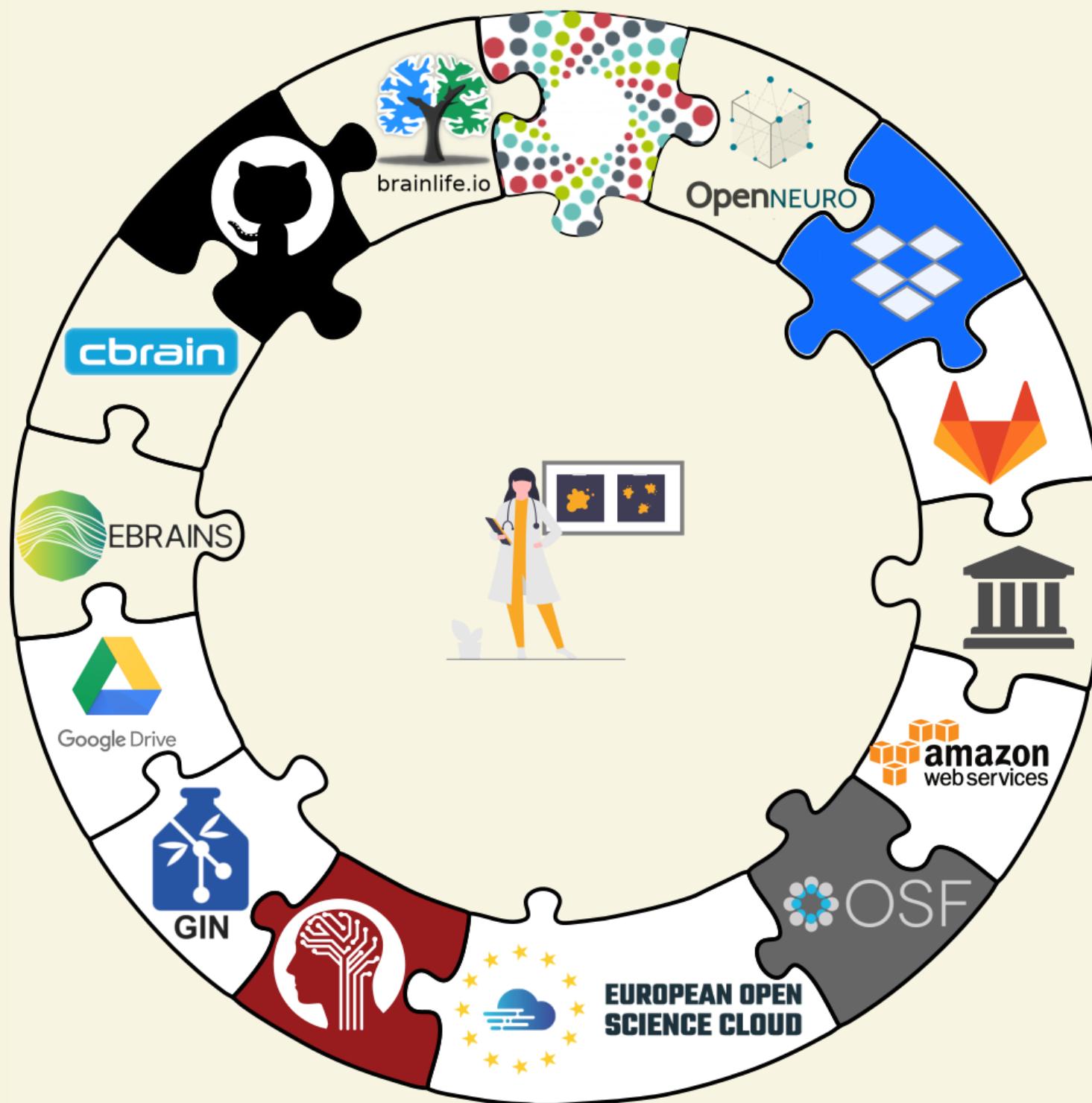
C-PAC



... and many more!

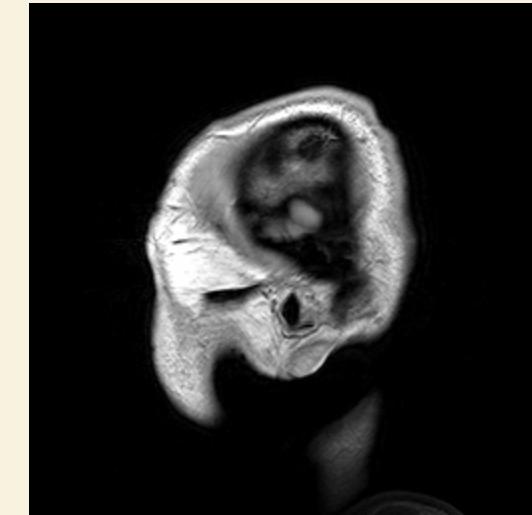
PERKS OF BEING A (NEURO)SCIENTIST...

Many readily available, often free, sometimes FOSS, services for data storage and collaboration



PERKS OF BEING A (NEURO)SCIENTIST...

Work on questions targeting understanding of and treatments for mental and neural illness



THE GOOD NEWS, THE BAD NEWS

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Data sharing

THE GOOD NEWS, THE BAD NEWS

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Heterogenous distribution and updating, scientists lack data management skills

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Reproducibility is threatened by intransparent, multi-stepped analyses & unstable results across software versions¹

¹ Kiar et al., 2020

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Collaboration

¹ Kiar et al., 2020

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Data sharing	Heterogenous distribution and updating, scientists lack data management skills
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Data analysis	Reproducibility is threatened by intransparent, multi-stepped analyses & unstable results across software versions ¹
Collaboration	Few interoperable workflows across institutes, rather: isolated solutions

¹ Kiar et al., 2020

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General underlying difficulties (distribution, updates, management, interoperability, reproducibility) also exist(ed) for software - what can we learn?

¹ Kiar et al., 2020

IMPROVE SCIENTIFIC WORKFLOWS, COMING FROM THE PERSPECTIVE OF SOFTWARE DISTRIBUTIONS

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"Share and treat data like sourcecode"

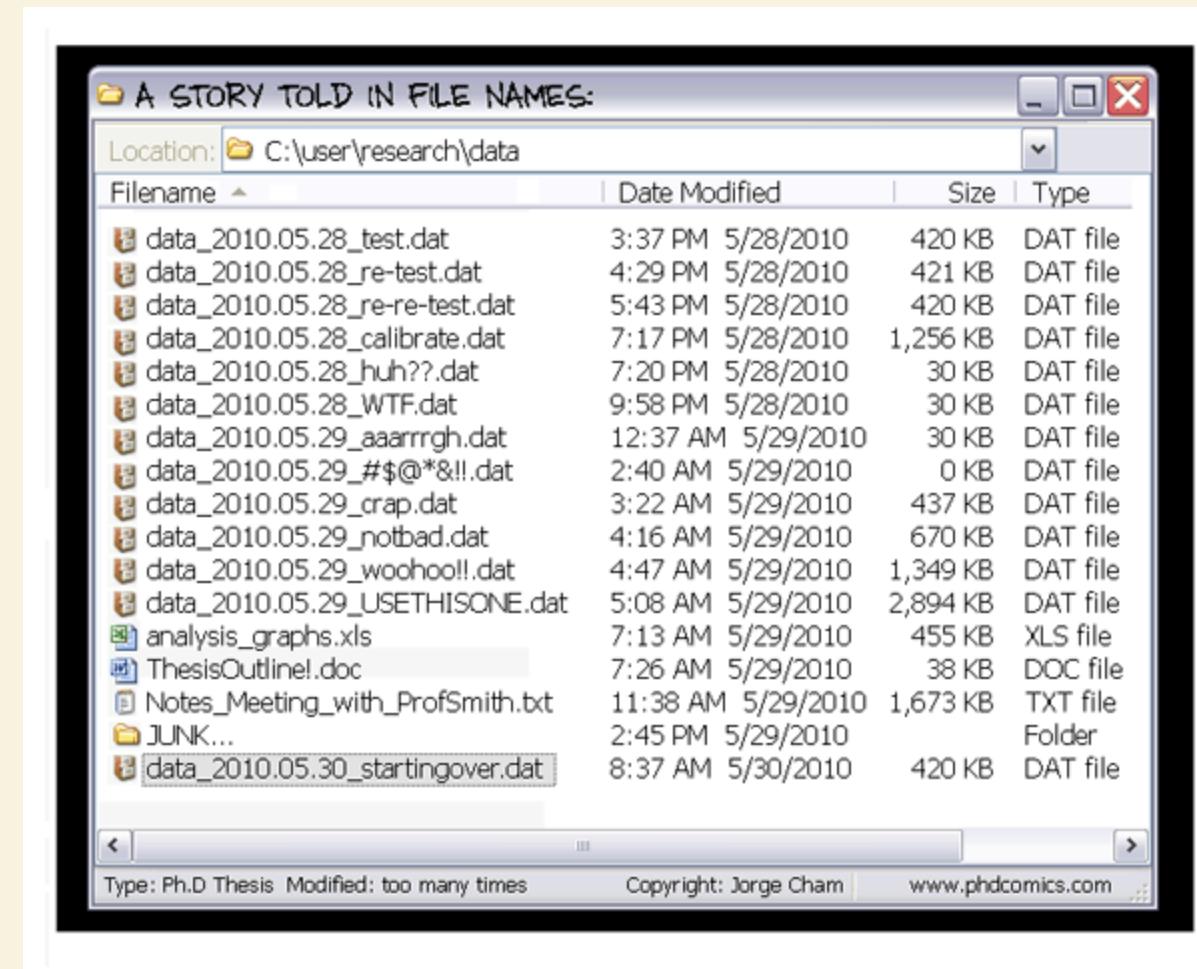
RETHINKING DATA

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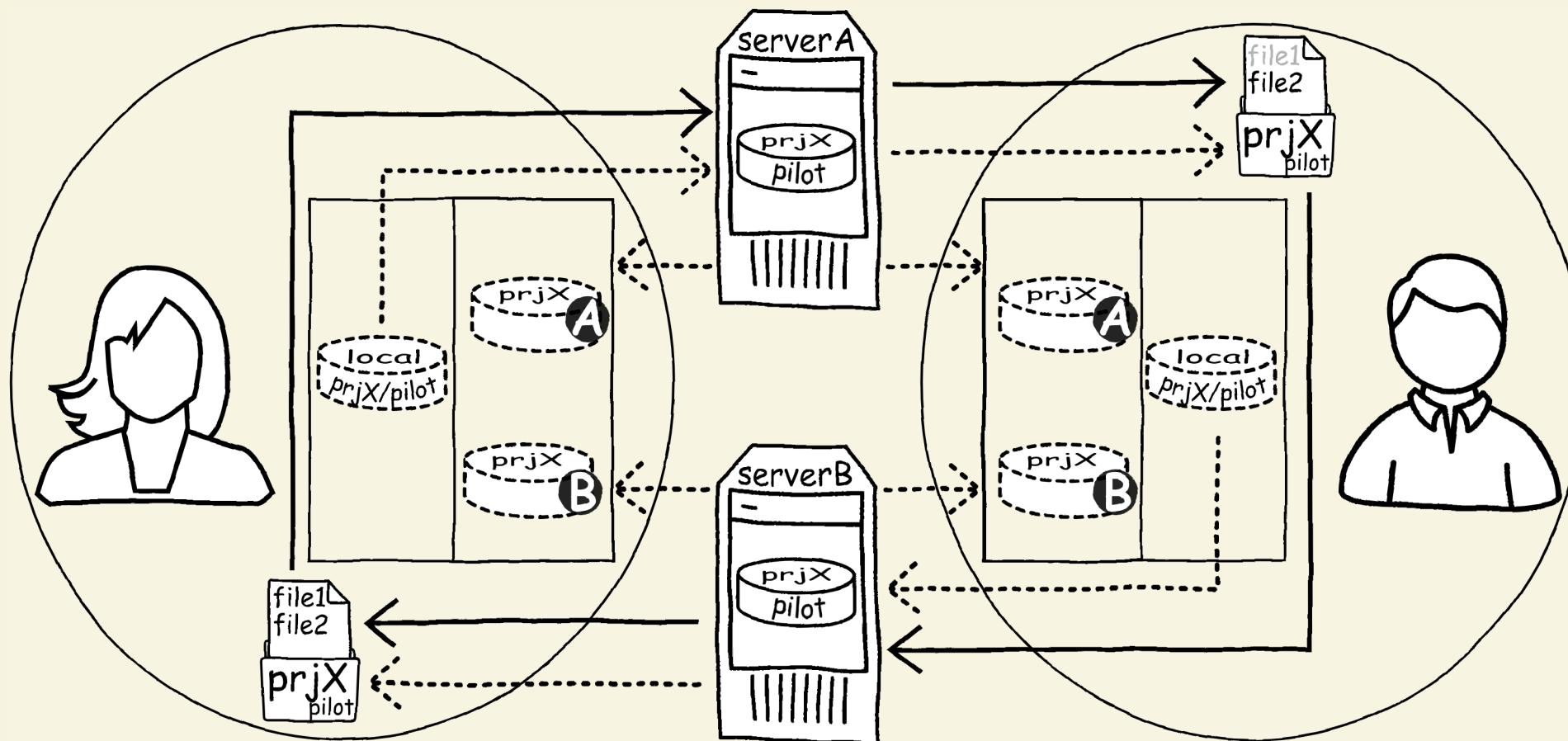


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- Just like code, data is subject to collaboration. It should be (publicly) sharable, and also update-able, with generic workflows similar to those in open-source software development

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DATALAD

- Joint management of digital objects through their entire life cycle
 - Version control
 - Transport logistics
 - Interoperability
 - Provenance capture
- Available in Debian
- Built on top of Git and `git-annex` (Joey Hess)
- Free and open source Python software (MIT licence)
- Python API and command line interface

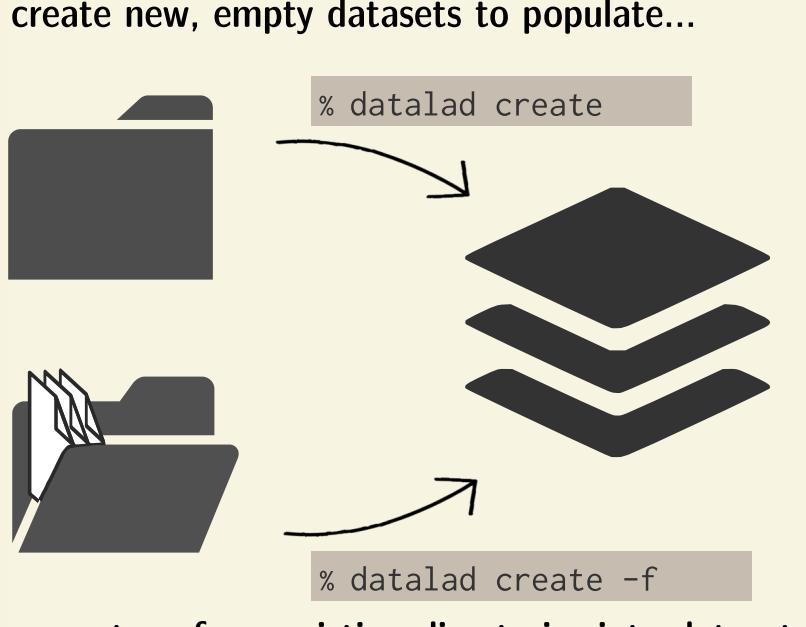
VERSION CONTROL

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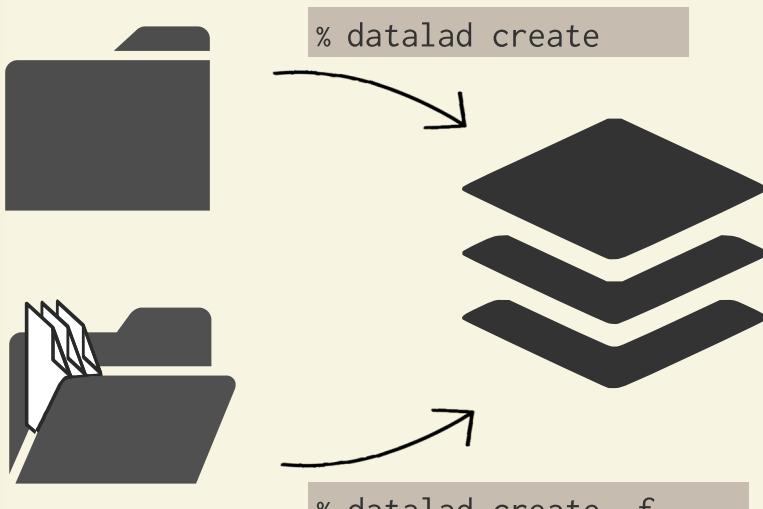


.... or transform existing directories into datasets

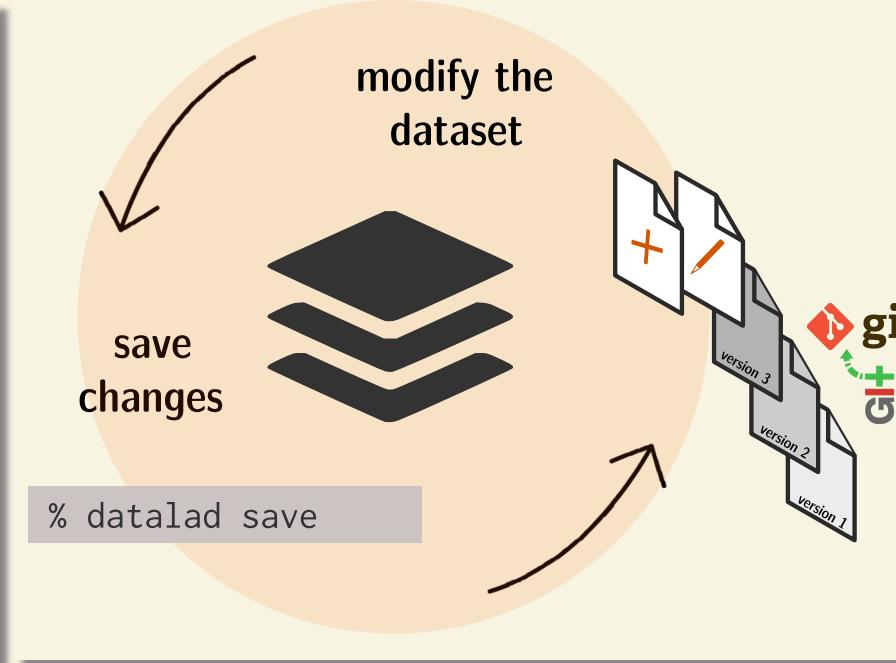
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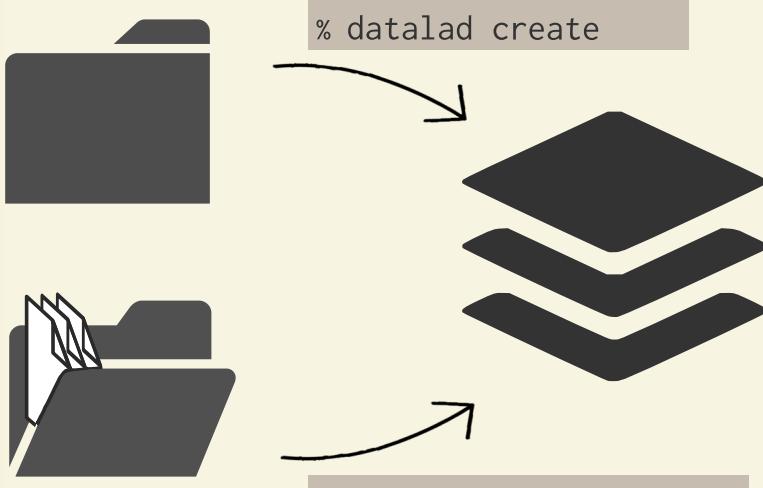
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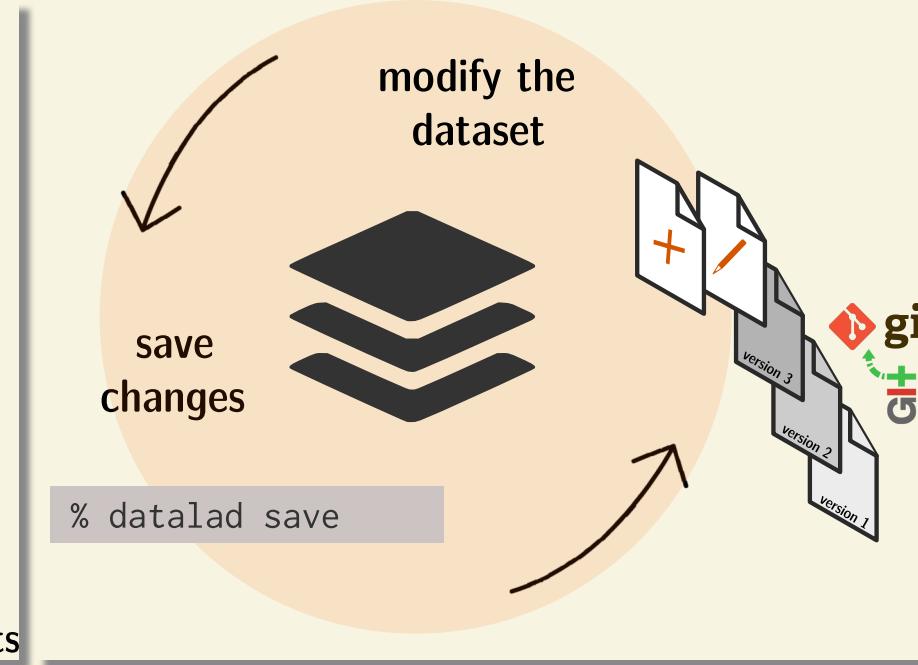
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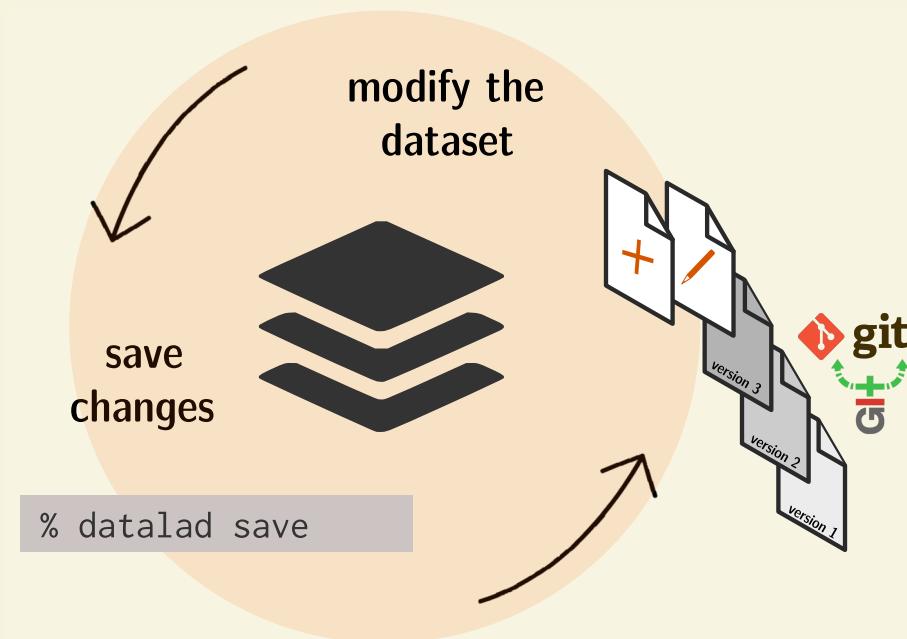
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- A DataLad dataset is an Git repository:
 - Content and domain agnostic
 - Minimization of custom procedures or data structures (**user must not lose data or data access of DataLad vanishes**)
 - **Uncompressed decentralization**

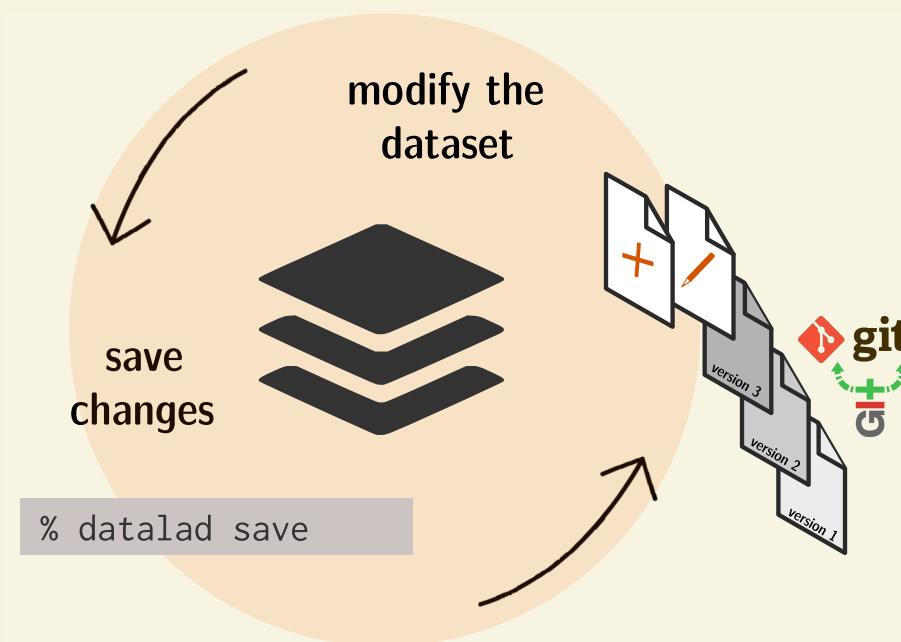
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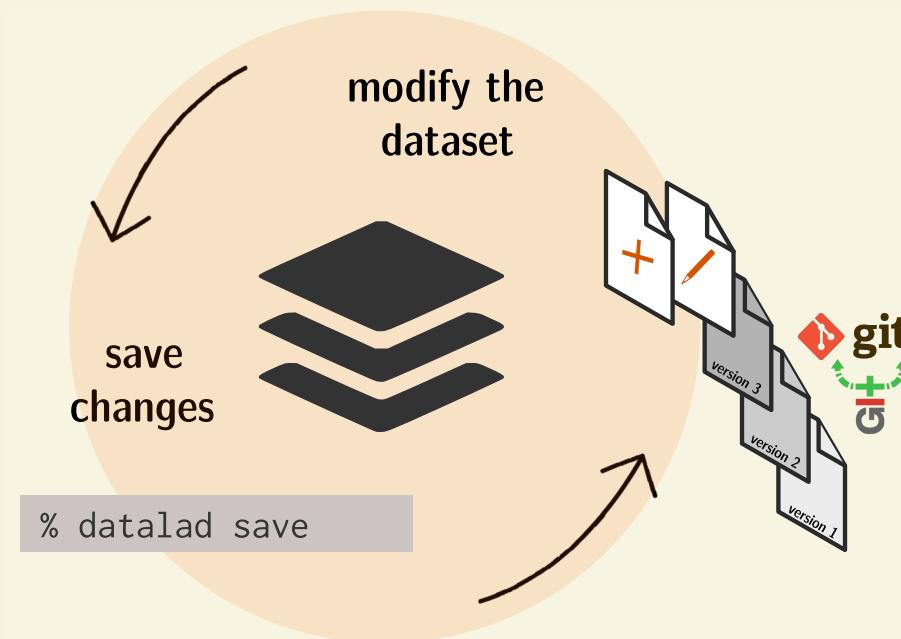
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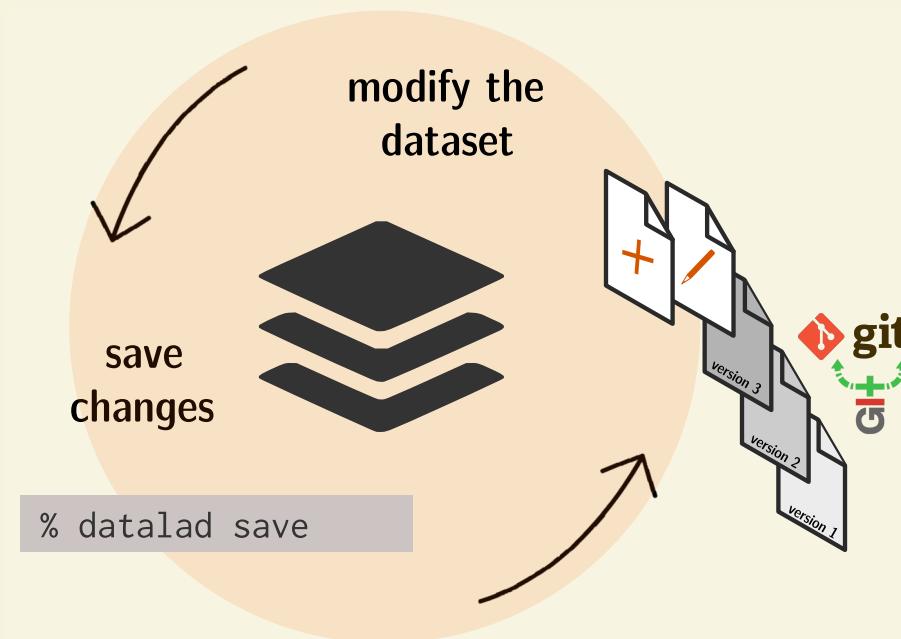
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- Datasets have an optional annex for (large) data.
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→ decentralized version control for files of any size.



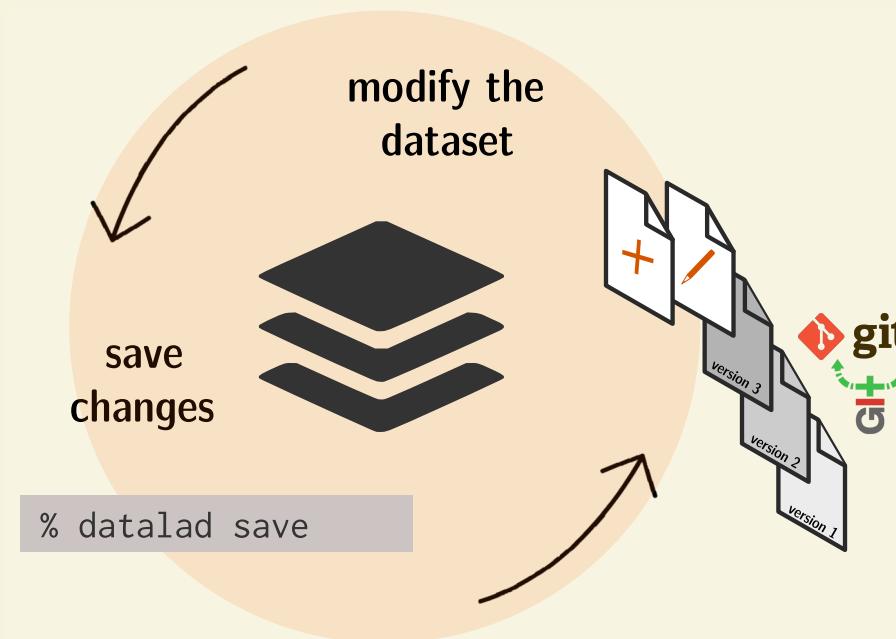
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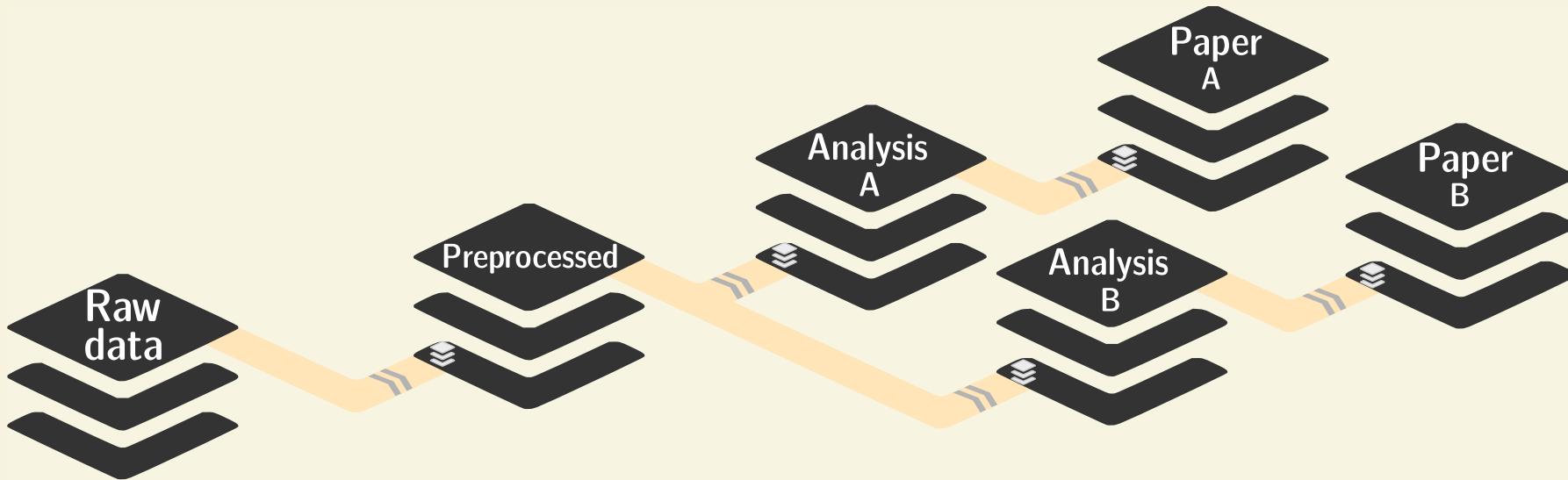
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- Flexibility and commands of Git and git-annex are preserved (useful for experienced Git/git-annex users)

VERSION CONTROL

- Seamless nesting mechanisms:

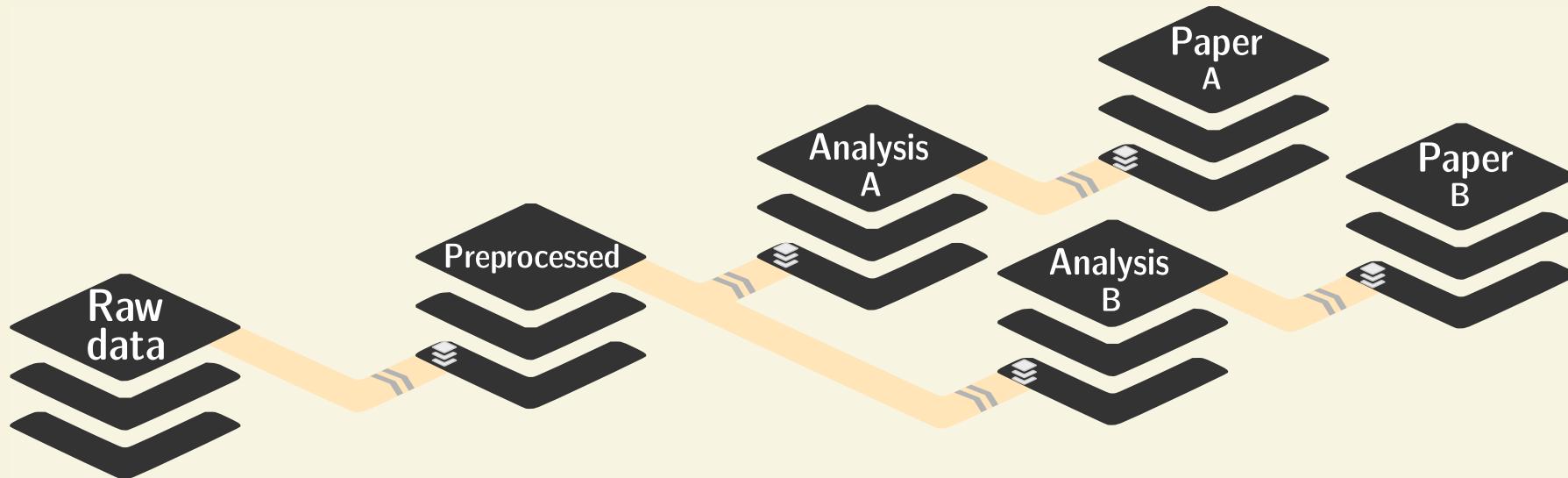


Nest modular datasets to create a linked hierarchy of datasets,
and enable recursive operations throughout the hierarchy

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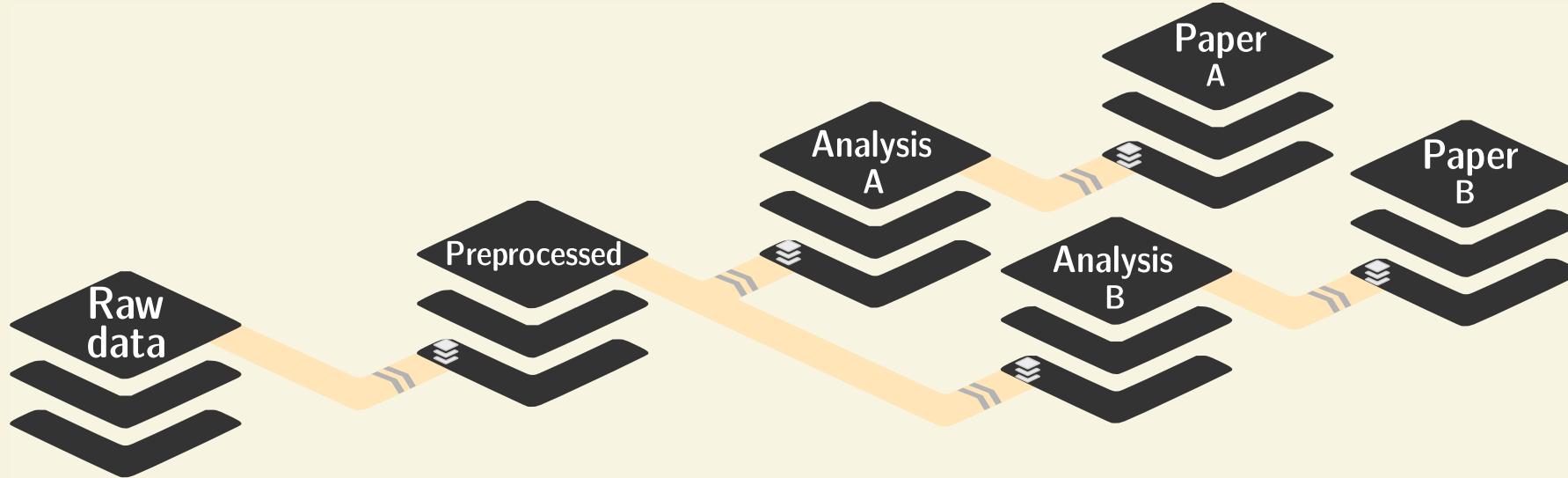
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- based on Git submodules, but seamless (recursive operations) and faster
- Overcomes scaling issues with large amounts of files

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

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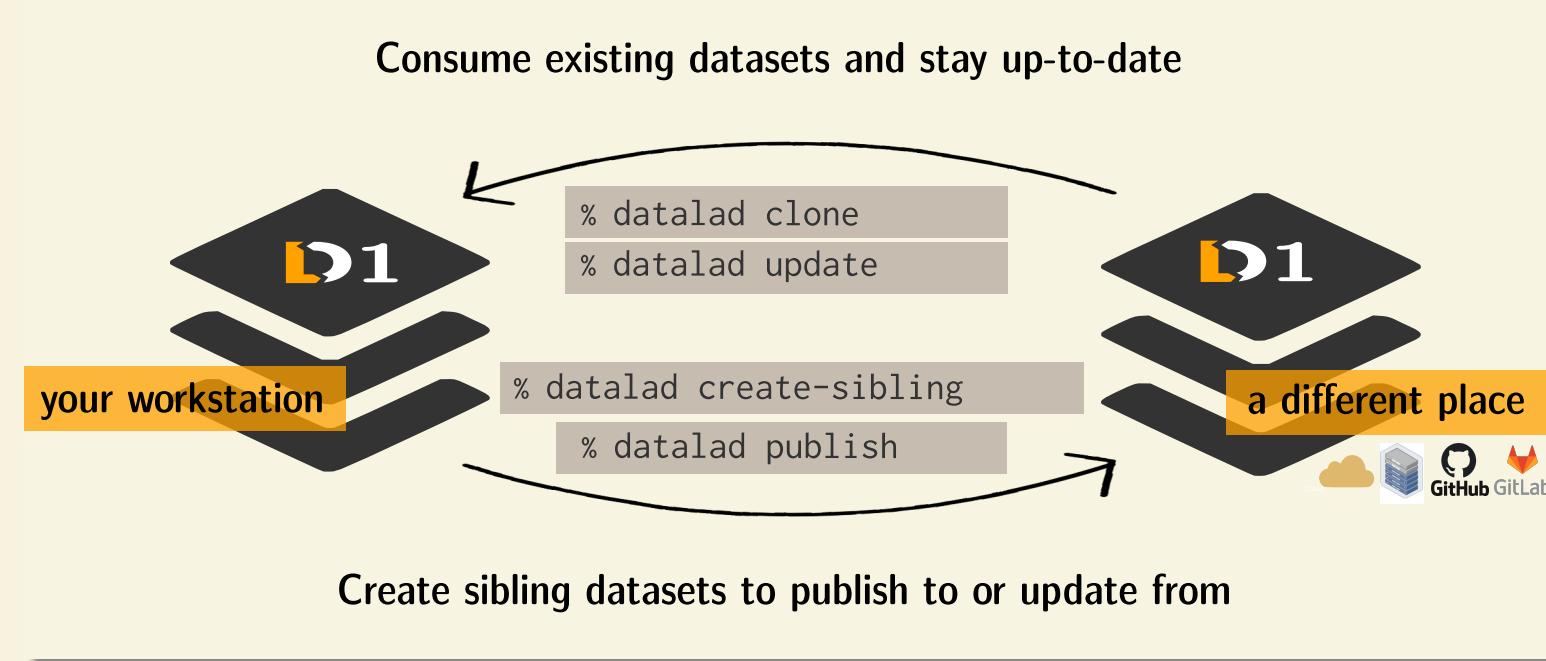
- Modularizes research components for transparency, reuse, and access management

TRANSPORT LOGISTICS

- Share data like source code

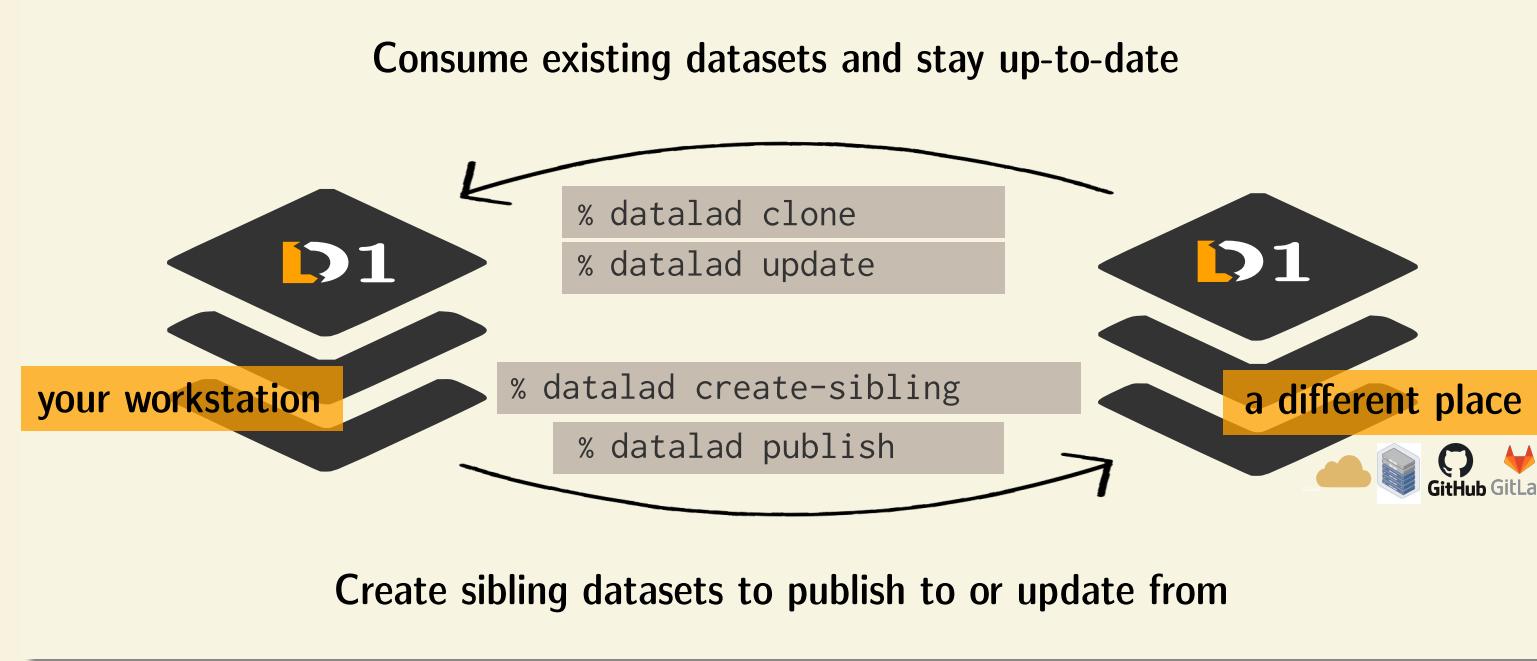
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- Flexible data access management for annexed file contents based on storage location

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```

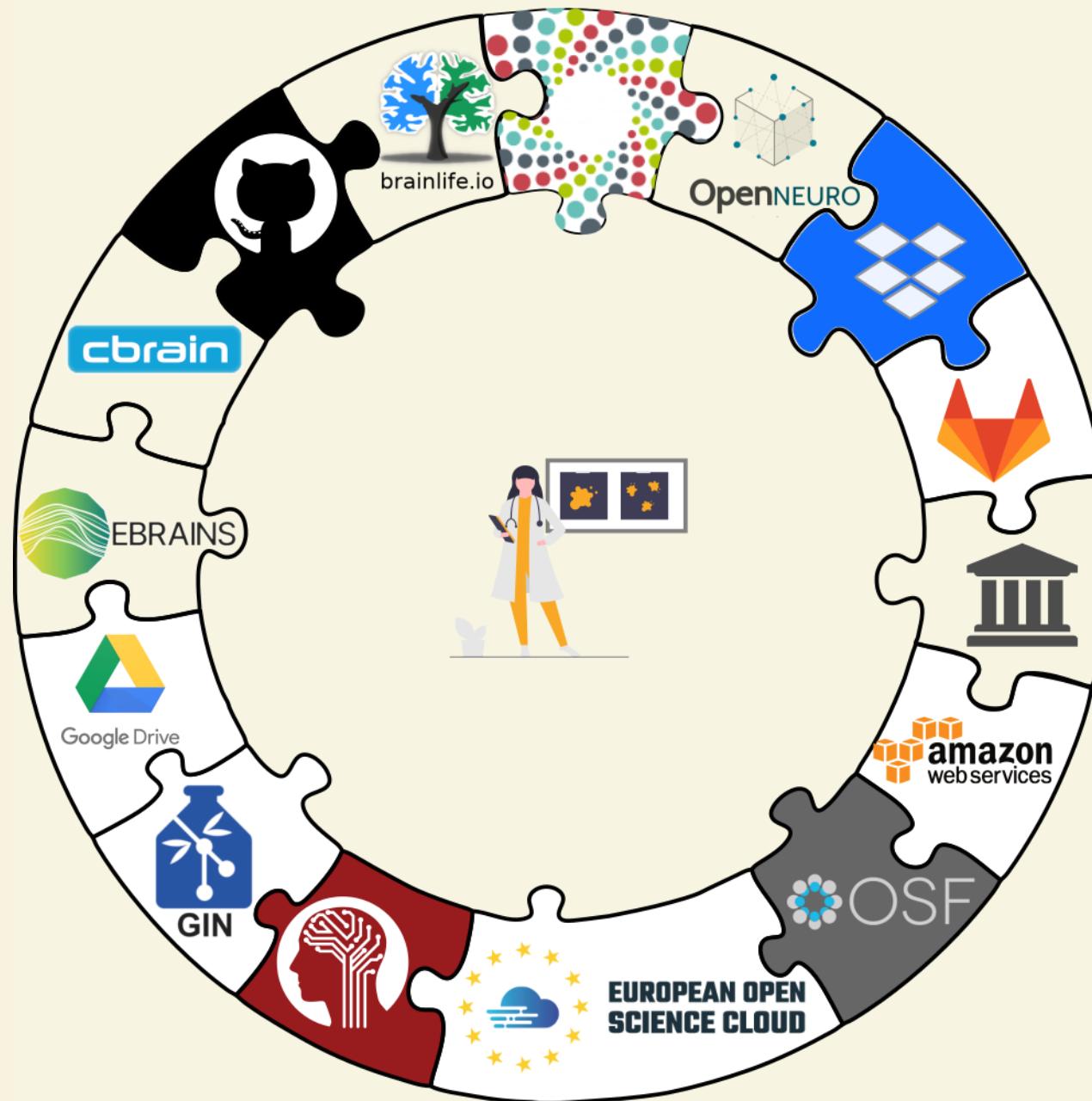
```
$ datalad drop A.Shashua-Introduction_to_Machine_Learning.pdf  
drop(ok): /tmp/machinelearning-books/A.Shashua-Introduction_to_Machine_Learning.pdf (file) [checking https
```

INTEROPERABILITY

- DataLad is built to maximize interoperability and use with hosting and storage technology

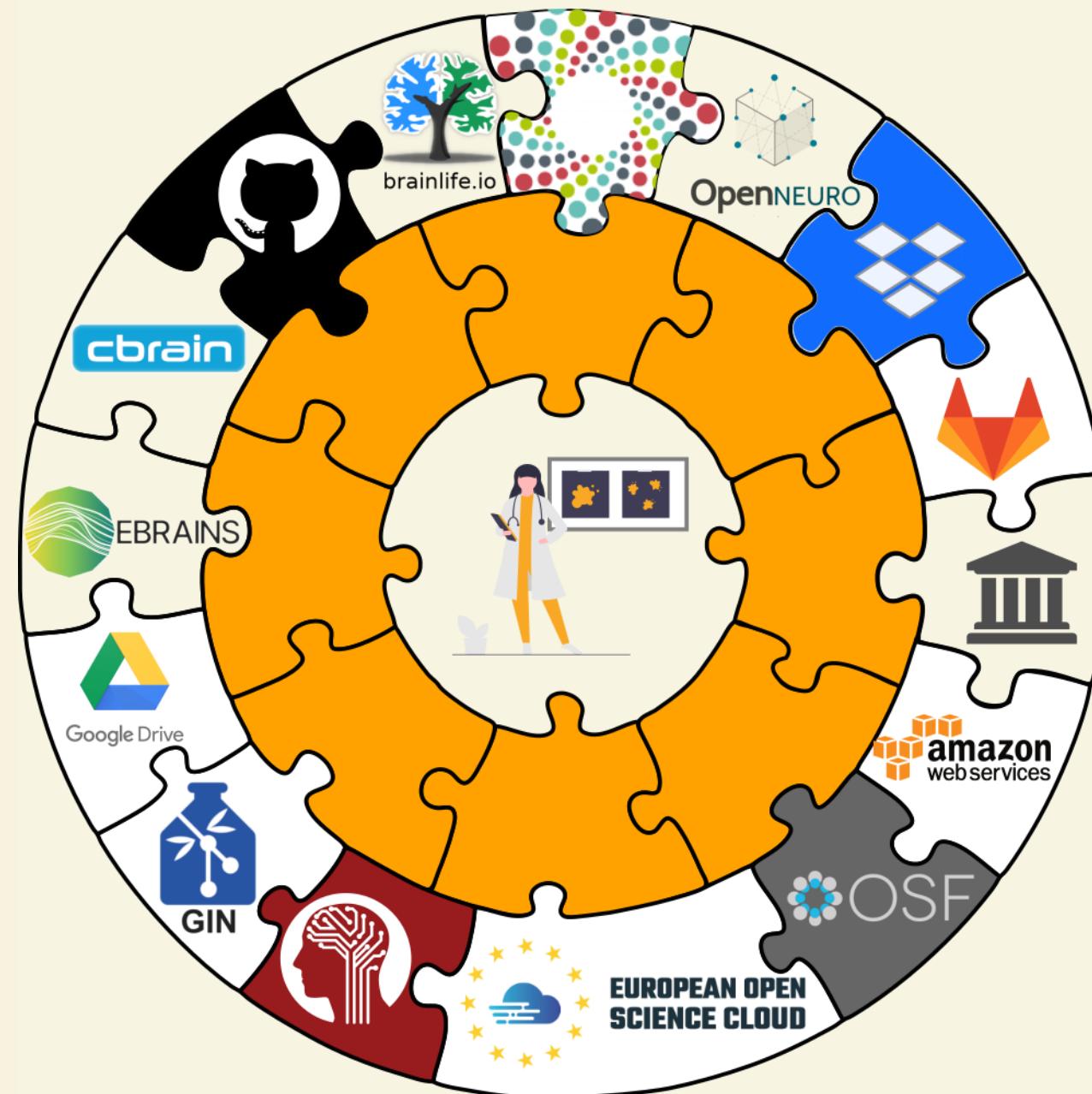
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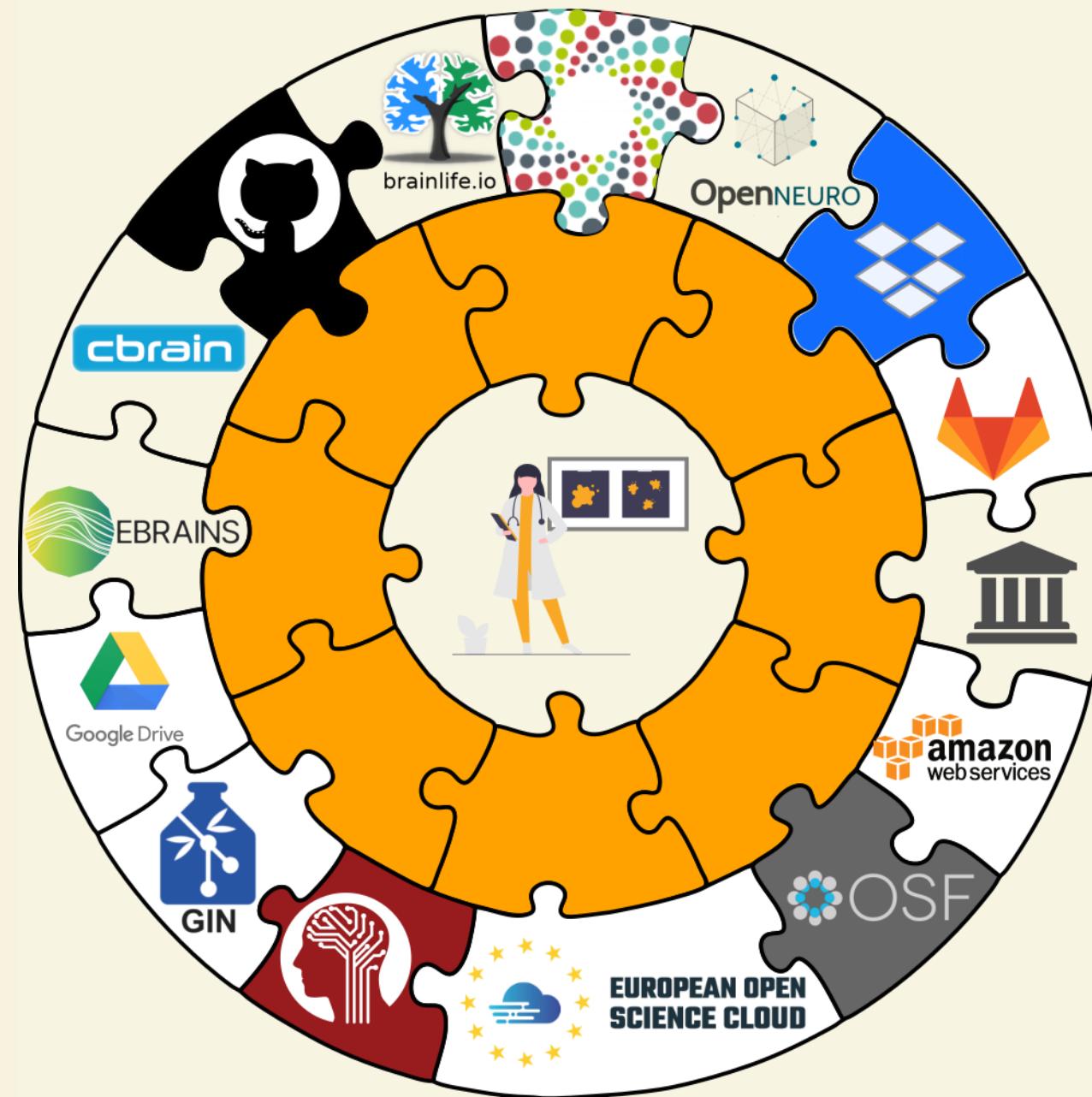
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- Uncompromised decentralization, no required central server or service.

INTEROPERABILITY

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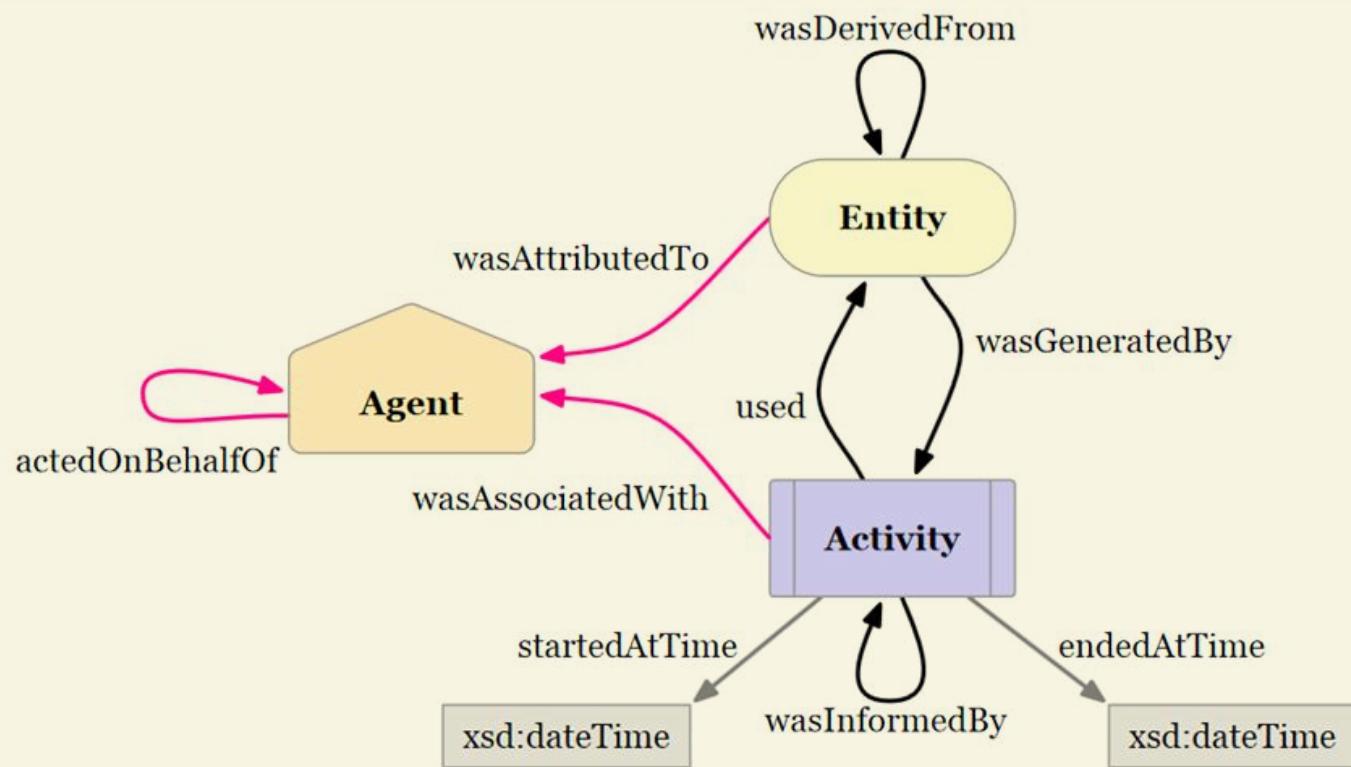
The screenshot shows a GitHub repository page for the user 'psychoinformatics-de' and the repository 'paper-remodnav'. The top navigation bar includes links for Pull requests, Issues, Marketplace, and Explore. Below the header, the repository name is displayed along with a star count (8), a fork count (2), and a 'Code' button which is highlighted in green. The main content area shows a list of recent commits:

Author	Commit Message	Date
adswa	Merge pull request #12 from psychoinformatics-de/fin...	6f09e35 on Jun 5
code	Merge pull request #12 from psychoinformatics-de/finalr...	2 months ago
data	Point to latest label dataset	15 months ago
img	Label panels in flowchart	5 months ago
remodnav @ d289118	Update remodnav with latest test dataset	16 months ago
.gitignore	Prevent permanent rebuilds of the figures	16 months ago

On the right side of the page, there are sections for 'About' (describing the repository as 'Code, data and manuscript for https://doi.org/10.1101/619254') and 'Releases' (indicating 2 tags). The bottom of the page features a yellow footer bar.

PROVENANCE CAPTURE

- Datasets can capture dataset **transformations** and their **cause** in order to track the entire evolution and lineage of files in datasets



- "How did this file came to be?", "What steps were undertaken to transform the raw data into the published result?", "Can you recompute this for me?"

PROVENANCE CAPTURE

- **Basic provenance:** DataLad can capture arbitrary dataset transformations (e.g., from computing analysis results) and record the cause of such a change

```
$ datalad run -m "Perform eye movement event detection" \
  --input 'raw_data/*.tsv.gz' --output 'sub-*' \
  bash code/compute_all.sh

-- Git commit -- Michael Hanke <...@gmail.com>; Fri Sep 21 22:00:47 2019
[DATALAD RUNCMD] Perform eye movement event detection
==== Do not change lines below ====
{
  "cmd": "bash code/compute_all.sh",
  "dsid": "d2b4b72a-7c13-11e7-9f1f-a0369f7c647e",
  "exit": 0,
  "inputs": ["raw_data/*.tsv.gz"],
  "outputs": ["sub-*"],
  "pwd": "."
}
^^^ Do not change lines above ^^^
---
sub-01/sub-01_task-movie_run-1_events.png | 2 ++
sub-01/sub-01_task-movie_run-1_events.tsv | 2 ++
...
```

PROVENANCE CAPTURE

- **Computational provenance:** Datasets can track **software containers**, and perform and record computations inside it:

```
$ datalad containers-run -n neuroimaging-container \
--input 'mri/*_bold.nii' --output 'sub-* /LC_timeseries_run-* .csv' \
"bash -c 'for sub in sub-*; do for run in run-1 ... run-8;
do python3 code/extract_lc_timeseries.py \$sub \$run; done; done'"

-- Git commit -- Michael Hanke <... @gmail.com>; Fri Jul 6 11:02:28 2019
[DATALAD RUNCMD] singularity exec --bind {pwd} .datalad/e...
==== Do not change lines below ===
{
  "cmd": "singularity exec --bind {pwd} .datalad/environments/nilearn.simg bash..",
  "dsid": "92e1faa-632a-11e8-af29-a0369f7c647e",
  "inputs": [
    "mri/*.bold.nii.gz",
    ".datalad/environments/nilearn.simg"
  ],
  "outputs": ["sub-* /LC_timeseries_run-* .csv"],
  ...
}
^^^ Do not change lines above ^^^
---
sub-01/LC_timeseries_run-1.csv | 1 +
...
```

PROVENANCE CAPTURE

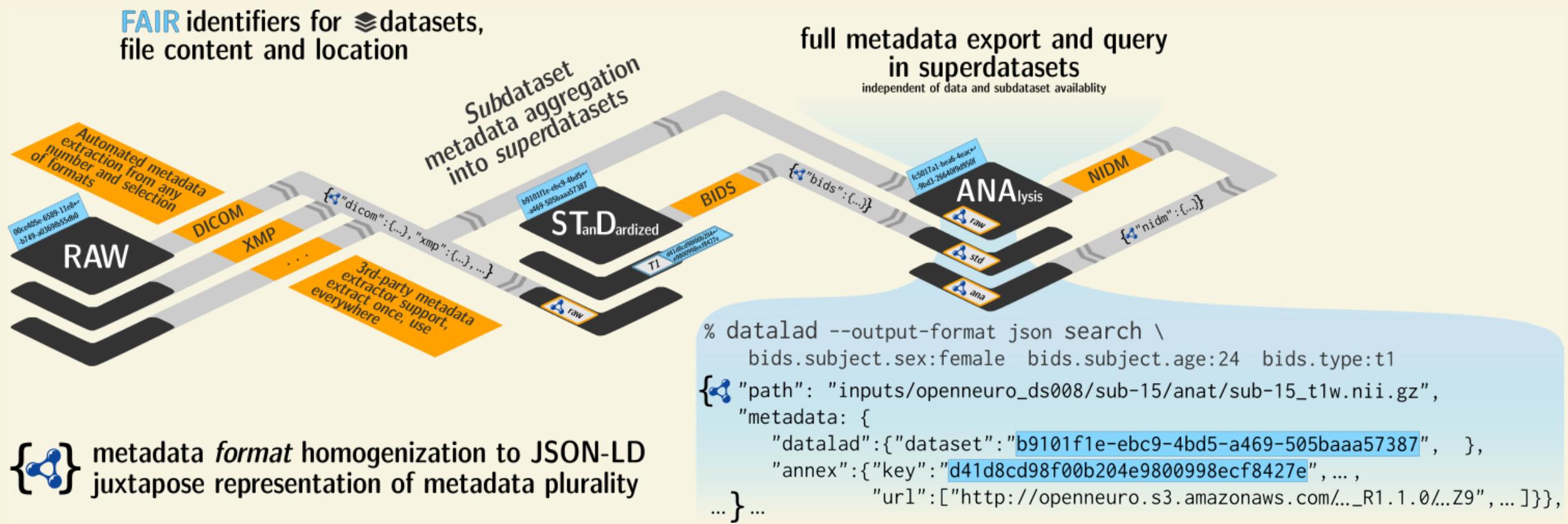
- All recorded transformations can be re-computed automatically

```
$ datalad rerun eee1356bb7e8f921174e404c6df6aadcc1f158f0
[INFO] == Command start (output follows) ====
[INFO] == Command exit (modification check follows) ====
add(ok): sub-01/LC_timeseries_run-1.csv (file)
...
save(ok): . (dataset)
action summary:
  add (ok: 45)
  save (notneeded: 45, ok: 1)
  unlock (notneeded: 45)
...
...
```

- Aid with the reproducibility of a result and verify it (via content hash)
- Use complete capture and automatic re-computation as alternative to storage and transport

AND THERE IS MORE...

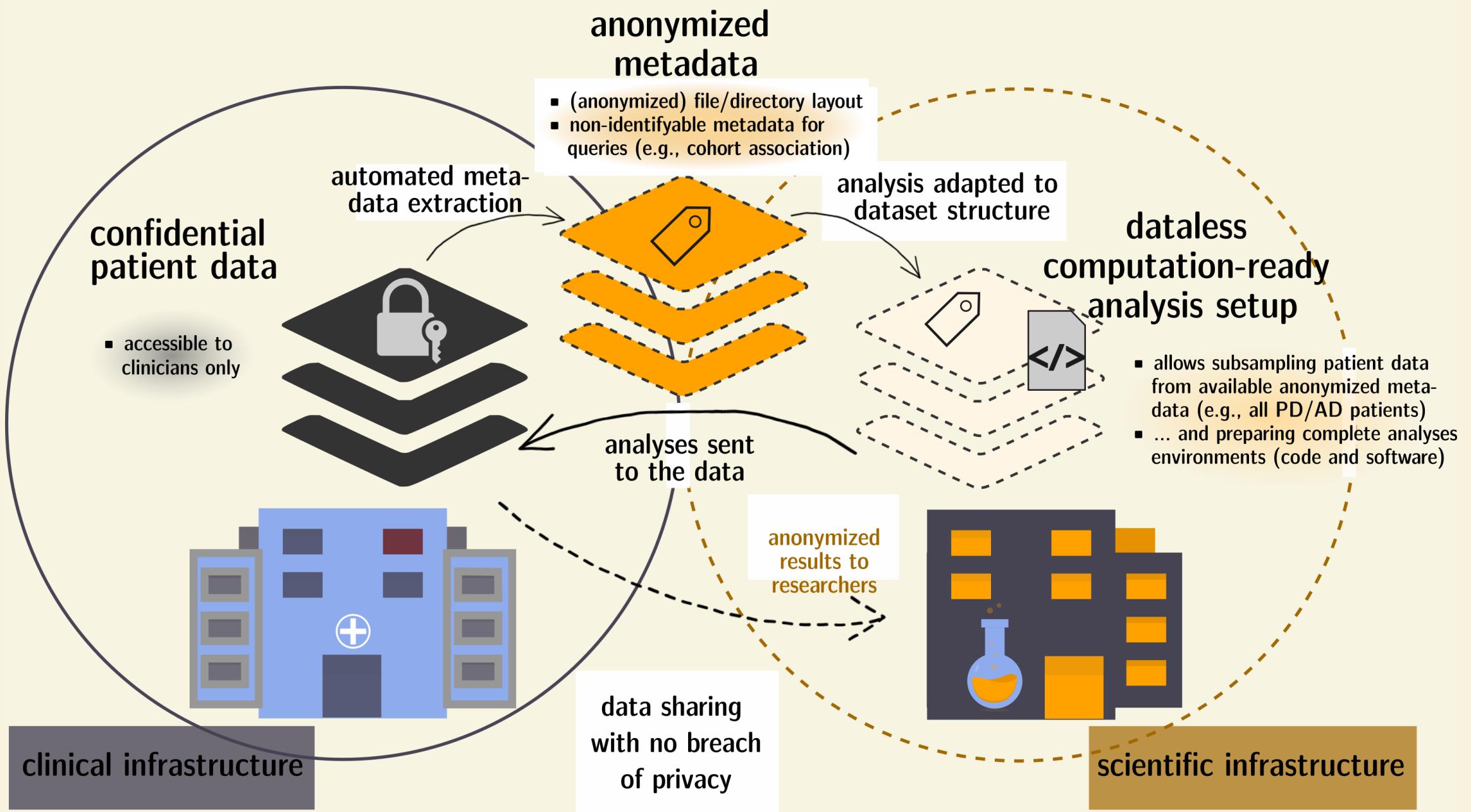
SCALABLE AND ACTIONABLE (META)DATA REPRESENTATIONS



- meta data logistics to generate, store, share, and search arbitrary meta data
- Sharing/retrieving only dataset meta data enables data discovery that doesn't require retrieving (potentially large) file contents first
- facilitates building metadata-driven applications

DEALING WITH SENSITIVE DATA

- Flexible data access management - file contents can be made available to none or selected few
- Share anonymized meta data not subject to privacy concerns
- Viable solution to bring the computation to the data



STILL MORE...

"RIA stores" for central data management, archival, or backup:

self-contained, plain file system storage for datasets, tuned for maintainability and use on systems with inode limitations (any-sized dataset \approx 25 inodes). More: handbook.datalad.org/r.html?RIA

Extensions with additional or domain-specific functionality:

Available as pip-installable Python packages. More: handbook.datalad.org/r.html?extensions

Open Data collection:

As of August 2020, about 250TB of open data: datasets.datalad.org/

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- Collaborate: Generic workflows, interoperability with established tools & services

FURTHER INFORMATION

- Source code: github.com/datalad/datalad
- Extensive user documentation, tutorials, and use cases: handbook.datalad.org
- Technical docs: docs.datalad.org
- Video tutorials: Youtube channel "DataLad"
- Matrix channel: DataLad

THANKS!