ETH-RAT

Enabling Reproducible, Repeatable and Reusable (Data) Science With the RENKU Platform

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Swiss Data Science Center by the numbers

- ~30 people, scaling up to ~40 by mid-2019
  - ~10 on Renku platform/software engineering
  - ~15 data scientists from variety of backgrounds
- 18 academic collaboration projects
  - Funding mix of infrastructure and personnel
- several industry collaborations, scaling up with addition of a dedicated industry component

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Reproducibility — what do we mean?

- The “reproducibility crisis”*
  - Lack of replication studies
  - Failure to reproduce published results
  - Publication bias (only publishing “good” results)
  - False positives in published research
  - Lack of transparency and completeness

The upside: “credibility revolution”

* from the Stanford Encyclopedia of Philosophy

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Reproducibility — what do we mean?

- Reproduce studies based on the “concept”
- Repeat entire experiments following published methods/ protocols (but with own implementation)
- Repeat the published computational procedures on original or new data
- Repeat computations “verbatim” (same code, environment)

Five FAQs in Data-Driven Research

1. How did I compute this result?

2. How does new data change this result?

3. How did you compute *your* result?

Can I use your data to reproduce it?
With your code?
On your infrastructure?

4. Has anyone ever used an <XYZ-algorithm> on this data? How?

5. Who is using my data? and my algorithm?

Why are they not citing me?!

If you can answer these questions confidently:

- You can collaborate easily
- Your team is efficient
- You participate in Open Science/Open Data
- You are properly acknowledged (and you acknowledge others!)
- You can be held accountable
- Your results are **trustworthy**

Public focus

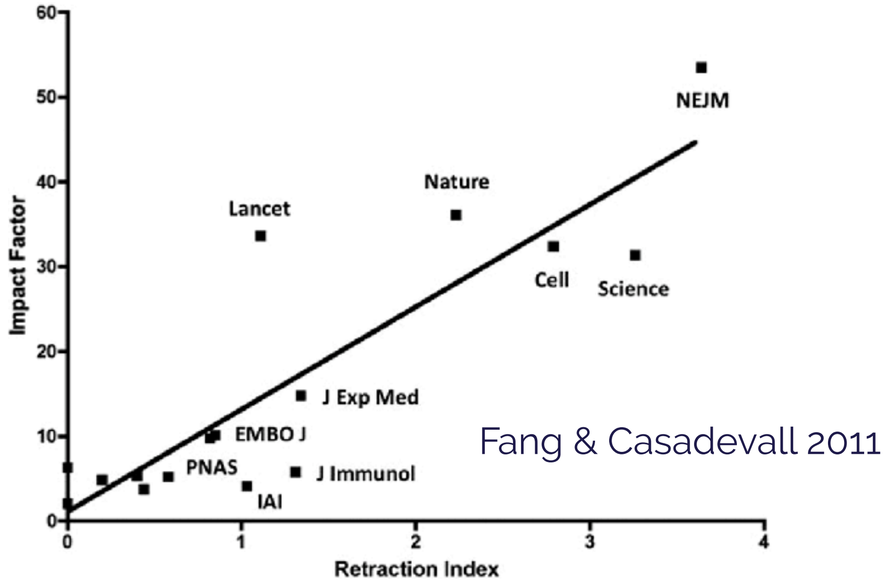
Kultur > Wissen >

Glaubwürdigkeit in Gefahr

Pimp my presentation: Wenn die Wissenschaft panscht

Viele Studien lassen sich nicht wiederholen. Das wirft ein schlechtes Licht auf die Wissenschaft. Was dagegen tun?

Montag, 03.09.2018, 15:33 Uhr



Fang & Casadevall 2011

- Increasingly, (failed) reproducibility in publicly-funded science under scrutiny
- Requirements for open science from funding agencies, governments (downward pressure)
- Some places (e.g. Switzerland) *openness* also across e.g. government data
  - But, is open useful in and of itself?
  - How can the open data be used?
  - How can the open science be reused? Reproduced?

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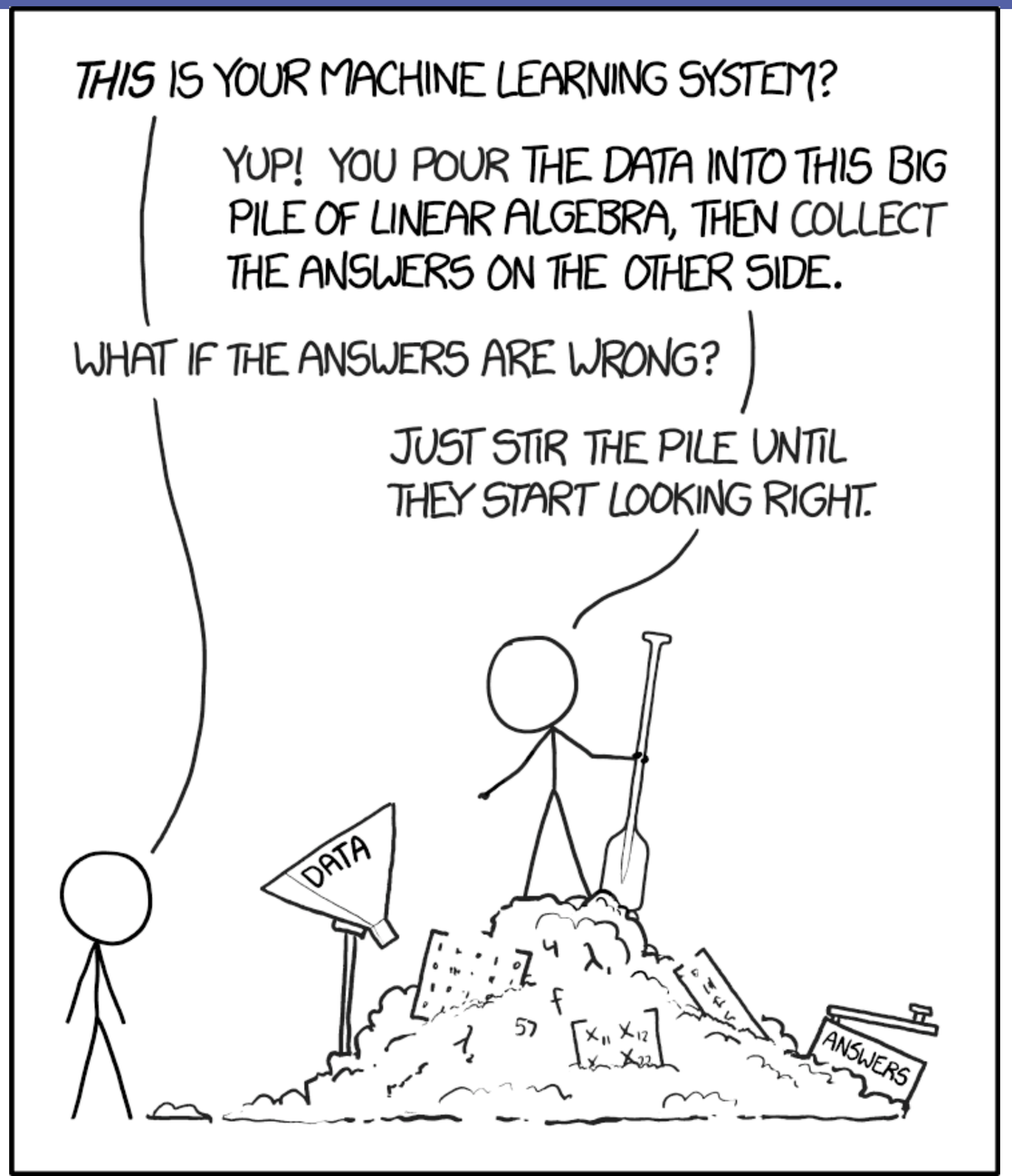
Situation to avoid...



Does “reproducible” mean “open”?

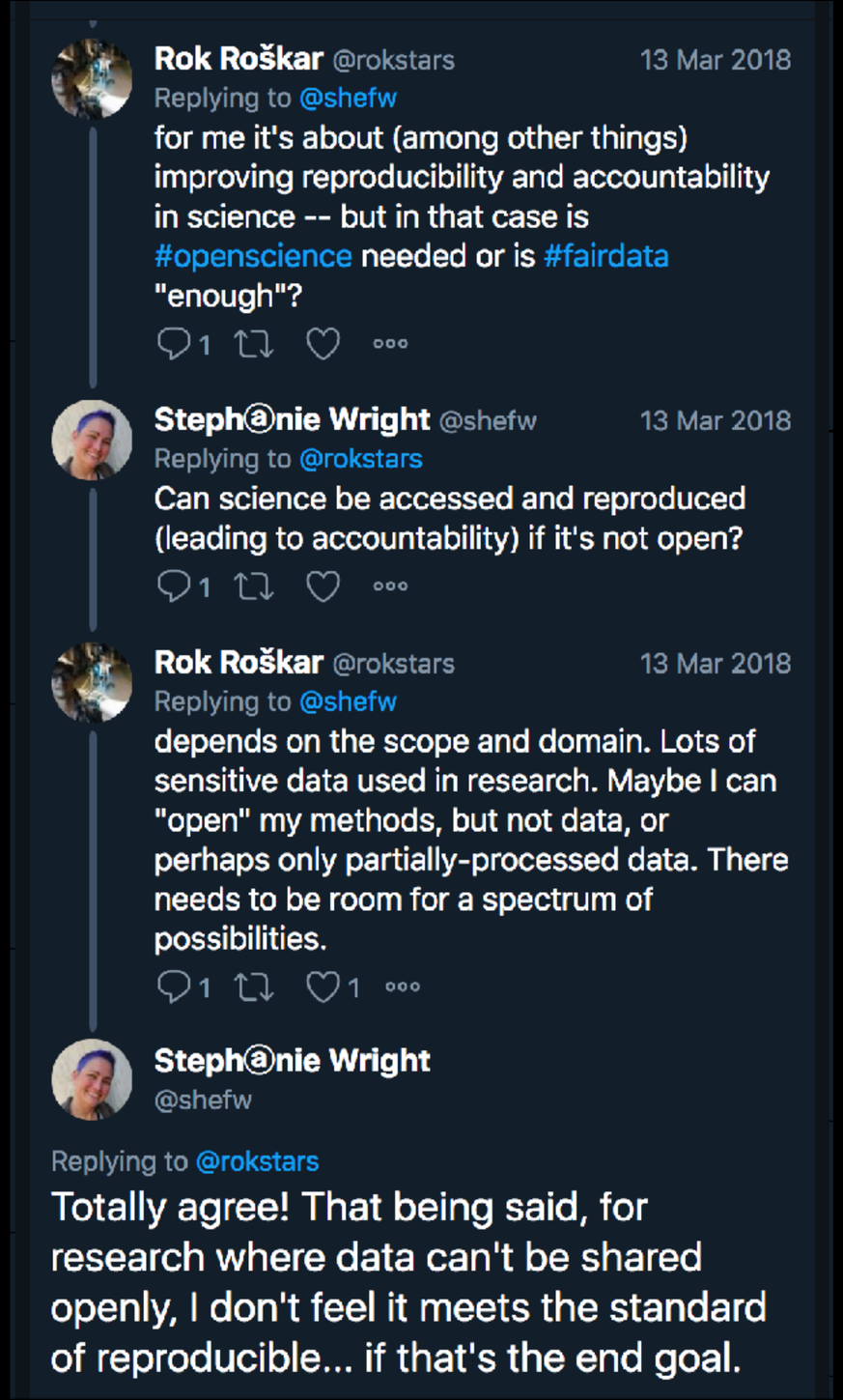
Does “open” mean “reproducible”?

Does FAIR mean “reproducible”?

Does FAIR mean “open”?

“reproducible” may depend on context and point of view…

Q: Which problem is Open Science fixing?



Rok Roškar @rokstars 13 Mar 2018
Replying to @shefw
for me it's about (among other things) improving reproducibility and accountability in science -- but in that case is #openscience needed or is #fairdata "enough"?
1

Steph@nie Wright @shefw 13 Mar 2018
Replying to @rokstars
Can science be accessed and reproduced (leading to accountability) if it's not open?
1

Rok Roškar @rokstars 13 Mar 2018
Replying to @shefw
depends on the scope and domain. Lots of sensitive data used in research. Maybe I can "open" my methods, but not data, or perhaps only partially-processed data. There needs to be room for a spectrum of possibilities.
1 1

Steph@nie Wright
@shefw

Replying to @rokstars
Totally agree! That being said, for research where data can't be shared openly, I don't feel it meets the standard of reproducible... if that's the end goal.

A Myriad of Tools

Hard **work** to make science reproducible, accessible, open etc…

- Version control (`git`)
- Code sharing (GitHub, GitLab, BitBucket)
- Data sharing (Zenodo, Figshare, institutional digital archives)
- Presentation and communication (Jupyter, RStudio)
- Correctness – testing (CI, e.g. travis)
- Packaging, containerization (docker, singularity)

Difficult to stay **productive** and worry about all of the above!

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FAIR + Open + ? Make it also practical!

- Findable, accessible, interoperable, reusable - data. What about the process?
- Top-down pressure for openness
  - It's in the public interest!
  - Is it in the interest of the individual researcher?
- Focus on the process also focuses on the scientist - making the process better will enable + incentivize
- **Scientists are practical - make "open" work for them!**

Reproducibility is critical here

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RENKU - 連句

A Platform for Reproducible, Reusable, Shareable, (Data) Science

Terminology

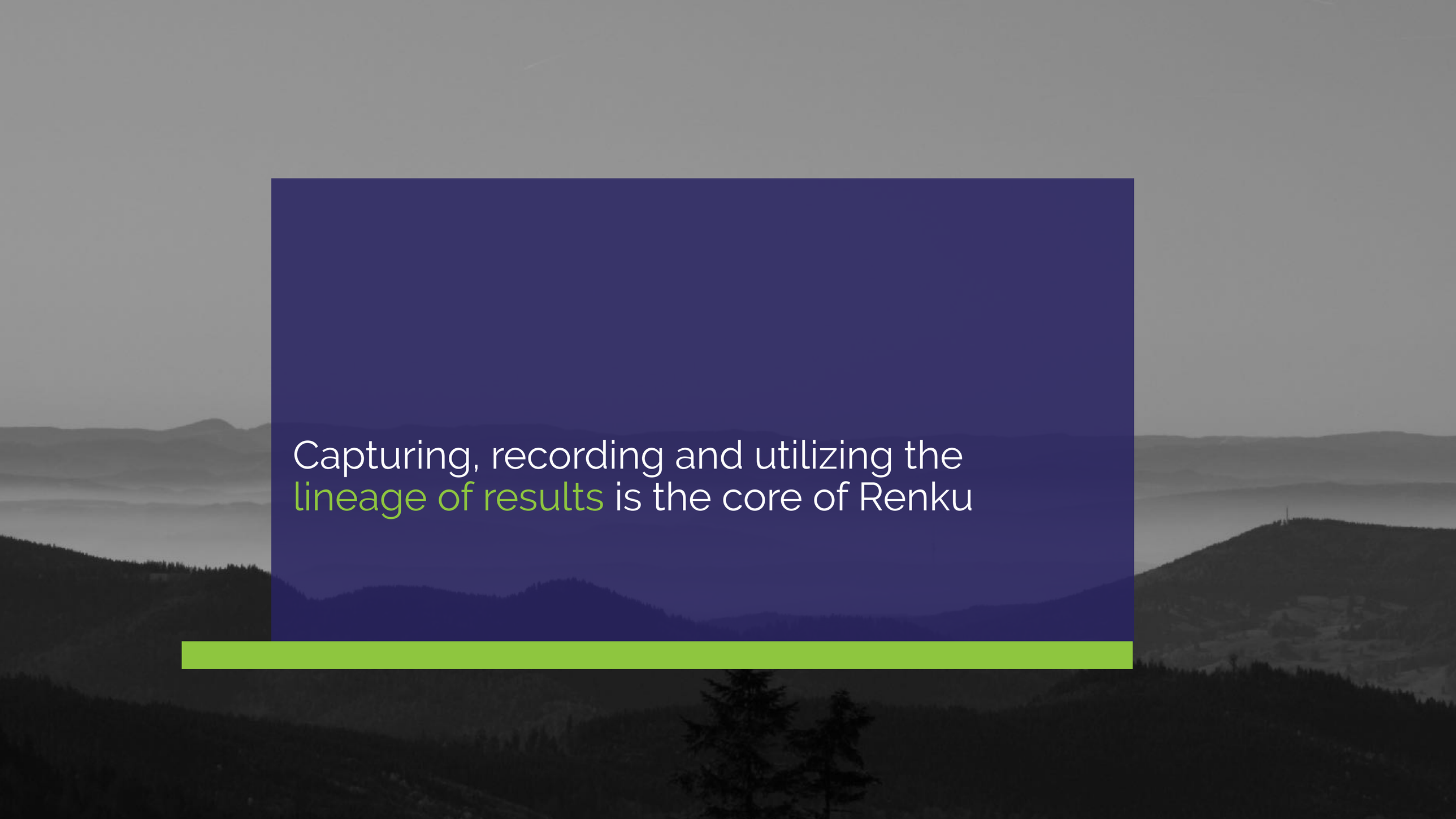
- We borrow the **Renku** name from the Japanese word for *linked-verse poetry*
- A "**ku**" is a verse in a renku poem
- We use "**ku**" to mean a piece of the data analysis process – includes discussion, code, and results

Five Questions → Three Words

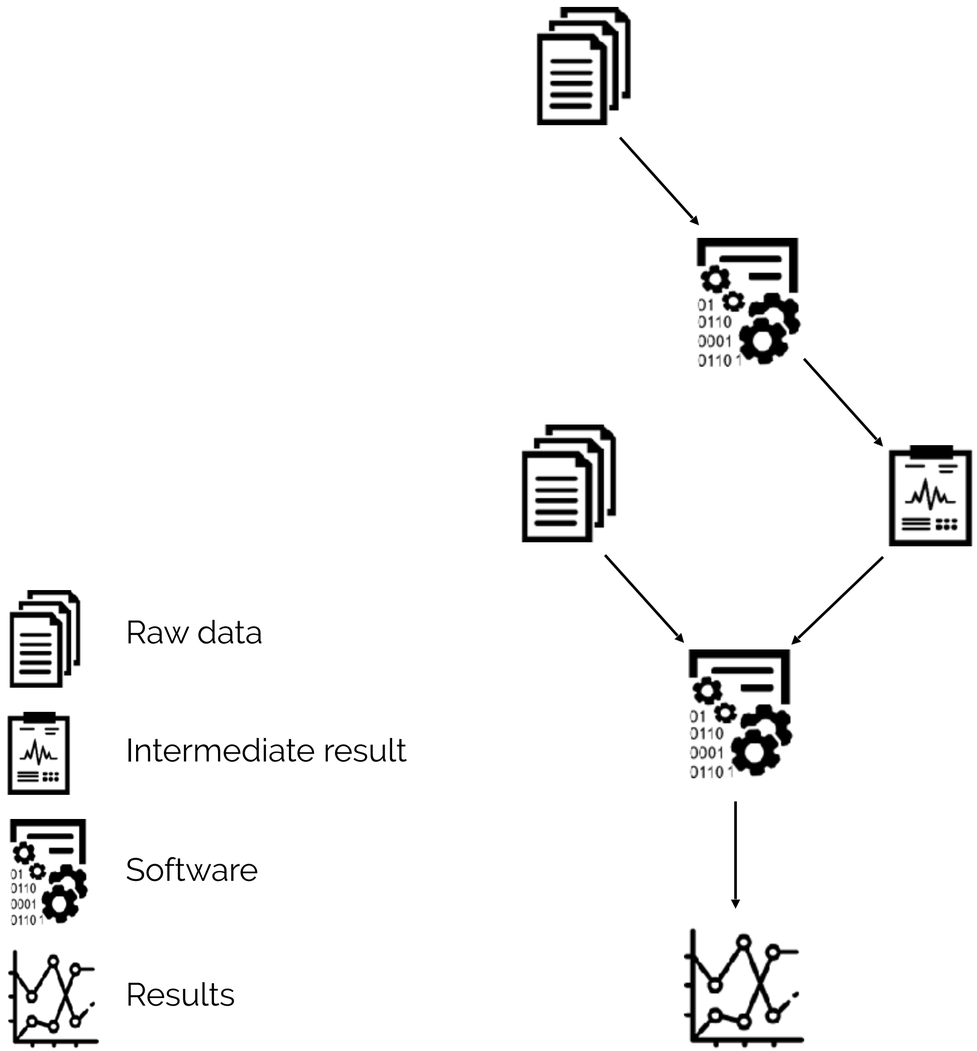
Reproducibility

Reusability

Collaboration


Capturing, recording and utilizing the
lineage of results is the core of Renku

Lineage of a simple analysis



- Inputs and outputs of analysis steps are recorded into a **knowledge graph** *as the work is being done*
- Steps can be **repeated** or integrated into more complex **workflows**
- **Provenance** of all data products is always accessible via simple tools
- **Version control** is built-in for data, code, and workflows

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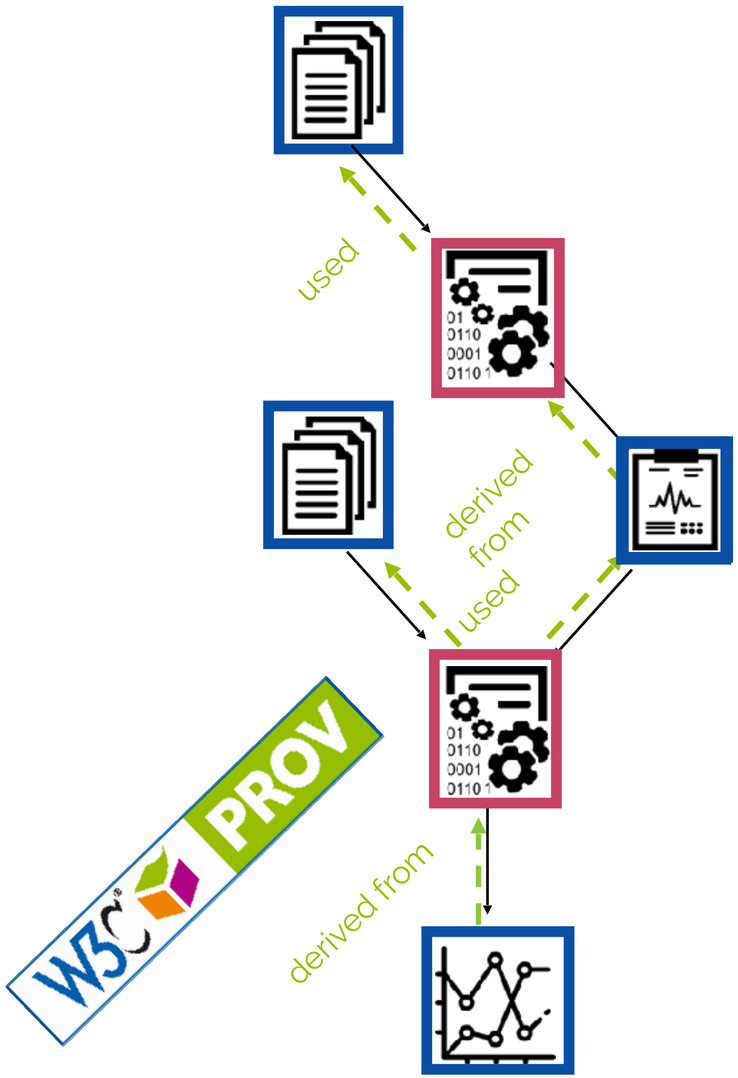
Capturing the Knowledge Graph

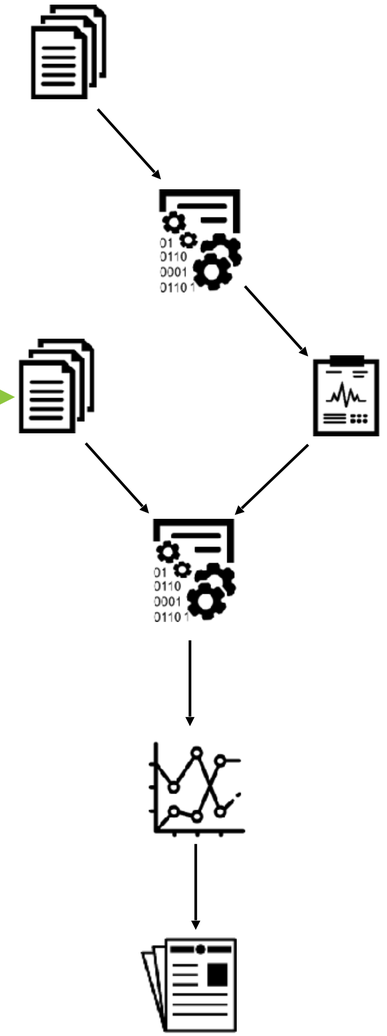
- Record the dependency graph using linked data standards e.g. Dublin Core, FOAF, Schema.org, PROV-O
- Capture the full semantic information to enable interoperability and domain-specific ontologies



- CWL for representing all computational steps
- Capture individual steps from user input
- Tools for constructing workflows from basic pieces
- Rely on container technologies to ensure consistent environment for reproducibility

Discover and understand the analysis process

Graph-based search…



Ex: search for **data** and explore the tools to efficiently generate results

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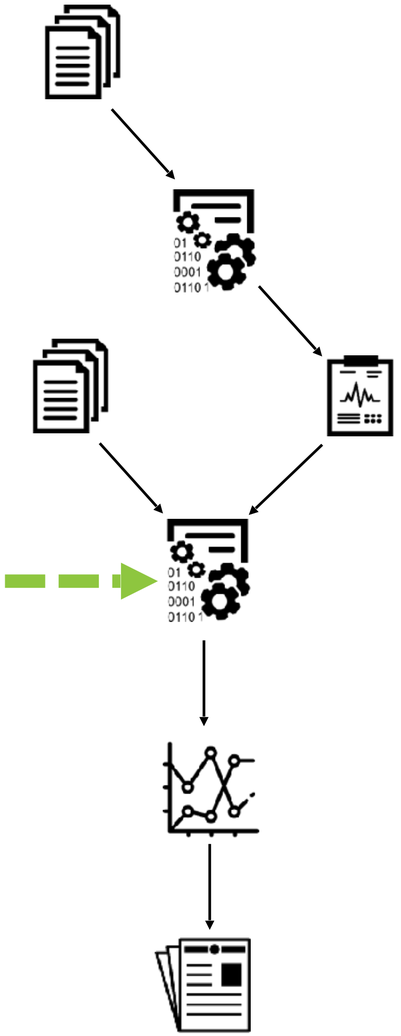
Discover and understand the analysis process

Graph-based search…



Ex: search for an **algorithm**
and see its applications

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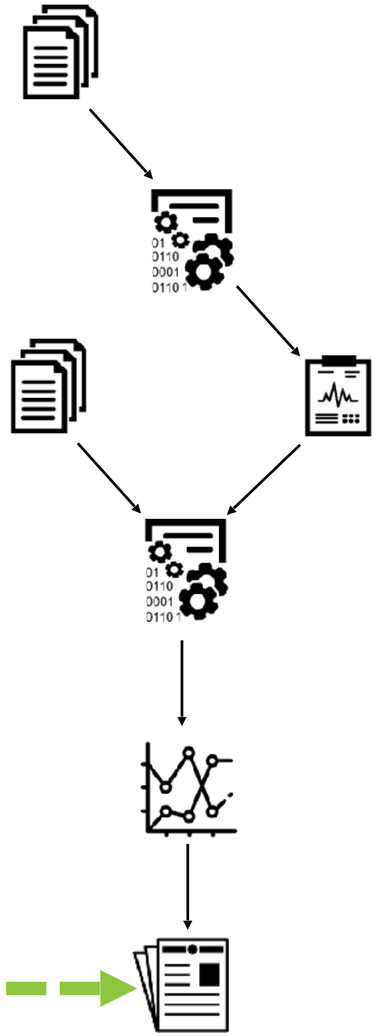
Discover and understand the analysis process

Graph-based search…

Ex: search for a **publication**, obtain a full view of how the results were obtained



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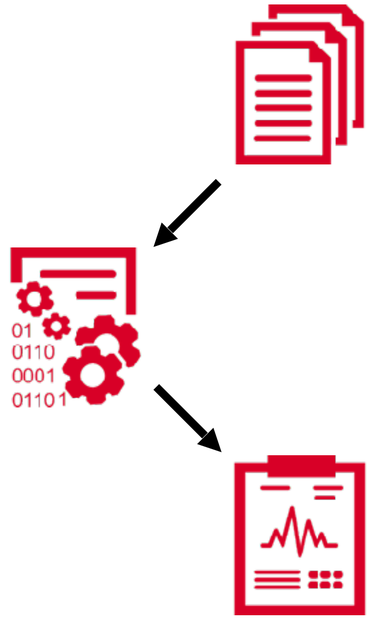
Reuse and repeat



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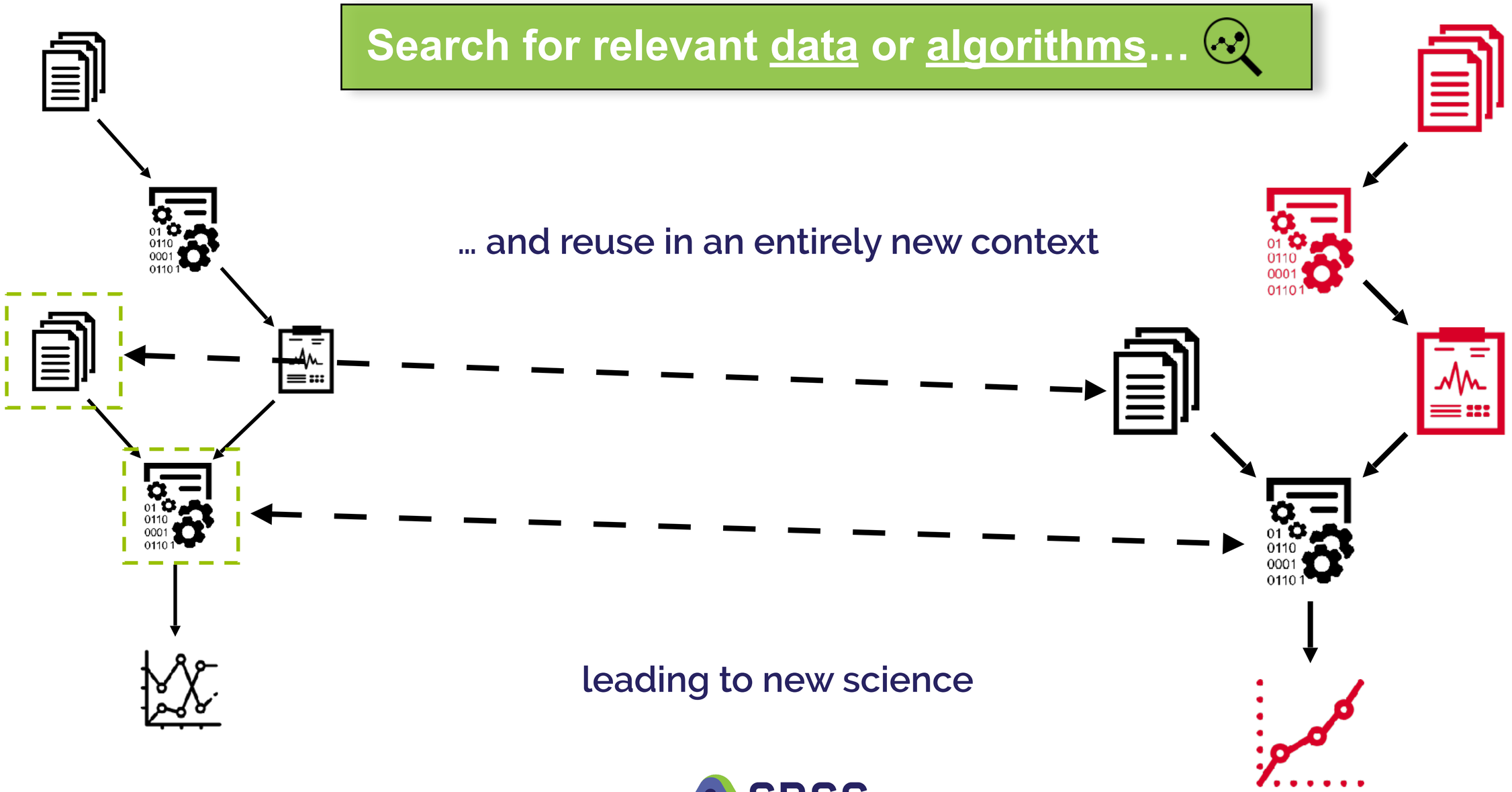
Reuse and repeat



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Explore the KG to answer questions

- Who is using the data and how?
- Which algorithms are used to answer which questions?
- How to regenerate results if new data becomes available? If old data is now off-limits?
- Who to credit?
- How popular is my work/the work of my lab/my unit?

Best-practices translate to immediate benefits for the scientist

Establish trust

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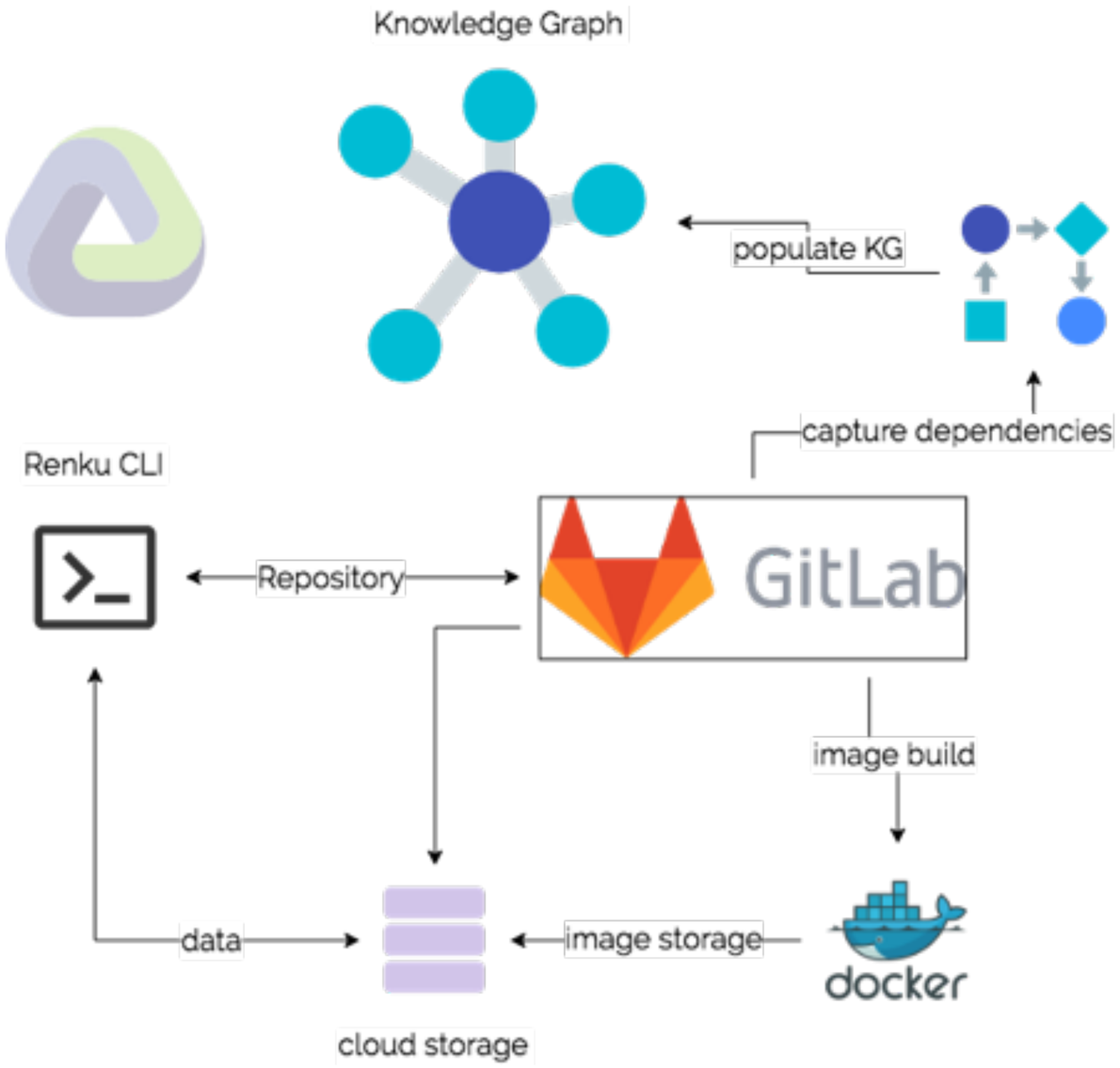
Technology

- Core is based on trusted tech like git, GitLab, Jupyter, docker
- Easily deploys on any cloud
- Designed to be as independent/closed as needed, but as open as possible
- Example public deployment on renkulab.io - try the demo!

Reproducibility



- CLI developed from ground up taking advantage of Git to capture lineage
- Designed with interoperability in mind, using linked data standards to express dependencies
- Using version control for data and code – overcoming usability challenges

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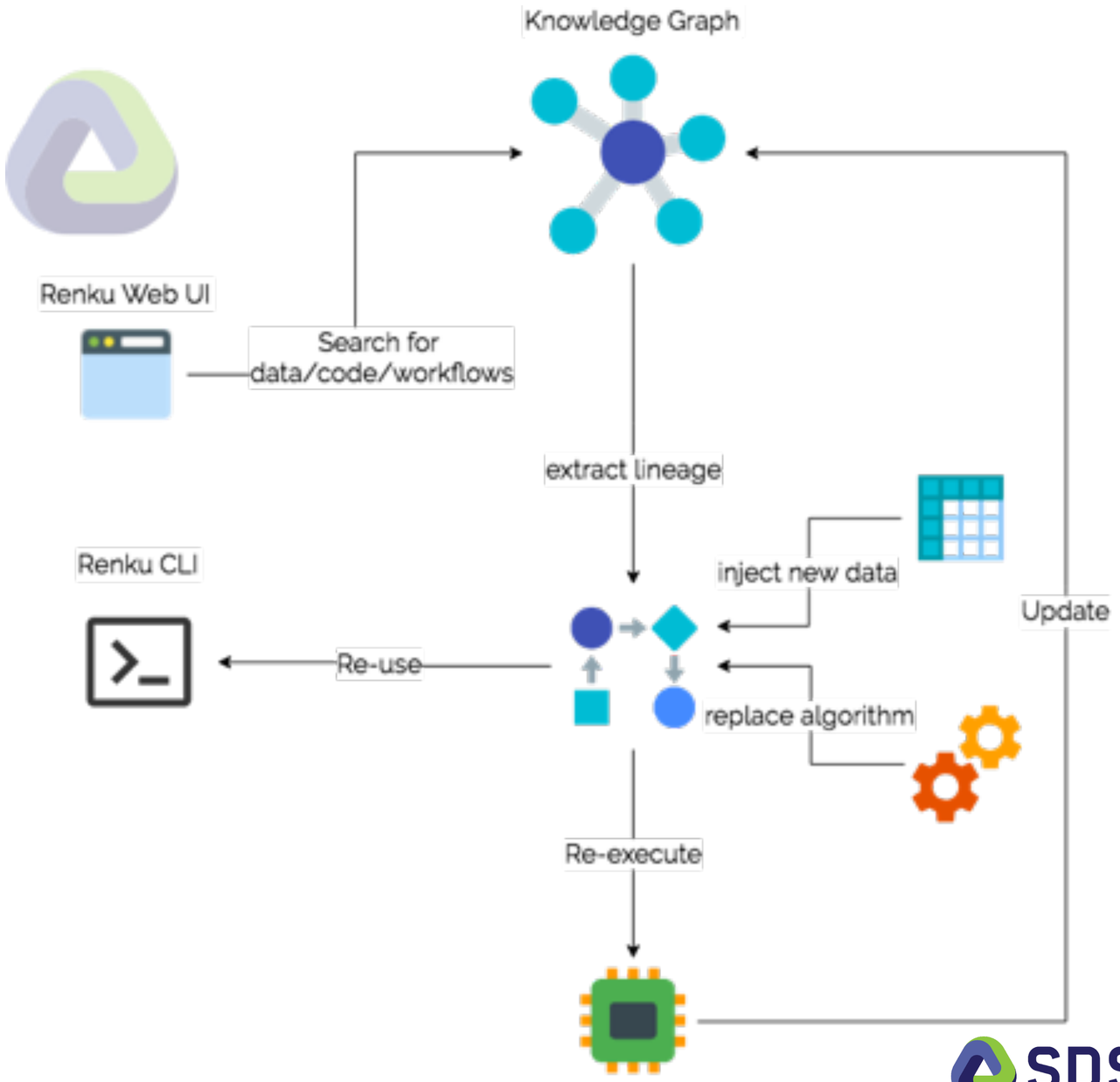
Reusability



- Understanding lineage means we can always re-execute and update results as methods or data change
- Workflow construction and re-execution possible with the local client
- Developing the means to execute workflows in the cloud and on HPC (CSCS)
- Search for graph artifacts being developed

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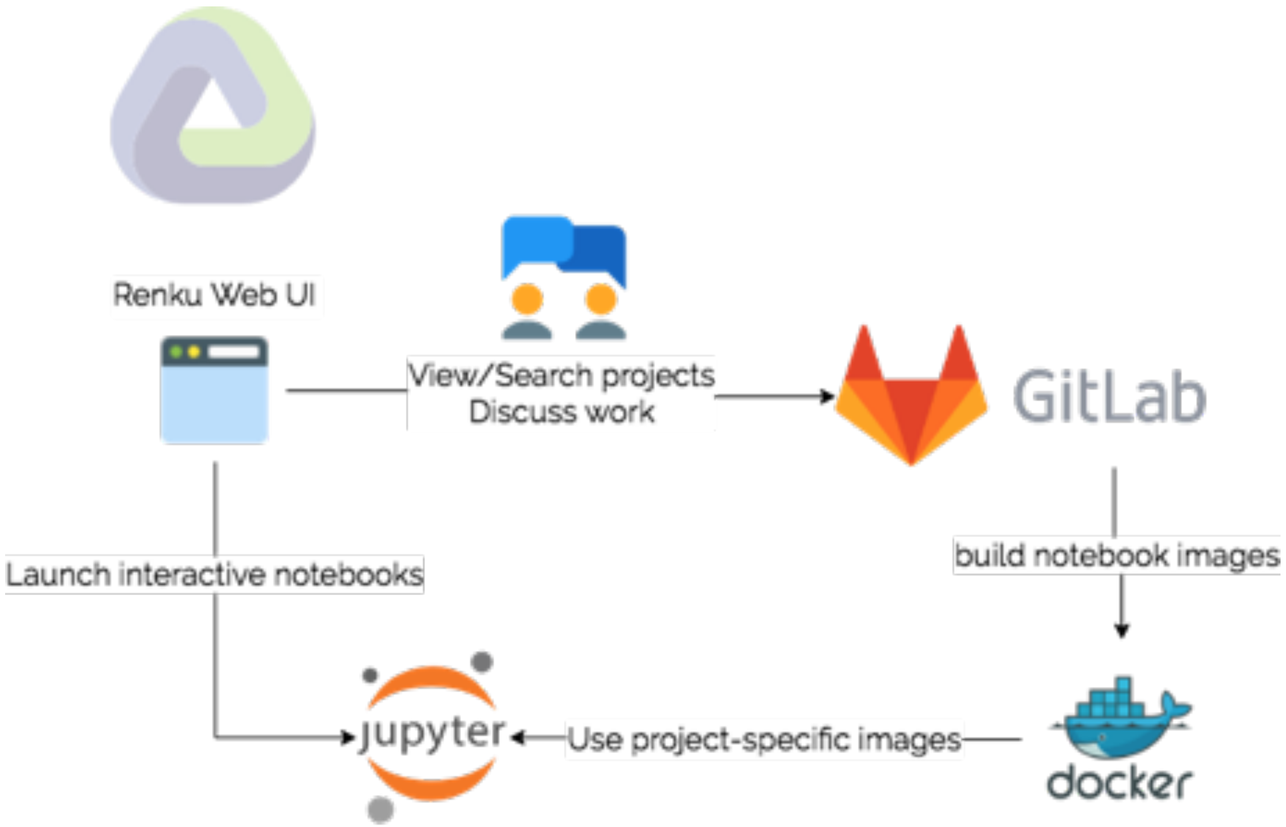
Collaboration



- Web UI serves as primary point of contact for users
- Allows creation of projects, discussions with media embedding
- Creation of hosted interactive sessions with version-controlled environments (docker images)
- Various supported languages, e.g. python, matlab (with GUI), R, Rstudio

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Renku platform

Goal: improve the scientific process by making use of best-practices simple

- Track the lineage of research artifacts
- Index lineage into a combined Knowledge Graph that can be queried
- Use the lineage through simple tools (e.g. update results with new data)
- Make all steps reusable and repeatable by others
- Provide a simple user interface for collaboration and exploration
- Enable on-line interactive environments for rapid prototyping

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Status and upcoming challenges

Status

- Platform is under very active development
- Releasing v0.4.0 within a few weeks - preview with tutorial at: https://renkulab.io
- All open-source: https://github.com/SwissDataScienceCenter

Challenges

- Knowledge representation/engineering
  - What questions will the users ask?
  - What is the optimal way to represent the graph (with FAIR+ in mind)?
- Community building and awareness
- Education - make scientists aware of and believe in “best practices”

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