

Reproducible machine learning

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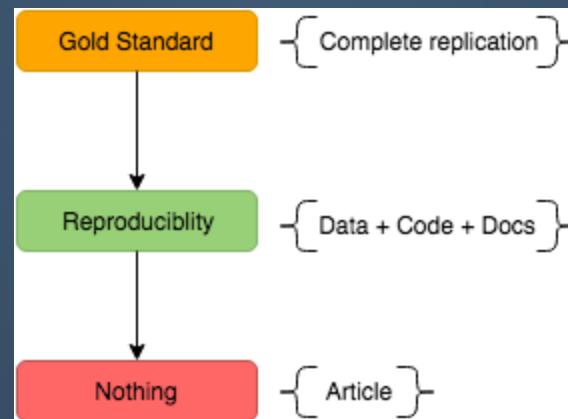
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Who we are

Triangle of reproducibility

- code
- data
- models

Reproduction vs Replication



[AP]

Why

- trust
- compliance
- auditing
- teams
- banking, healthcare, transportation, insurance

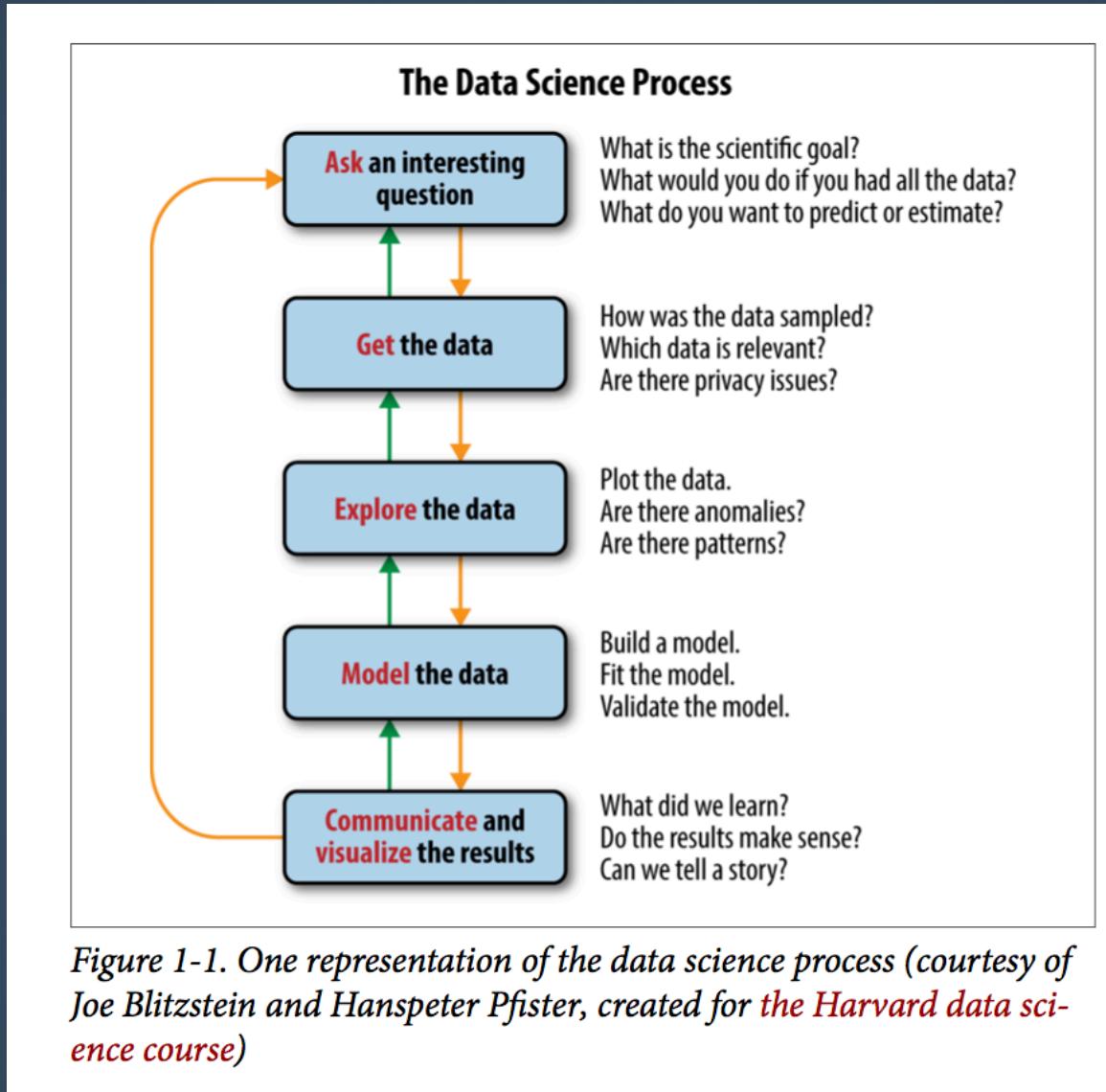


Figure 1-1. One representation of the data science process (courtesy of Joe Blitzstein and Hanspeter Pfister, created for [the Harvard data science course](#))

[CB]

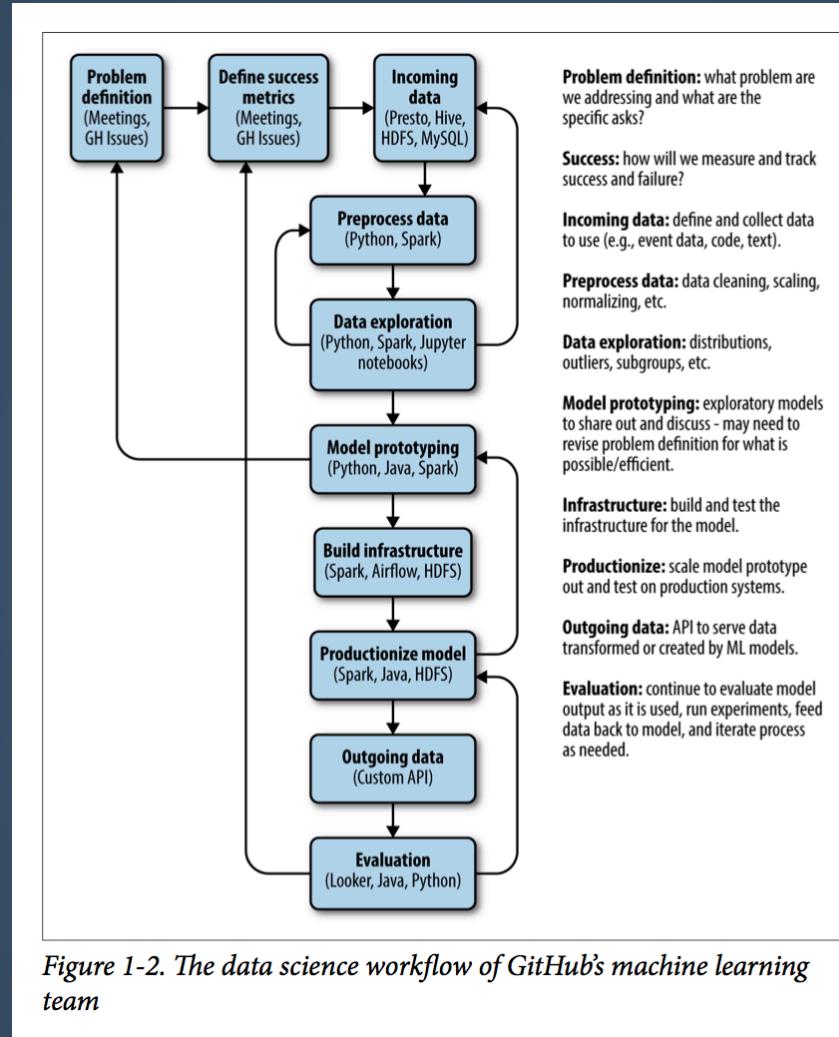


Figure 1-2. The data science workflow of GitHub's machine learning team

[CB]

Out of scope

- Deploying models to production
- Big data (Spark, Hadoop)
- But many of the tools discussed still apply

Tools for reproducibility

- code = conda + git + jupyter + *Docker
- data = pandas + quilt
- models = scikit + TensorFlow + quilt

conda

- packages + environments
- run from the command line
- do not install in root env
- `conda create -n MY_ENV python=3.6`
- `pip freeze`

pip or conda?

- pip - python packages in any env
- conda - any package in conda envs
- Never do this: sudo pip install

Don't put data in git

- Slows down repo
- Does not serialize
- Does not quickly handle large data (incl. LFS)
- Conflates code and data changes

Demo

TensorFlow

- Alpha - in development
- Virtual File System (in addition to standard API)
- Release in 2-4 weeks

Quilt + Keras/PyTorch/TF

- Reproducibility = specific data version, verified hashes
 - load input data + model/checkpoints from Quilt (vs local files)
 - saving+sharing model checkpoints in Quilt
- Example:
 - Download CIFAR-10 data; "quilt build" package and push to data repo

```
# map local directories/files to Quilt packages
import quilt.vfs
quilt.vfs.setup("<PKGNAME>:version",
mappings={...})
```

Demo

Resources

<https://github.com/quiltdata/reproducible-ml>

Further learning

- A tour of artificial intelligence and its limitations
- [CB] Development Workflows for Data Scientists, Claire Byrne
- [AP] Reproducible Research in Computational Sciences, Arnu Pretorius
- [JV] Installing Python Packages from a Jupyter Notebook, Jake VanderPlas
- [TM] Machine Learning, Tom Mitchell