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Reproducible Computational Science with Popper Workflows

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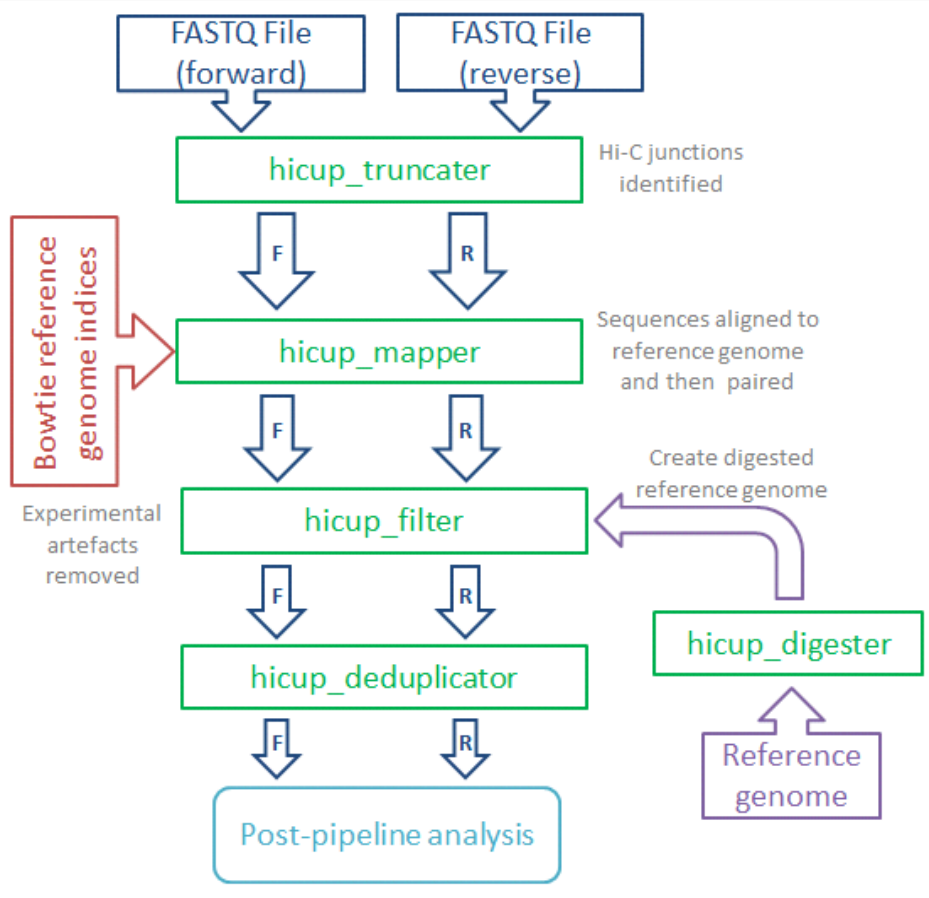
Common Reproducibility Issues (1)

Python statistics libraries

- Research using statistical and/or machine learning tools depends on increasingly complex software stacks
- Replicating a result is difficult due to incomplete dependencies, platform incompatibilities, ...

Common Reproducibility Issues (2)



A bioinformatics data pipeline

- Data processing pipelines have many interdependant steps from the raw data to the final result
- Replicating a workflow requires difficult guesswork if these steps not properly documented

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Popper

Popper is a container-native workflow execution engine which addresses these issues:

- Containerizing workflows avoids problems due to different software environments
- Specifying steps explicitely in a Popper workflow file avoids problems due to data pipeline complexity

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Limitations

However . . .

- Popper requires fluency in DevOps tools (in particular container engines)
- Steep learning curve for users with no prior experience in these tools, who would nonetheless benefit from more reproducible workflows

→ My goal was to create a collection of tools and tutorials to smooth out this learning curve for users in computational fields

Contributions: Tutorials

Tutorial for developing Popper workflows oriented to Python and R users:

- Computational notebooks with Popper
- Dependency management
- Project structure

Contributions: Templates

cookiecutter templates to bootstrap Popper workflows in Python and R including starter Docker images

```
├── LICENSE
├── README.md                    <- The top-level README.
├── data                         <- Data used in workflow.
├── paper                        <- Generated paper as PDF, LaTeX.
├── wf.yml                       <- Workflow starter
├── containers                   <- Definitions of containers used in workflow
│   └── exploration              <- Container used for exploratory work.
│       ├── exploration.dockerfile  <- Default dockerfile used in workflow.
│       └── exploration_env.yml     <- Defines conda environment used by container.
├── results
│   ├── models                   <- Model predictions, serialized models, etc.
│   └── figures                  <- Graphics created during workflow.
└── src                          <- Source code for this project.
    ├── notebooks                <- Jupyter notebooks.
    ├── data                     <- Scripts to download or generate data.
    ├── models                   <- Scripts used to generate models.
    └── figures                  <- Scripts to generate graphics.
```

Structure generated by cookiecutter for Python workflows

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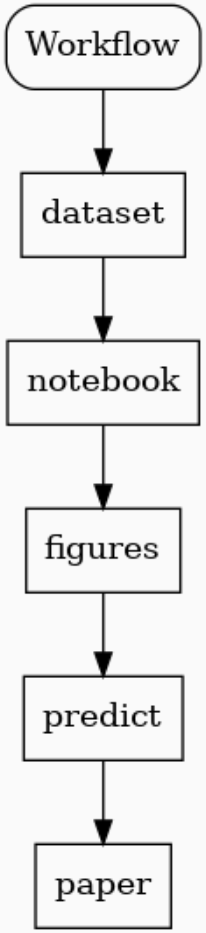
Contributions: Sample Workflows



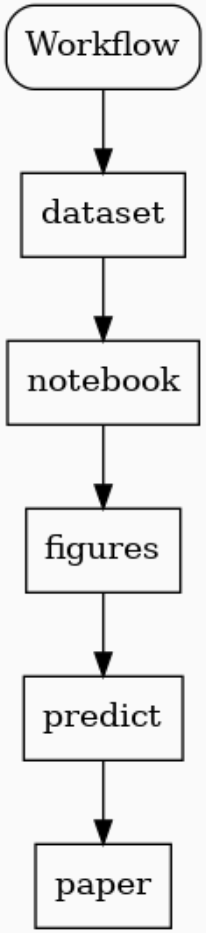
Workflow diagram generated by Popper

Sample Popper workflows in Python and R demonstrating an end-to-end machine learning project with data acquisition and transformation, model fitting and evaluation

Highlights (1)

- **Key idea in DevOps**: minimize the distance between development and production environments
- Users in computational research should be able to develop from the beginning their workflows in Popper
- This is done using Popper's interactive execution feature

Highlights (2)



Workflow diagram generated by Popper

- Users in computational fields use computational notebooks to prototype workflows
- I added configuration options to the core popper CLI to support running a computational notebook server

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