Continous benchmarking of single-cell tools using RENKU

A framework for open and continuous community benchmarking of bioinformatic tools

Project Website: https://renkulab.io/projects/omnibenchmark
Source code: https://renkulab.io/gitlab/omnibenchmark
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BACKGROUND

Benchmarking is a critical step for the development of bioinformatic methods and provides important insights for their application.
The current benchmarking scheme has many **limitations**:

– it is a `snapshot` of the available methods at a certain time point.
– it can be `outdated`, already at the time of a publication.
– `low comparability`: different procedures, different datasets, different evaluation criteria.
– all of the above can lead to `different conclusions` among benchmarks made at different time points or at different groups.

CONCEPT

✓ Here we propose a new `modular` and `extensible` framework based on a free open-source analytic platform, `RENKU`, to offer a continuous and open `community benchmarking system`.

✓ The framework consists of `data`, `method` and `metric` repositories (or "modules") that are connected via a `knowledge graph` from the `RENKU system`.

✓ The results could then be displayed in an `interactive dashboard` to be openly explored by any analyst looking for recommendations of tools.

✓ Any new data, method or metric can be added by the `community` to extend the benchmark.

Key features of the developed benchmarking framework:

- Periodic updates to provide the community with the latest recommendations
- Easy extendable thanks to templates for data, methods or metrics
- Follow the `FAIR principles` thanks to a Docker image system, an integration with Gitlab and the full `provenance` (tracking of inputs, commands and generated files)
- Use `independent (docker) environments` and flexibly connect and share modules within and between benchmarks.
- Use a `variety of programming languages` commonly used in bioinformatics: R, Python, Bash, Julia,...

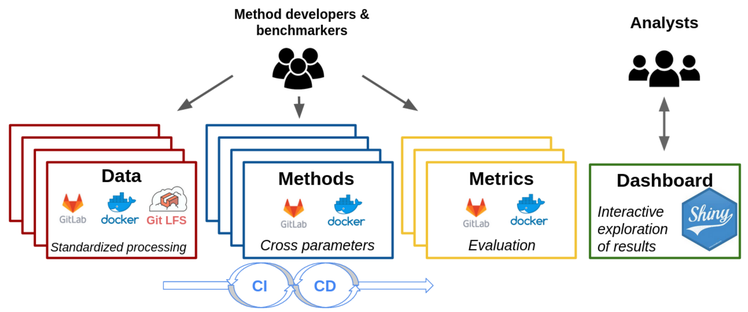


Figure 1: Overview of the proposed benchmarking framework on the RENKU platform. Each step of the benchmark consists of a set of repositories (a.k.a "modules") that perform a coordinated task (e.g. standardized data processing). Any new data, method or metric can be easily integrated in the framework by the scientific community to trigger a continuous delivery to the analysts with up-to-date recommendations. Each component of the framework is automatically tracked by the knowledge graph of RENKU and contain Docker images to provide fully reproducible results.

PROTOTYPE

Based on the above concept, we are currently building a prototype for community-based benchmarking of single-cell batch correction methods. Research in **single-cell RNA-seq (scRNA-seq)** is a perfect use case, where 900 tools have been developed in only a few years [1] and where the benchmarking efforts are often **not** `coordinated`, **not** `extendable` and **not** `reproducible`.

Our prototype consists of:

- Two datasets of 2370 genes x 3613 cells separated in 2 batches and 1401 genes x 13575 cells separated in 3 batches [2, 3].
- Common preprocessing consisting of normalization, highly-variable genes selection, dimensionality reduction.
- An integration using the MNN method [4].
- Evaluating batch-effect using the LISI metric [5] and cms score [3].
- Exploring the results using the interactive browser bettR [6].

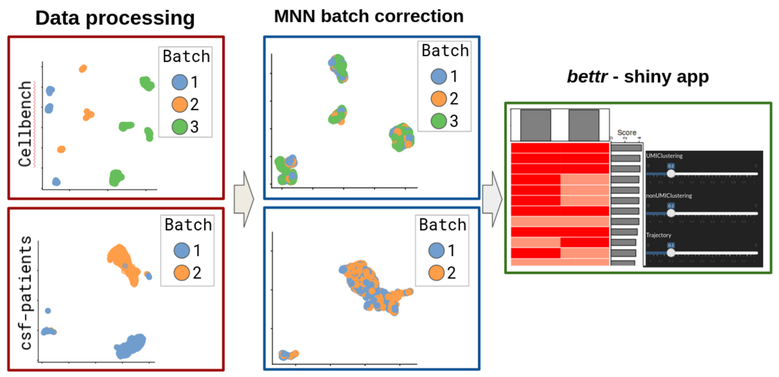


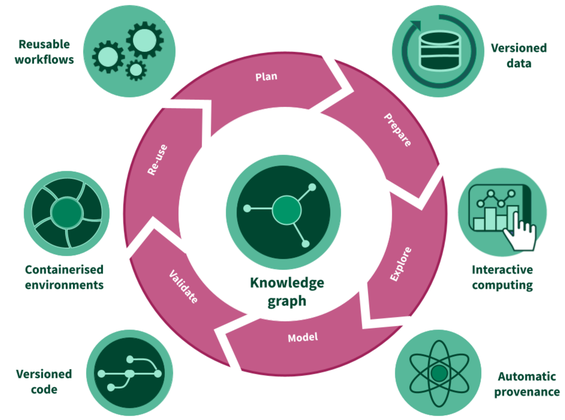
Figure 2: Example of the proposed framework applied to benchmark batch correction methods of scRNA-seq data. Datasets are uniformly processed and passed to a batch-correction method of a separated module. Results are displayed in a shiny app for an interactive exploration of the results. All modules are connected through the RENKU knowledge graph, which allows to track workflows from a set of repositories using different environments and programming languages.

renku

RENKU is an open and collaborative platform which provides a knowledge infrastructure for the entire research life cycle. The platform and its tools are built on top of a stack of open-source components and aims to make data science reproducible.

On **RENKU**:

- As RENKU is based on cloud computing fully interactive sessions can be accessed through the browser, with no local installation needed or through a CLI.
- Versioning and containers ensure precise and reproducible computational environments.
- Datasets and workflows are automatically tracked in a `knowledge graph`, which can be queried from within a project, a group of projects or even across deployments.
- Workflows can be re-run or updated automatically when inputs such as datasets or scripts change.
- CI/CD can be leveraged to automate cumbersome tasks, such as fetching results of a piece of analysis to integrate into a dashboard.



References

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