Versioning of data and code using Git

Introduction to Data Management Practices course

NBIS DM Team

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https://nbisweden.github.io/module-versioning-dm-practices/

Data storage and processing

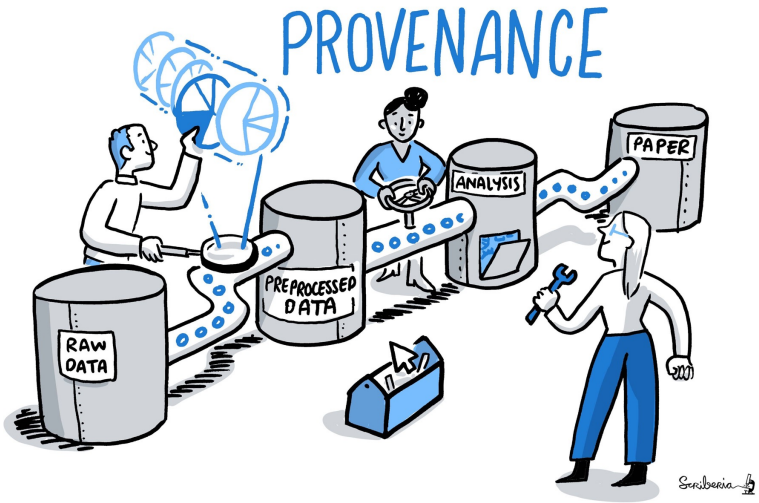
- Data has a life cycle

  Raw (experiment) data – produce, collect, license, get access, …

  Processed – generate, clean, aggregate, label, transform, analyse, …

  Archived – document, select, convert, package, submit, …

  Published – FAIRify, promote reuse, …
- Maintain data integrity and authenticity
- Plan a storage strategy
- Plan a backup and disaster recovery strategy



Data integrity and authenticity

- **Keep original (raw) versions** of data files, or keep documentation that allows the reconstruction of original files
- **Track the location of files** if they are stored in a variety of locations
- Establish **terms and conditions of data use** within the project team and beyond
- Keep a ‘master file’ of the data and take measures to preserve its authenticity
- Decide **how many and which versions to keep** for how long
- **Document changes** that were made in any version
- **Record relationships between items** where needed, for example between code and the data file it is run against

(UK Data Service, 2017a; Krejčí, 2014)

Local storage

- When working on different (local) workstations, e.g. laptop at home and the desktop in the office:
  - **always make sure that you are working on the most current version**, for example with the help of versioning software or guidelines
  - make sure that the most **current version is always backed up somewhere else**
- Only suitable as a primary storage for projects involving very few people
- Avoid if data will be moved back and forth between personal computers frequently

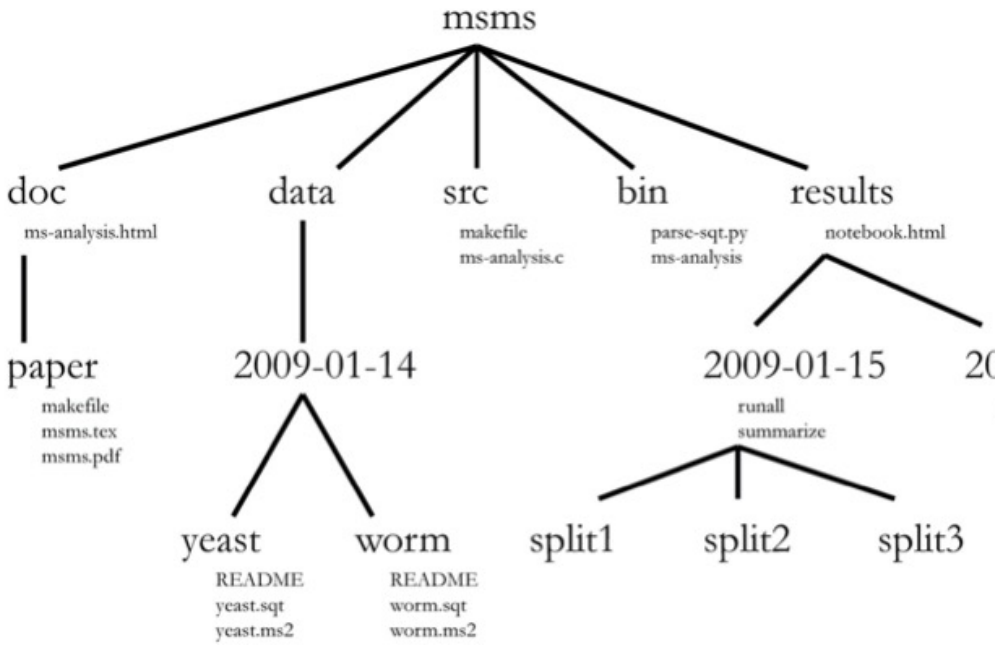
Cloud storage

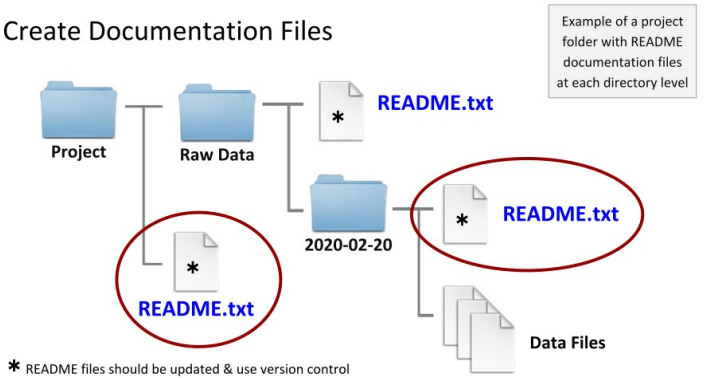
- Granting **shared, remote and easy access to data and other files** to all involved in the project
- **Read the terms of service**. Especially focus on rights to use content given to the service provider
- **Opt for European, national, or institutional** cloud services which store data in Europe if possible

- **Not your only storage and backup solution**
- **Not for unencrypted (sensitive) personal data**

Also be careful with passwords and other secrets!

Organising files and folders





Folder structure, docs and naming conventions are important!

Example from: Noble WS (2009) A Quick Guide to Organizing Computational Biology Projects. *PLoS Comput Biol* 5(7): e1000424. https://doi.org/10.1371/journal.pcbi.1000424

Fundamentals of versioning

- Snapshot projects and files

  Infinite undo, traceability, reproducibility

  Software, data, documents, scripts, manuscripts, …
- Copy–rename–describe

  Duplicate / rename files and folders

  Changes.txt
- Software assisted

  Projectplace, Google Docs, Sharepoint, Dropbox, but there is more…
- Collaborative versioning

  On your computer, on the web, from a single line of text to a complete project

https://stackoverflow.com/questions/1408450/why-should-i-use-version-control

Git is free and widely used

git --distributed-even-if-your-workflow-isnt

Search entire site...

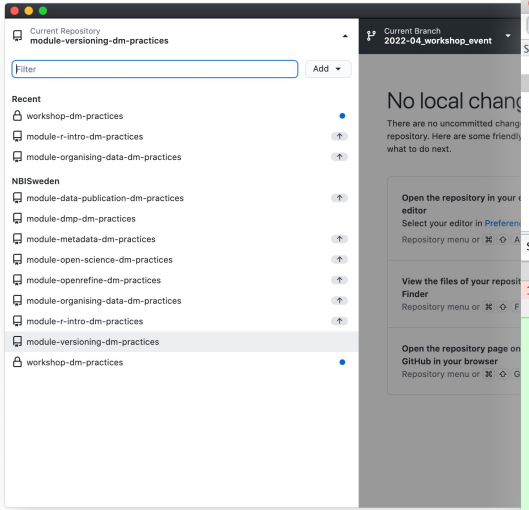
Shared — -zsh — 80×24

```
$ git
usage: git [--version] [--help] [-C <path>] [-c <name>=<value>]
           [--exec-path[=<path>]] [--html-path] [--man-path] [--info-path]
           [-p | --paginate | -P | --no-pager] [--no-replace-objects] [--bare]
           [--git-dir=<path>] [--work-tree=<path>] [--namespace=<name>]
           <command> [<args>]

These are common Git commands used in various situations:

start a working area (see also: git help tutorial)
   clone     Clone a repository into a new directory
   init      Create an empty Git repository or reinitialize an existing one

work on the current change (see also: git help everyday)
   add       Add file contents to the index
   mv        Move or rename a file, a directory, or a symlink
   restore   Restore working tree files
   rm        Remove files from the working tree and from the index

examine the history and state (see also: git help revisions)
   bisect    Use binary search to find the commit that introduced a bug
   diff      Show changes between commits, commit and working tree, etc
   grep      Print lines matching a pattern
   log       Show commit logs
```

https://git-scm.com/

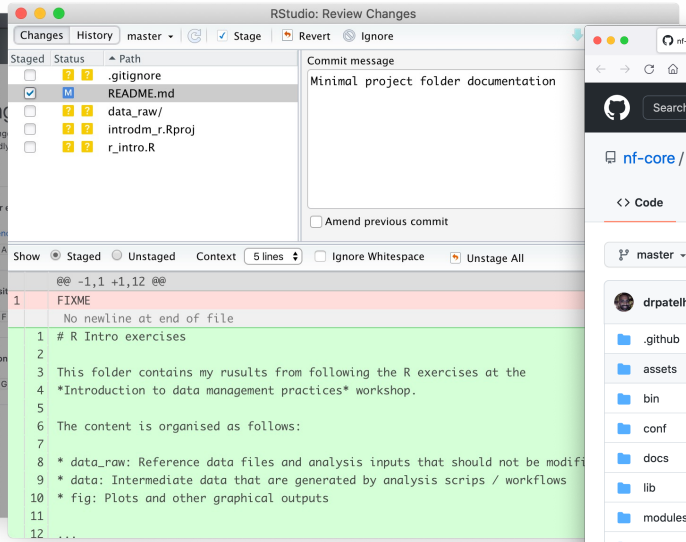
Alternative interfaces

GitHub Desktop



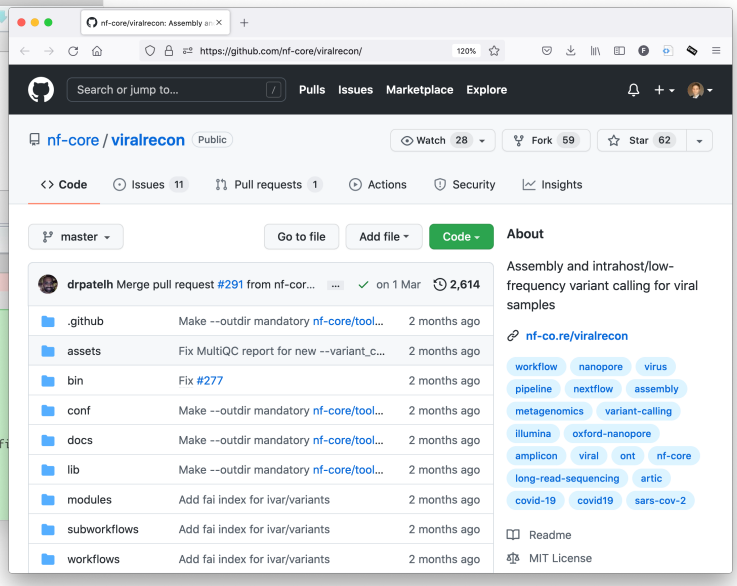
Keeping track of all your local copies in one place

RStudio



Managing changes for a specific file or project type

GitHub.com



Managing collaborations and access to shared versions of your files

Managing parallel versions

- Not a replacement for back-ups
- Write informative commit messages
- Establish conventions for using and naming branches
- Best out-of-the box experience with text-based files (lines)
- Use tags / hashes to reference a specific revision
- Use data archives to preserve important revisions, e.g., Zenodo or Figshare