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Reproducible workflows with R and GitHub

Ceres Barros

July 12th, 2023 2023 MacroBrum Birmingham UK

Outline

1. The importance of repeatability, reproducibility, reusability and transparency – R³T

2. General guidelines

3. A working example in R and GitHub

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Repeatability ≠ Reproducibility ≠ Reusability

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agreement of results obtained by the <u>same individual</u> using <u>same</u> methods

Repeatability ≠ Reproducibility ≠ Reusability

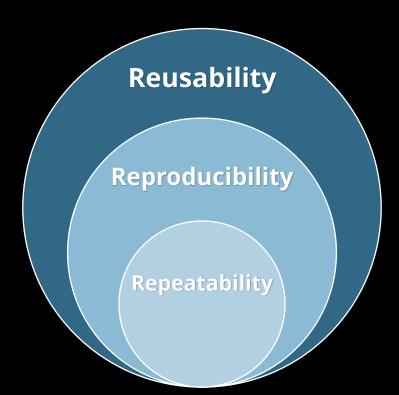
agreement of results obtained by the <u>same individual</u> using <u>same</u> methods

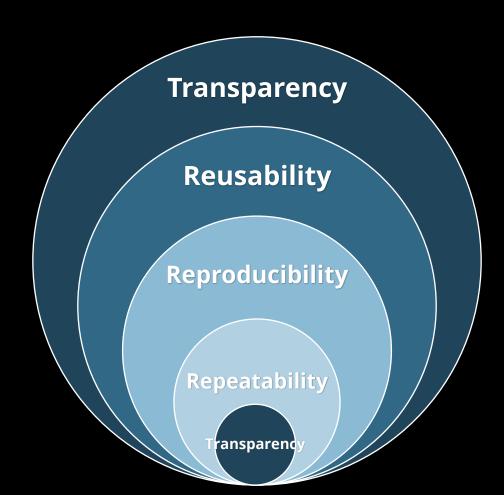
agreement of results obtained by two individuals/groups using same methods

Repeatability ≠ Reproducibility ≠ Reusability

agreement of results obtained by the <u>same individual</u> using <u>same</u> methods ability to <u>re-use the same methods</u> in a <u>different context</u> (e.g. new study area)

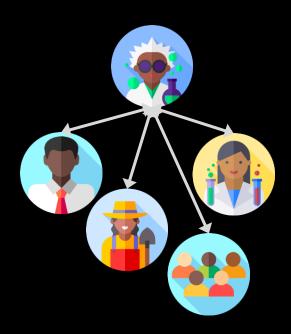
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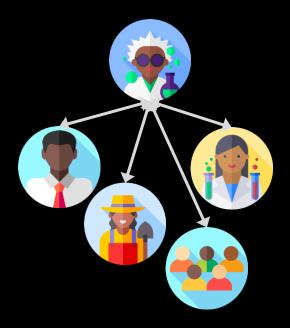


R³T analyses, What? models... data results **Transparency** forecasts, effect sizes, field, survey, publications, reports... experimental... Reusability Reproducibility Repeatability ransparend

Trust



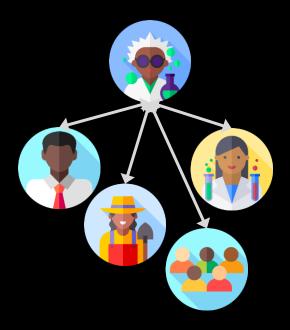
Trust



Benchmarking & meta-analyses



Trust



Benchmarking & meta-analyses



Building-on & improving analyses/models/workflows



Depends on **context**

- Project type and size
- Purpose
- Audience

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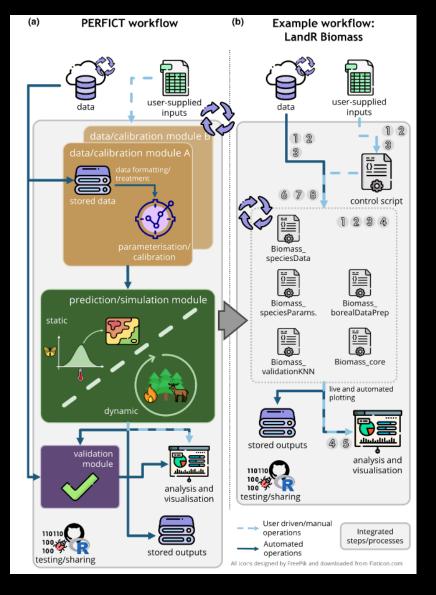
Data (both input and output) types Input and output management Suitable workflow Repeatability, reproducibility, reusability and transparency

How?

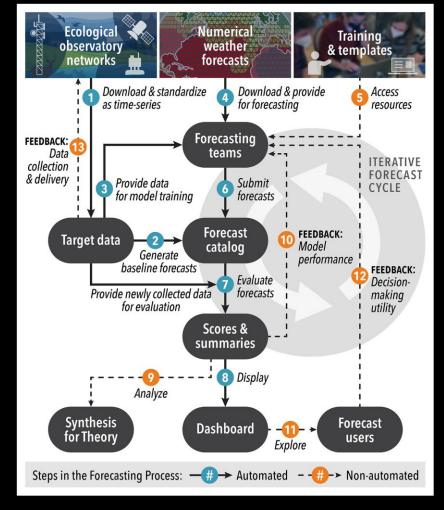
RESEARCH ARTICLE
Realising the Promise of Large Data and Complex Models

Empowering ecological modellers with a PERFICT workflow:
Seamlessly linking data, parameterisation, prediction, validation and visualisation

Ceres Barros¹® | Yong Luo¹,2,3® | Alex M. Chubaty⁴® | Ian M. S. Eddy²® |
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Steven G. Cumming⁶® | Eliot J. B. McIntire¹,2®



How?



Ecological (iterative) forecasting (continuous and integrated) workflow based on monitoring data

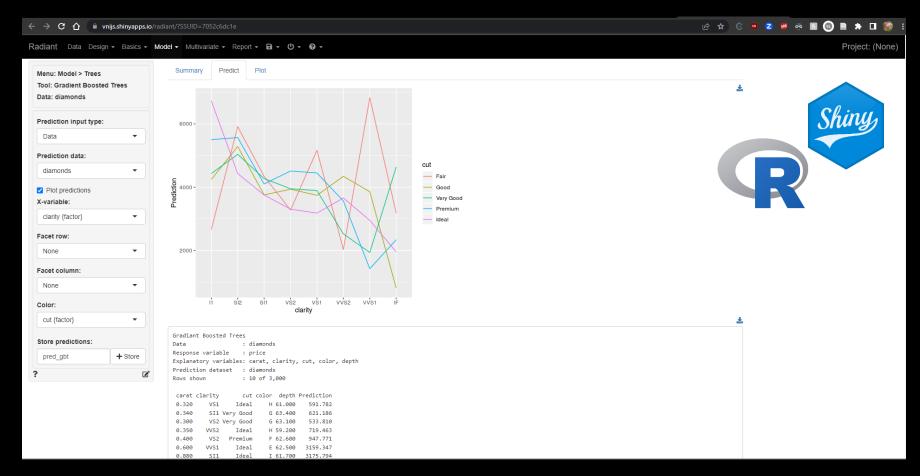
NEON Forecasting Challenge workflow Thomas et al. (2023)

Repeatability, reproducibility, reusability and transparency

How?

engagement/education point of view

R-shiny apps can be useful for education, engaging stakeholders/public and delivering an interactive product to end-users



https://vnijs.shinyapps.io/radiant/?SSUID=03eddd27f4

Most ecological research likely benefits from using a R³T approach, but the tools used to accomplish it can be varied



https://ceresbarros.github.io/reproducibleworkflowsWS

All steps, from processing *raw data* to producing *final figures* are integrated and automated*

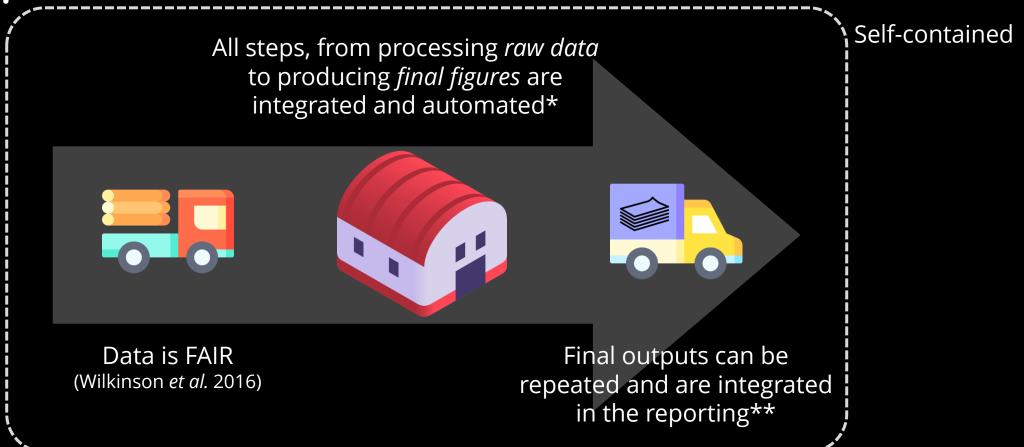


Data is FAIR (Wilkinson *et al.* 2016)

Final outputs can be repeated and are integrated in the reporting**

*as much as possible
**directly, or indirectly via links

How?



*as much as possible
**directly, or indirectly via links

Outline

1. The importance of repeatability, reproducibility, reusability and transparency – R3T

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General guidelines 1. Scripting/executing the workflow

1.1. Script, script, script

- **Goal**: no "secret handshakes" + record all steps of an analysis
- ALL steps this includes package/library installation/loading and sourcing data

DOComment your code



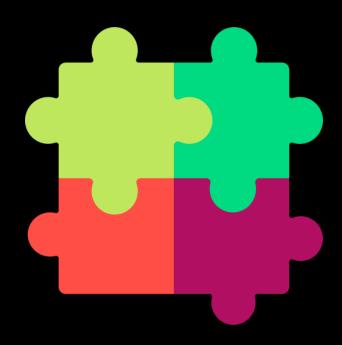
1. Scripting/executing the workflow

1.1. Script, script, script

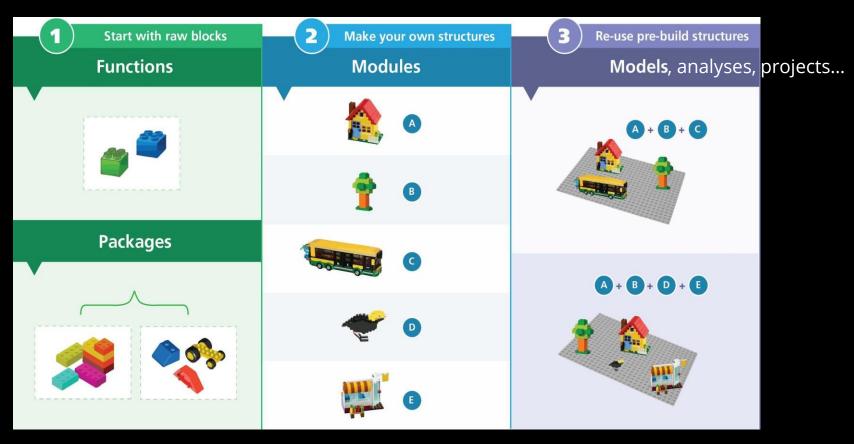
1.2. Minimise software/languages used

- **Goal**: increase workflow robustness fewer "moving parts", fewer "secret handshakes", fewer manual operations
- Interpreted languages (real-time user interaction) R, Julia, Python...
- Compiled languages (pre-compiled programs)
 C, C++, C#, Fortran,... <u>Do you really need this</u>?

- 1. Scripting/executing the workflow
- 1.1. Script, script, script
- 1.2. Minimise software/languages used
- 1.3. Modularise and "functionise" (!)
 - Goal: code organisation/readability; easier propagation of code updates/changes
 - Avoid loooooooong scripts
 - Break scripts into logical pieces
 - Encapsulate code into functions, especially when used multiple times/in multiple places
 - Consider "packaging" your functions.

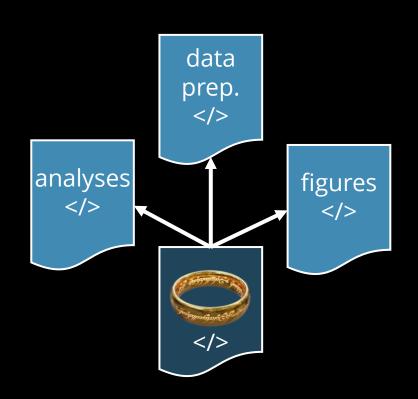


1. Scripting/executing the workflow



Functions and modules as key tools for R³T, but also for building integrated and continuous workflows
McIntire *et al.* (2022)

- 1. Scripting/executing the workflow
- 1.1. Script, script, script
- 1.2. Minimise software/languages used
- 1.3. Modularise and "functionise" (!)
- 1.4. Centralise workflow in a single script
 - Goal: no "secret handshakes" all scripts are utilised in correct way/sequence
 - Call/execute scripts/steps from central ("control") script



General guidelines 2. Project structure

2.1. Project-oriented workflows

- **Goal:** the entirely workflow can be re-run easily, and without changing code or files
- Choose a structure that is self-explanatory
- Relative paths vs. absolute paths
- Project-libraries

```
Legend: folder, file, comment
         10_data
                            discharge.tsv # built from get_discharge.R
                  raw
                            sites txt # site list emailed from collaborators
                            README.md # notes on email date, source for sites.txt
                  src
                           get discharge.R # downloads data from web
         15_process_climate
                           climate_2.tsv, climate 2.st
                  out
                           process climate.R
         20 clean
                            calibration data.Rds
                            estimation_data.Rds
                            combine CQ.R
         40 forecast
                            model_parameters.yml # no need for job dir when models are reliable, simple
                           model_02.Rds
                            model 68.Rds
                            flux model.R # makefile runs this 68 times
                           helpers-flux_model.R
         60 visualize
                            fig_annual_flux_forecast.png
                            plot_fluxes.R
         90 model archive
                           metadata_parent.yml
                           create_metadata.R, package_models.R, post_models.R # creating metadata for forecasts
         95 report
                           limnology-and-oceanography.csl, style.docx # journal-specific formatting
                           map.png, droughts.png, regression.png
                           model stats.Rmd
                           manuscript.Rmd, supplement 1.Rmd
                           manuscript.docx, supplement_1.docx
                  Makefile, 1_dat_spatial.mak, 1_dat_timeseries.mak, 2_process_climate.mak, ..., 9_report.mak
         explore
                  170802_check_boundaries
                  170807_compare_climate_data_sources
                                                                 [...files...] # Analyses to determine which drivers to use
                  download helpers.R # functions for downloading data from web
                  process_helpers.R
```

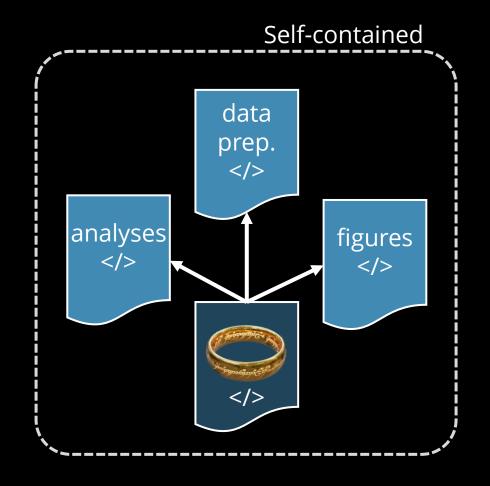
Source: https://ecoforecast.org/reproducible-forecasting-workflows/

General guidelines 2. Project structure

- 2.1. Project-oriented workflows
- 2.2. Self-contained workflows
 - Goal: ensure reproducibility
 - E.g. RStudio-projects
 - Containerisation encapsulates the whole system (even OS) – e.g. Docker



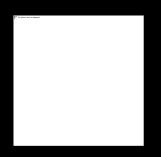




General guidelines 3. Project management

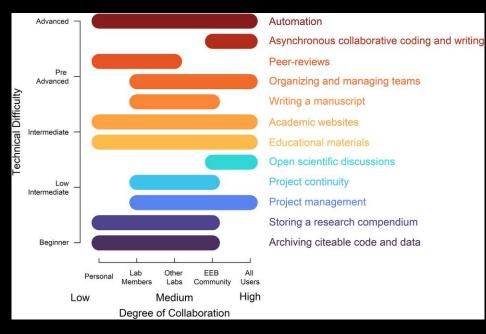
3.1. Version control

- **Goal:** <u>change tracking</u> in code/files + continuous and <u>collaborative</u> development
- Keeps a formal record of all changes
- Allows recovering old versions
- Allows keeping/working on multiple versions of the same code/project
- E.g. Git, CVS, SVN, ...



We'll come back to this!





GitHub is a multifaceted tool that can be appropriate to manage, track and collaborate on projects for various purposes and at various levels of complexity.

(Braga et al. 2023)

General guidelines 3. Project management

3.1. Version control

3.2. Integrated testing

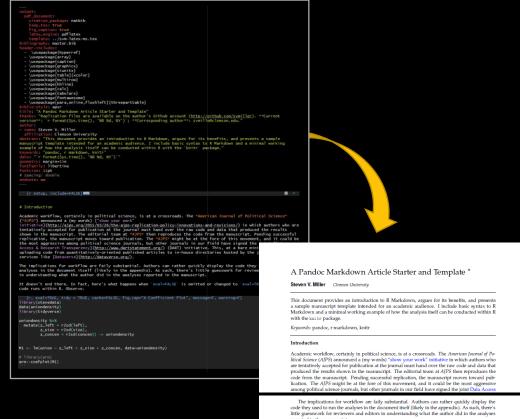
- Goal: enhance code robustness and longevity
- Not always necessary, but always a good idea;)
- Integration tests vs unit tests vs assertions
- Manual vs automated execution
- E.g.
 - testthat in R (unit tests)
 - simple code/object checks (assertions)
 - GitHub Actions and Travis CI for automated testing

 all types.

General guidelines 4. Literate programming

4.1. Integrate code and reporting/publication

- Goal: establishing explicit links between report/publication, data and analyses
- Integrates code and text in a single file
- Enhances transparency/reproducibility of reported outputs.
- E.g.
 - RMarkdown, Quarto static or interactive; multiple languages in a single file
 - Jupyter interactive; single language at a time (Julia, R or Python)

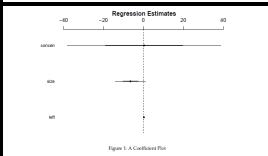


little guessorofs for reviewers and editors in understanding what the author did in the analyses reported in the manuscript.

It doesn't end there. In fact, here's what happens when eval=FALSE is omitted or changed to eval=FBLE. Now, the code runs within R. Observe.

library(stevemisc)
data(unicodemaity)

Mi < ln(unico "left + size + concen, data = unicodensity)
library(stevemisc)
coseplo(mi)



Outline

1. The importance of repeatability, reproducibility, reusability and transparency – R3T

2. General guidelines

3. A working example in R + RStudio + GitHub

Shall we try this?

What we will cover:

Project structure and management

- Version control using GitHub and GitKraken
- Self-contained workflows using R and Rstudio

Scripting/executing the workflow

- Script, script, script
- Modularise and "functionise" (!)
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The order is variable; it depends on the stage of the project and your own preference

Tools used in each step can also vary







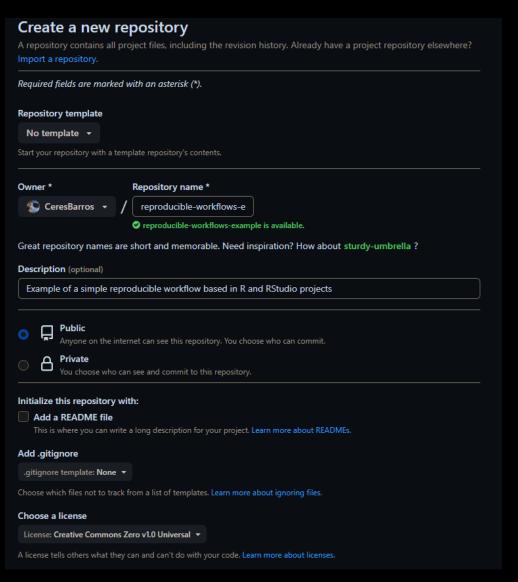
*you can do this in...





Assuming you already have an account on GitHub.com...

Create a repo

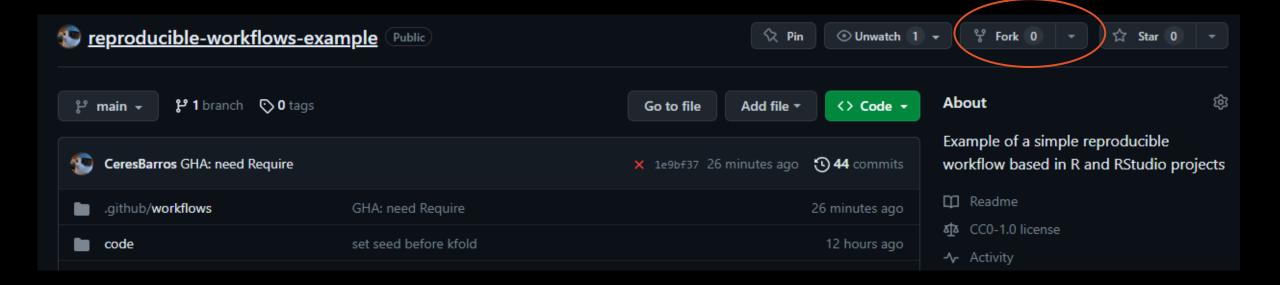




1. Create a repository for your project

Assuming you already have an account on GitHub.com...

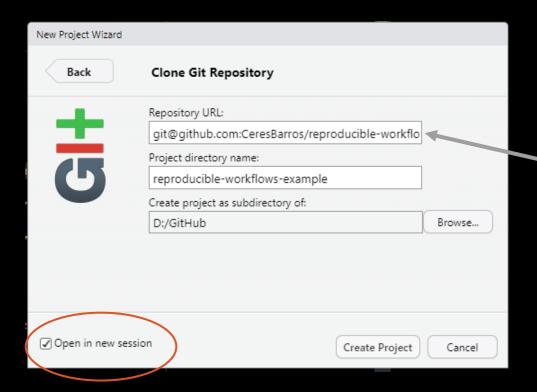
Or fork someone else's



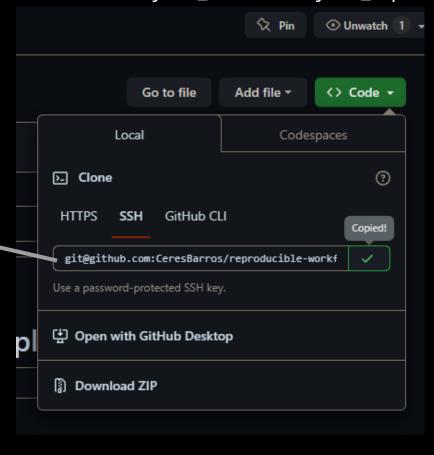
2. Create a self-contained project



In RStudio, go to File > New Project... > Version Control > Git



Get repo URL from
GitHub.com/your_username/your_repo

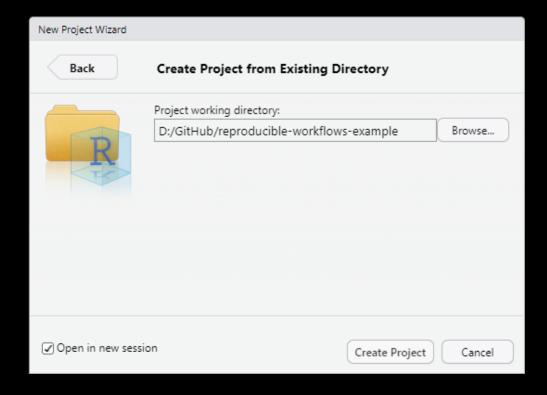


2. Create a self-contained project



If you already have a project folder (e.g. created by GitKraken, or from an existing project):

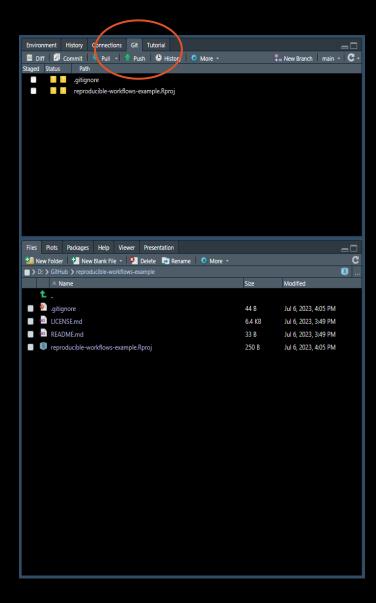
In RStudio, go to File > Existing Directory



2. Create a self-contained project

You can now manage your Git repo from RStudio

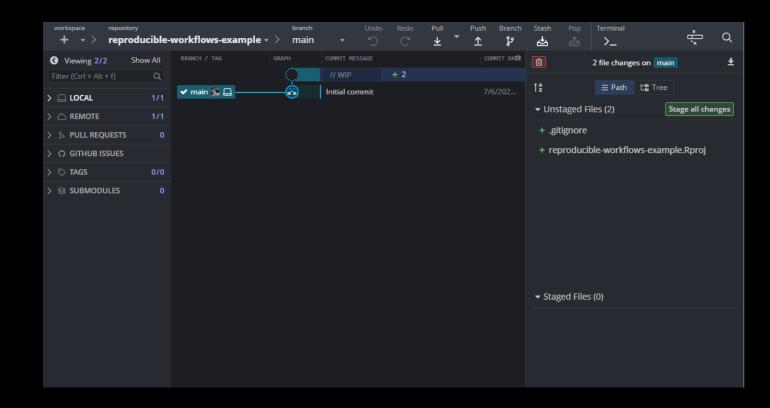






2. Create a project

You can now manage your Git repo from RStudio, GitKraken





2. Create a project



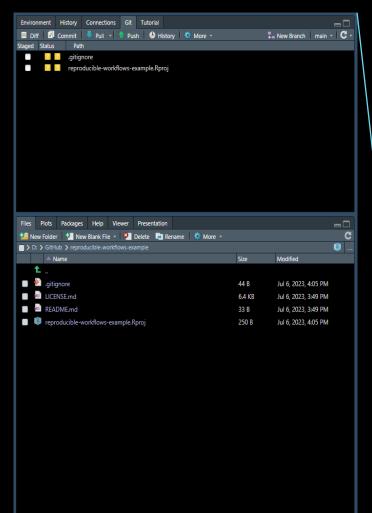
You can now manage your Git repo from RStudio, GitKraken, or even the command-line (e.g., git bash for Windows)

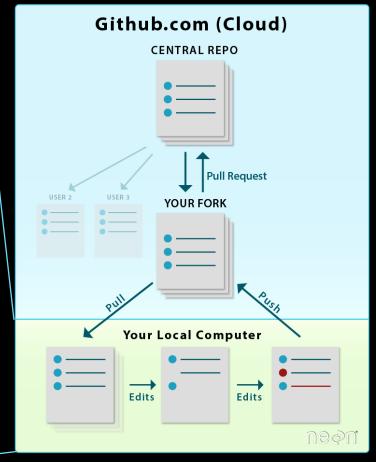


- ✓ keep master/main branch clean; develop in other branches
- ✓ small, incremental, commits
- ✓ .gitignore sensitive and large files – think about data storage
- ✓ pull first, push after



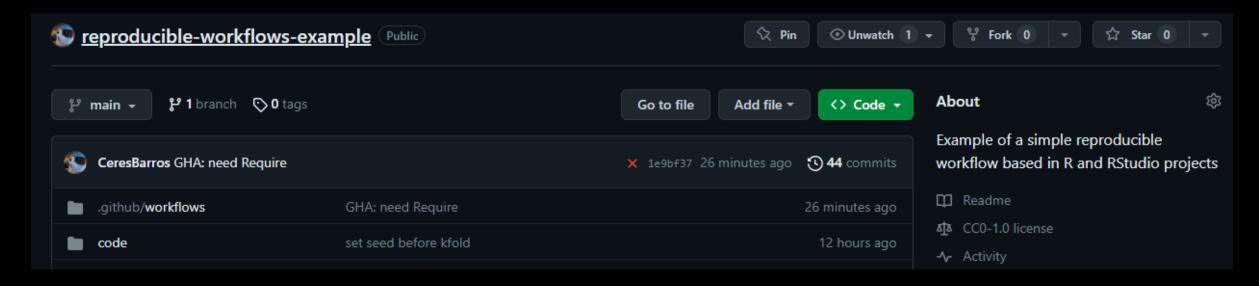






https://ceresbarros.github.io/reproducibleworkflowsWS

3. Example of a reproducible workflow in R, RStudio and GitHub



https://github.com/CeresBarros/reproducible-workflows-example

Useful resources

Peer-reviewed:

- Barros, C., Luo, Y., Chubaty, A.M., Eddy, I.M.S., Micheletti, T., Boisvenue, C., et al. (2023). Empowering ecological modellers with a PERFICT workflow: Seamlessly linking data, parameterisation, prediction, validation and visualisation. Methods Ecol Evol, 14, 173–188.
- Braga, P.H.P., Hébert, K., Hudgins, E.J., Scott, E.R., Edwards, B.P.M., Sánchez Reyes, L.L., et al. (2023). Not just for programmers: How GitHub can accelerate collaborative and reproducible research in ecology and evolution. Methods in Ecology and Evolution, 14, 1364–1380.
- Brousil, M.R., Filazzola, A., Meyer, M.F., Sharma, S. & Hampton, S.E. (2023). Improving ecological data science with workflow management software. *Methods in Ecology and Evolution*, 14, 1381–1388.
- Ellison, A.M. (2010). Repeatability and transparency in ecological research. *Ecology*, 91, 2536–2539.
- McIntire, E.J.B., Chubaty, A., Cumming, S., Andison, D., Barros, C., Boisvenue, C., et al. (2022). PERFICT: a Re-imagined Foundation for Predictive Ecology. Ecology Letters.
- Thomas, R.Q., Boettiger, C., Carey, C.C., Dietze, M.C., Johnson, L.R., Kenney, M.A., et al. (2023). The NEON Ecological Forecasting Challenge. Frontiers in Ecology and the Environment, 21, 112–113.
- Wilkinson, M.D., Dumontier, M., Aalbersberg, Ij.J., Appleton, G., Axton, M., Baak, A., et al. (2016). The FAIR Guiding Principles for scientific data management and stewardship. Sci Data, 3, 160018.

Reproducible workflows:

- Ecological Forecasting Initiative. (2020). Reproducible Forecasting Workflows. Ecological Forecasting Initiative. Available at: https://ecoforecast.org/reproducible-forecasting-workflows/. Last accessed 6 July 2023.
- The Practice of Reproducible Research (http://www.practicereproducibleresearch.org/)
- R Markdown: The Definite Guide (https://bookdown.org/yihui/rmarkdown/)
- R Markdown cheat sheets (https://www.rstudio.com/wp-content/uploads/2015/02/rmarkdown-cheatsheet.pdf)
- GitHub Quickstart (https://docs.github.com/en/get-started/quickstart/hello-world)

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RStudio

R

GitKraken

Git

References

GIFs/Images:

- https://www.reddit.com/r/gifs/comments/4a3exq/cat_typing_a_document_on_laptop/
- https://en.wikipedia.org/wiki/One_Ring#/media/File:One_Ring_Blender_Render.png
- All icons designed by Freepik and downloaded from Flaticon.com

Literature

- Barros, C., Luo, Y., Chubaty, A.M., Eddy, I.M.S., Micheletti, T., Boisvenue, C., et al. (2023). Empowering ecological modellers with a PERFICT workflow: Seamlessly linking data, parameterisation, prediction, validation and visualisation. *Methods Ecol Evol*, 14, 173–188.
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- Ecological Forecasting Initiative. (2020). Reproducible Forecasting Workflows. Ecological Forecasting Initiative. Available at: https://ecoforecast.org/reproducible-forecasting-workflows/. Last accessed 6 July 2023.
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- Thomas, R.Q., Boettiger, C., Carey, C.C., Dietze, M.C., Johnson, L.R., Kenney, M.A., et al. (2023). The NEON Ecological Forecasting Challenge. Frontiers in Ecology and the Environment, 21, 112–113.
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