FAIR_bioinfo : Open Science and FAIR principles in a bioinformatics project

How to make a bioinformatics project more reproducible

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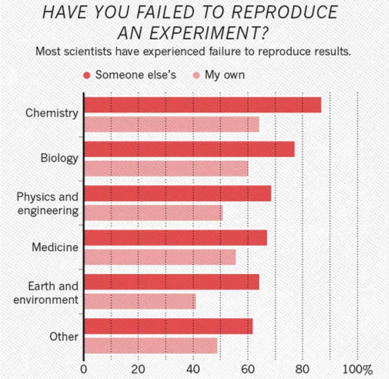
June 2021

Reproducibility

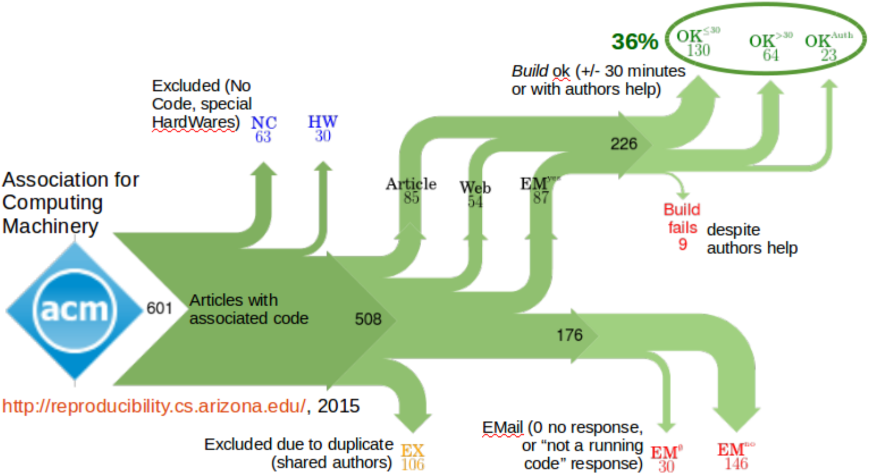
A reproducibility problem, Biology

70% of the analyses in Experimental Biology are not reproducible



Monya Baker, 1,500 scientists lift the lid on reproducibility, *Nature*, 2016

A reproducibility problem, Computer Sciences


36%
$\text{OK}^{\leq 30}$ 130
$\text{OK}^{>30}$ 64
OK^{Auth} 23
Build ok (+/- 30 minutes or with authors help)
Excluded (No Code, special HardWares)
NC 63
HW 30
Association for Computing Machinery
acm
601
Articles with associated code
508
Article 85
Web 54
EM^{yes} 87
226
Build fails 9
despite authors help
176
Excluded due to duplicate (shared authors)
EX 106
EMail (0 no response, or "not a running code" response)
EM^{0} 30
EM^{no} 146

http://reproducibility.cs.arizona.edu/, 2015

A reproducibility problem, Bioinformatics

TEN YEARS REPRODUCIBILITY CHALLENGE
RESCIENCE SPECIAL ISSUE
FREE TO READ - FREE TO PUBLISH
Workshop
June 22, 2020
BORDEAUX
Would you dare to run the code from your past self ?
(the one that does not answer mail)
SUBMISSION DEADLINE 01/04/2020
http://rescience.github.io/ten-years
In association with Inria, CNRS, Software Heritage, ReScience, Comité pour la Science Ouverte, URFIST Bordeaux & Mission de la pédagogie et du numérique pour l'enseignement supérieur.
Contact: nicolas.rougier@inria.fr

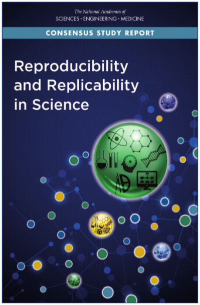
Ten-Year Reproducibility Challenge, Konrad Hinsen
Can your 2009 code still run?
special issue of ReScience and result comments in *Nature*

Who's never wanted to take over a protocol, a pipeline, or a tool without running into it?

- unable to install tools: not compatible OS, not availability of dependencies
- tool update ⇒ codes unusable: python 2 vs. 3, change of function arguments (R)
- inability to reproduce the results of computational analysis: package versions, IDE: stable version of the language different according to the OS (Rstudio)

Reproducibility in science

Reproducible research, Repeatability, Replicability, Reproducibility, Replication: overlapping semantics ⇒ a plethora of definitions![a]


The National Academies of
SCIENCES · ENGINEERING · MEDICINE
CONSENSUS STUDY REPORT
Reproducibility and Replicability in Science

National Academies of Sciences, Engineering, and Medicine (2019).[b]

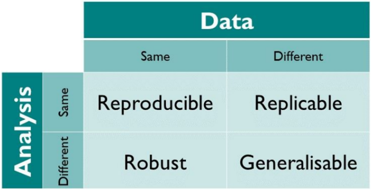
ACM definition (2016):

Repeatability Same team, same exp. setup

Replicability Different team, same exp. setup

Reproducibility Different team, different exp. setup

Whitaker's matrix of reproducibility (2017):[c]



		Data	
		Same	Different
Analysis	Same	Reproducible	Replicable
	Different	Robust	Generalisable

a: https://www.researchgate.net/publication/323118701_Terminologies_for_Reproducible_Research

b: National Academies of Sciences, Engineering, and Medicine. 2019. Washington DC. The National Academies Press, https://www.nap.edu/read/25303/chapter/1

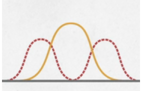
c: https://doi.org/10.6084/m9.figshare.5443201.v1, Slide number 7

FAIR_bionfo’s finding

Depends on the object of study x
what needs to be ”memorized” to replay the experience:

Raw Data
FAIR data principles & Data Management Plans

→



Statistical or bioinformatic analysis
Codes - parameters - workflows

→

Validation
Publication: thesis, article, report, etc

How to gain in reproductibility?

Focus on codes, parameters, and workflows used throughout the analysis process

Monya Baker, 1,500 scientists lift the lid on reproducibility, *Nature*, 2016

A solution

Divert FAIR data principles towards processes

Findable

Third party tools used = ref. in their field

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Easy to find analysis protocol (Github pages)

Accessible

Available codes (Github, dockerhub)

.

Third party open source tools

Interoperable

Cooperation of tools (snakemake, docker) as well as locally than on servers (cloud or cluster)

Reusable

Protocol replayable (snakemake) identically (Rshiny) in a virtual environment (docker)

Promote learning

FAIR bioinfo

Our objective

FAIR raw data

$+$

FAIR scripts

$=$

FAIR processed data

Course

Take your first steps with several companion tools to gain in reproducibility

Example based

Just the beginning of an NGS analysis
A full analysis is given as bonus (The NGS analysis is simply used as an example and not explained)

Ressources

- awesome a curated list of reproducible research case studies, projects, tutorials, and media
- The Role of Metadata in Reproducible Computational Research
- Towards reproducible computational biology
- A very similar sweden courses with git, conda, snakemake, jupyter, r-markdown, docker, singularity