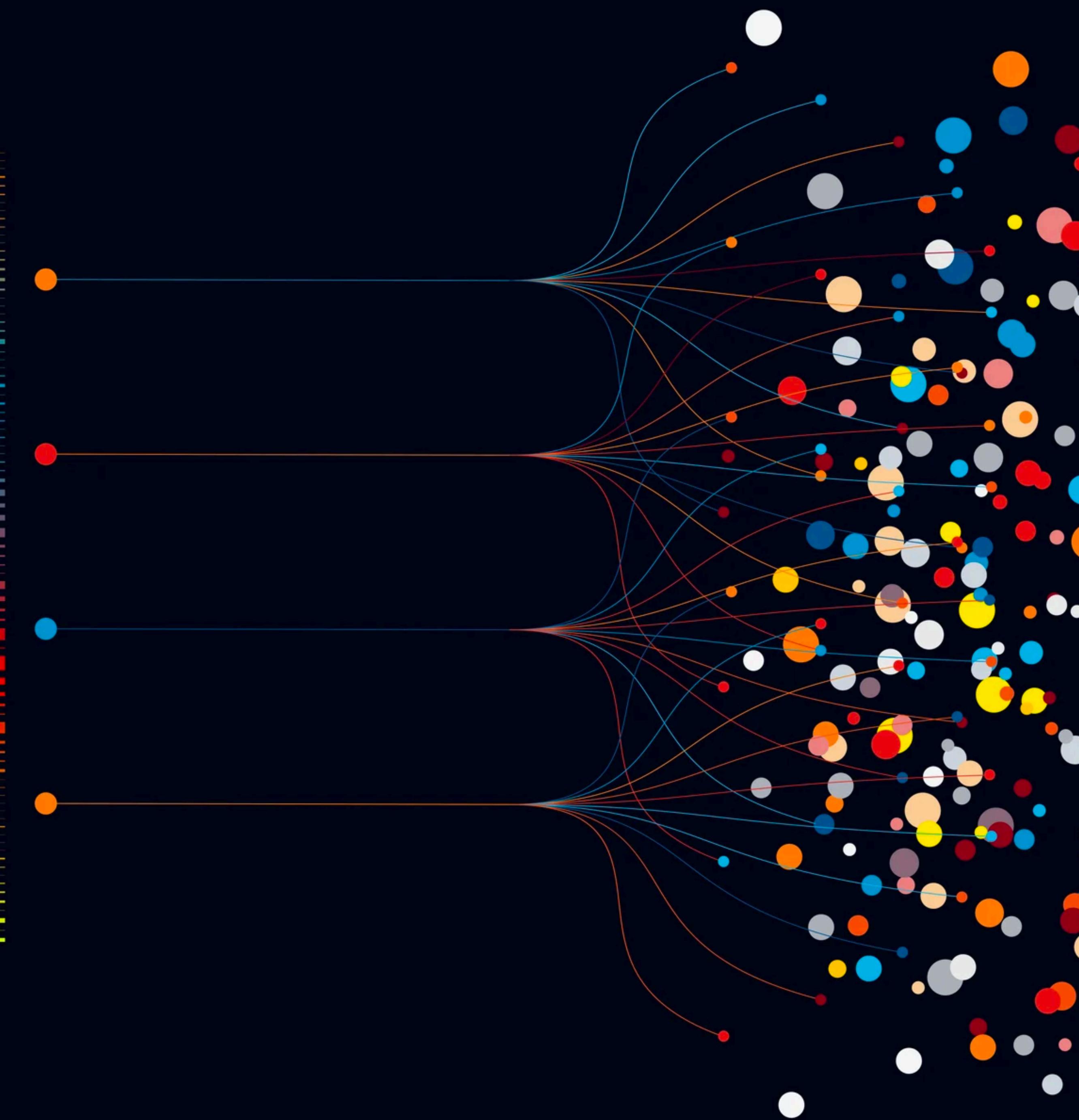


Module 4 - day 1

Reproducible data analysis and workflows

Antonio Fernandez-Guerra
antonio@metagenomics.eu

Fundamentals Data Analysis | May 27 2024 - Copenhagen

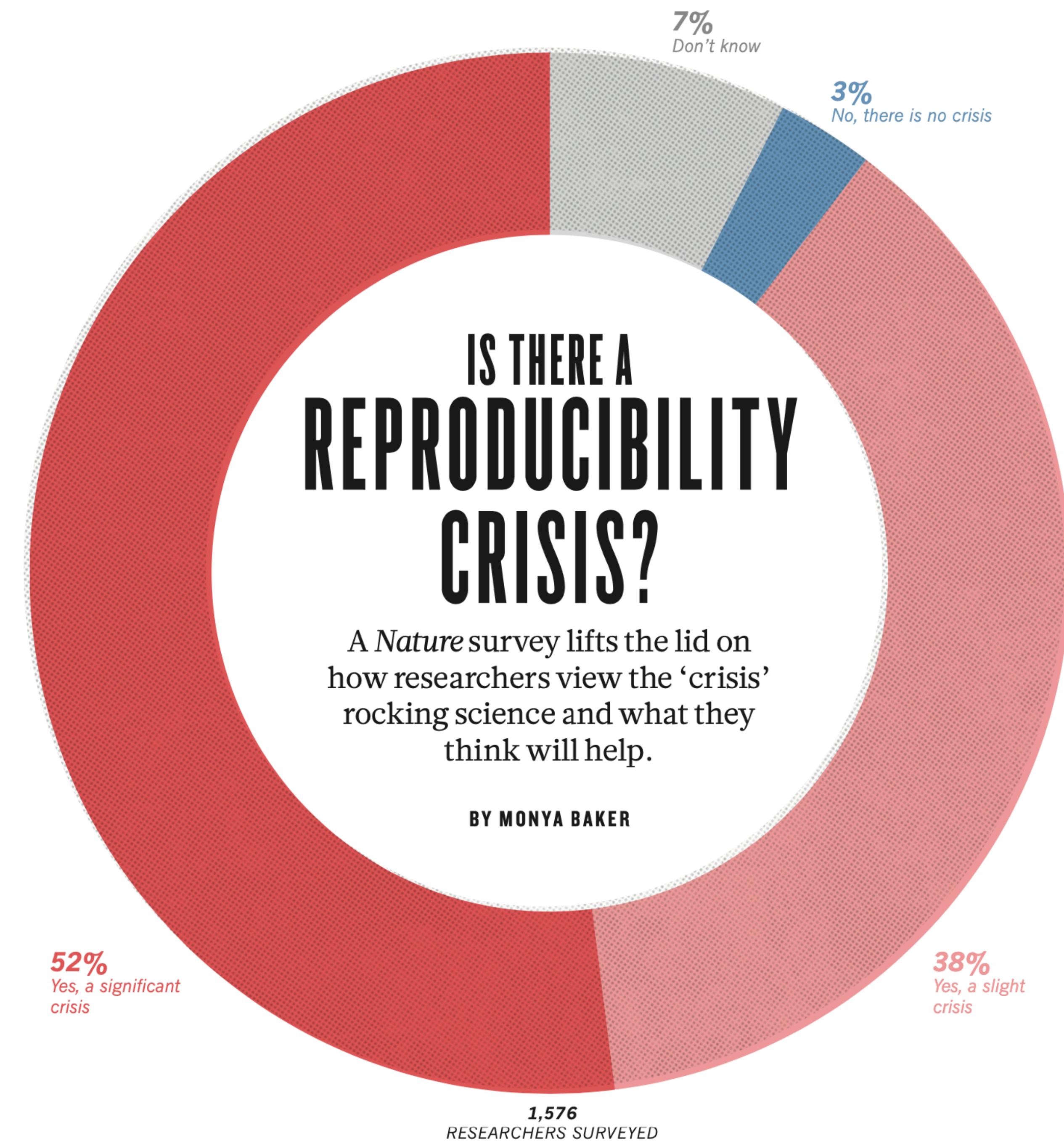


Objectives

- 1. The Reproducibility Crisis in Science**
Understanding the Problem and Finding Solutions
- 2. Ensuring Reproducibility in Scientific Research**
Best Practices and Strategies
- 3. Setting Up a Computational Research Project**
Tips and Techniques for Success
- 4. Git Version Control for Scientific Computing**
Managing Code and Collaborating Effectively
- 5. Introduction to BASH Scripting**
Automating Tasks and Streamlining Workflows

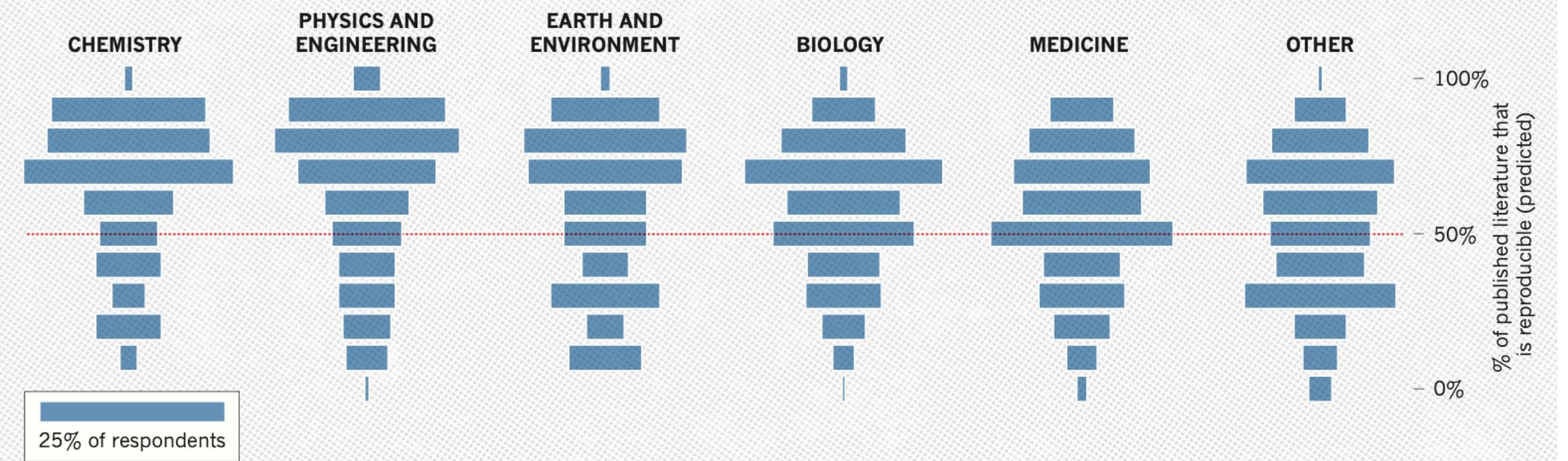
The Reproducibility Crisis in Science

Understanding the Problem and Finding Solutions



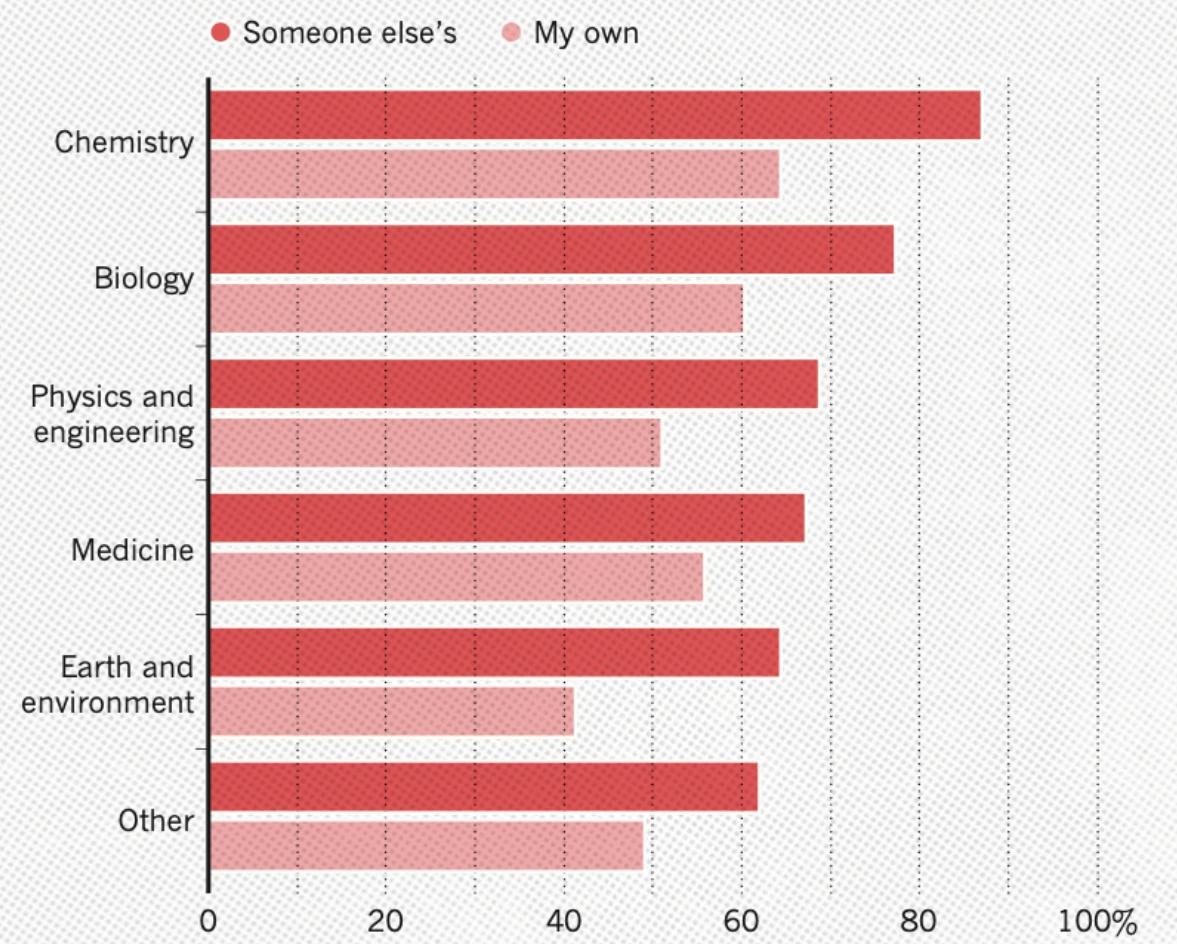
HOW MUCH PUBLISHED WORK IN YOUR FIELD IS REPRODUCIBLE?

Physicists and chemists were most confident in the literature.



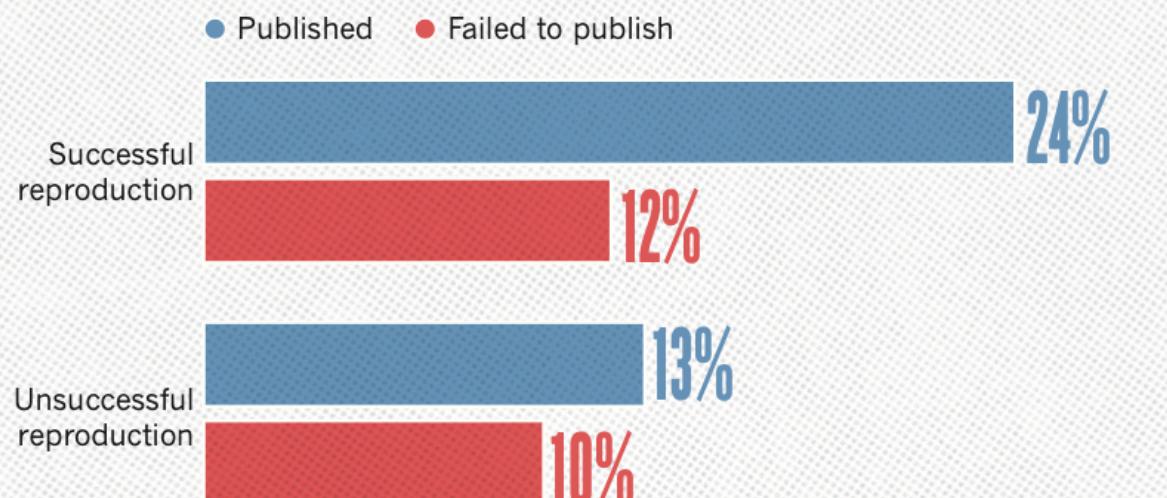
HAVE YOU FAILED TO REPRODUCE AN EXPERIMENT?

Most scientists have experienced failure to reproduce results.



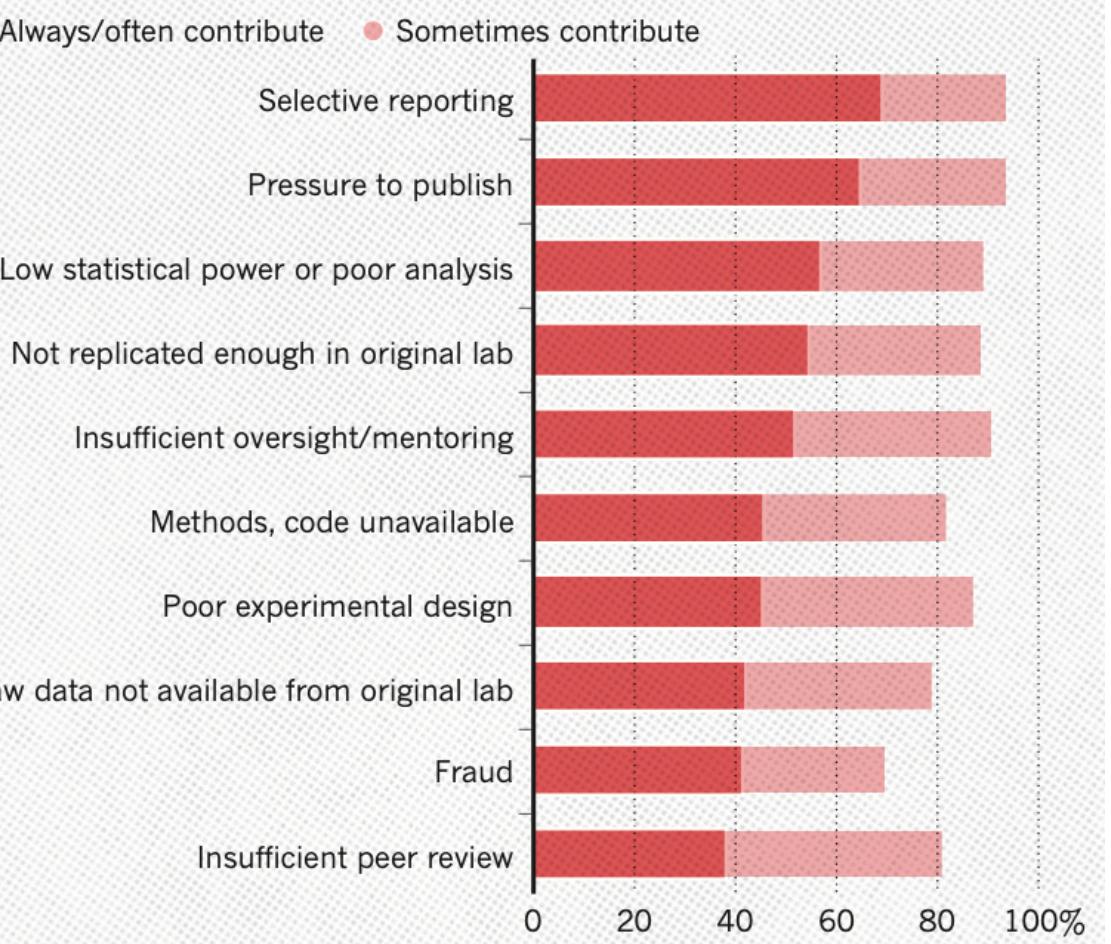
HAVE YOU EVER TRIED TO PUBLISH A REPRODUCTION ATTEMPT?

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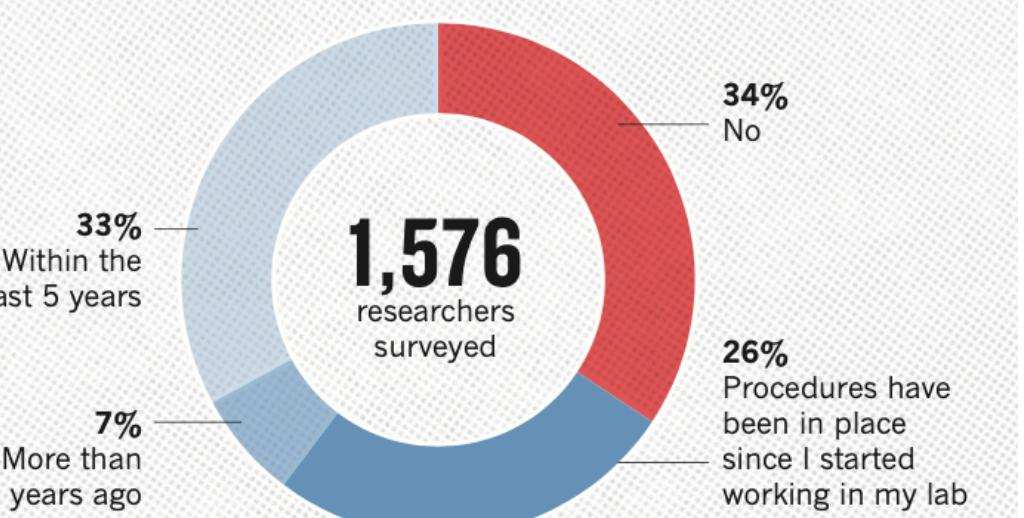
WHAT FACTORS CONTRIBUTE TO IRREPRODUCIBLE RESEARCH?

Many top-rated factors relate to intense competition and time pressure.



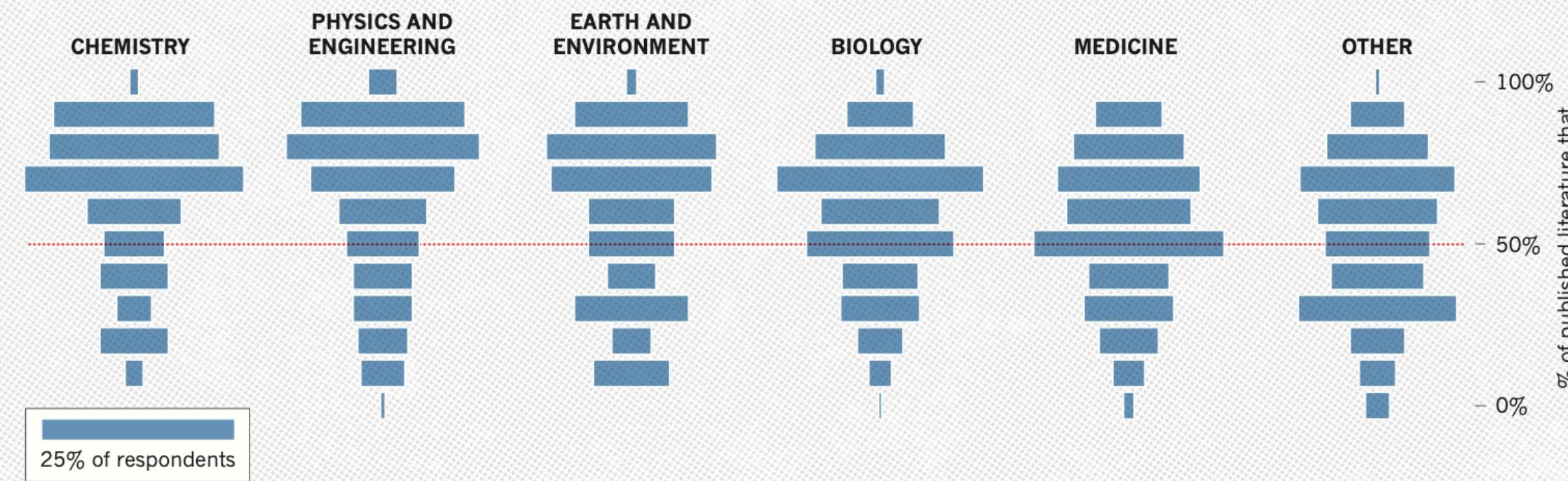
HAVE YOU ESTABLISHED PROCEDURES FOR REPRODUCIBILITY?

Among the most popular strategies was having different lab members redo experiments.



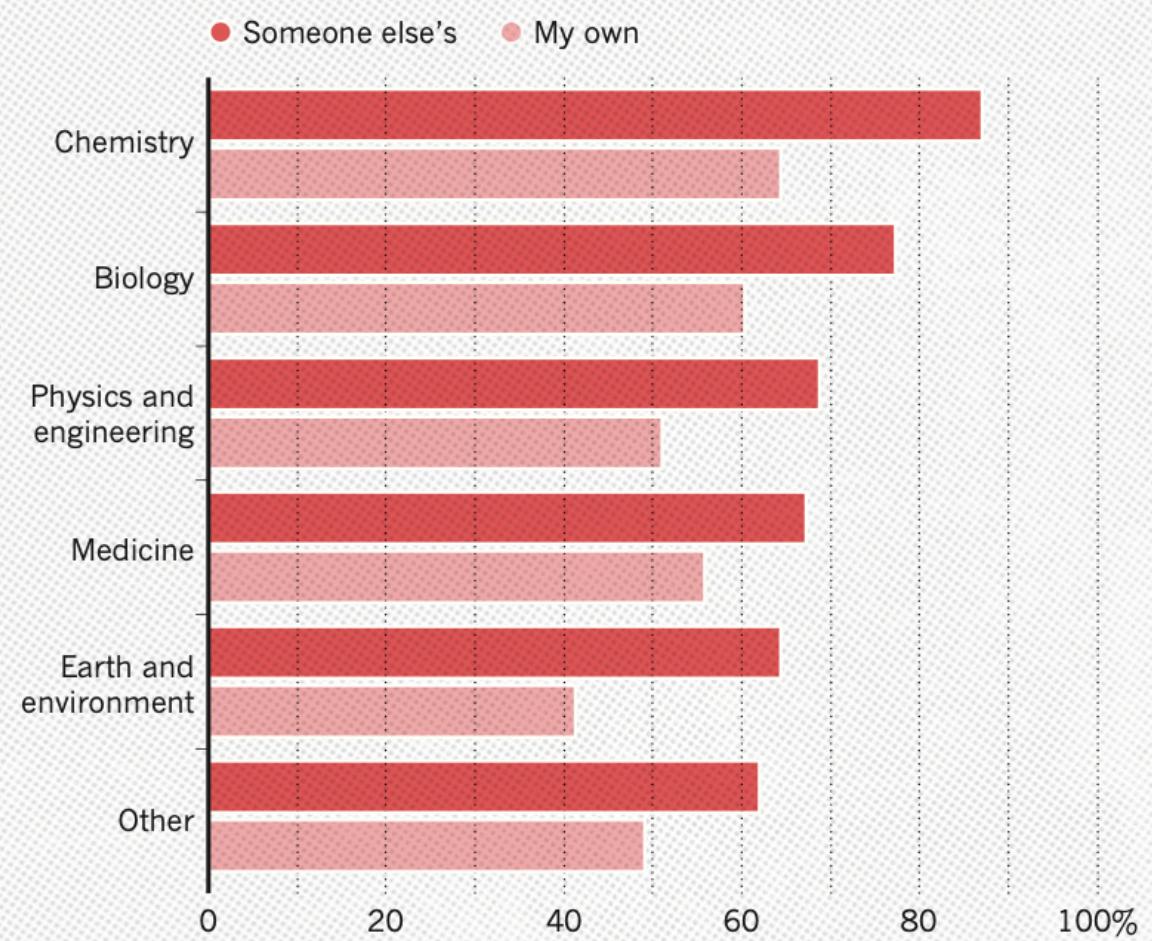
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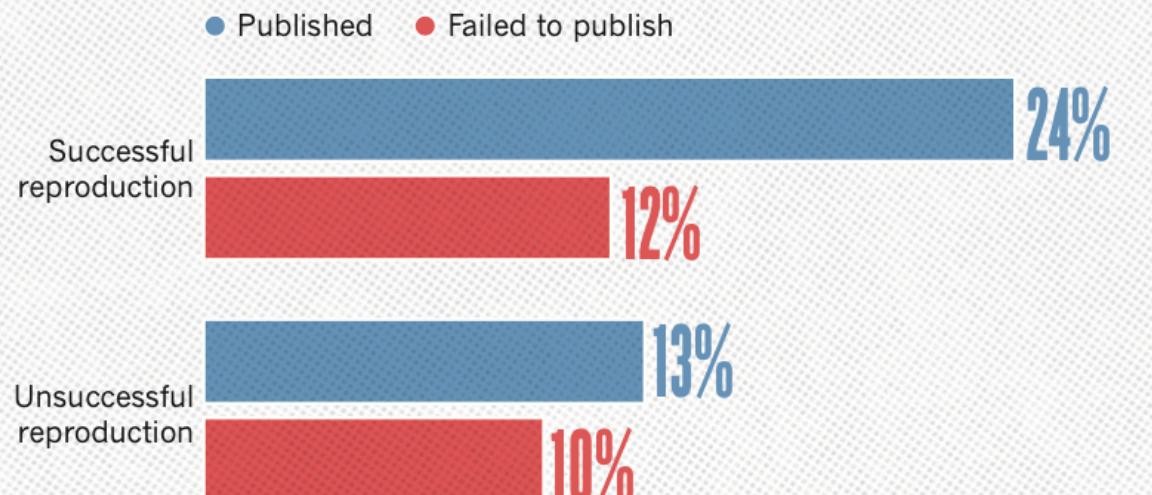
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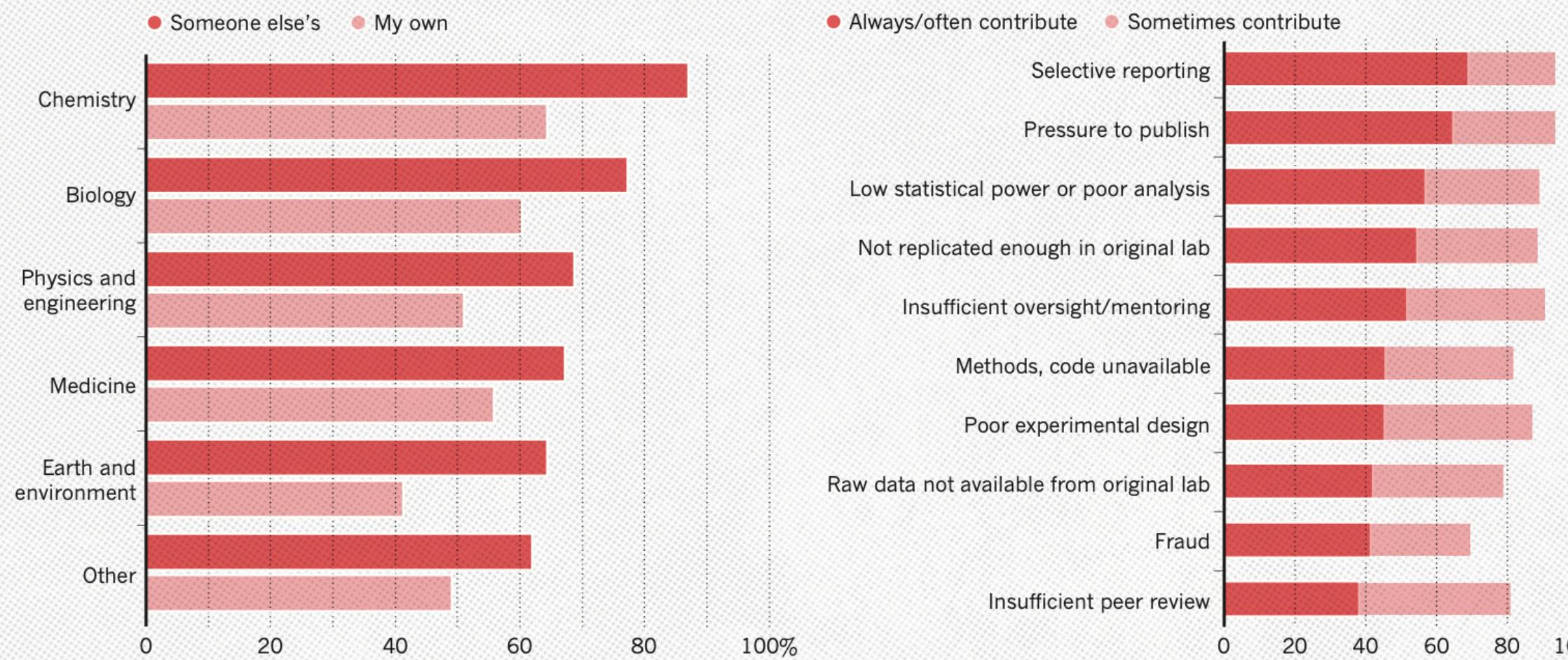
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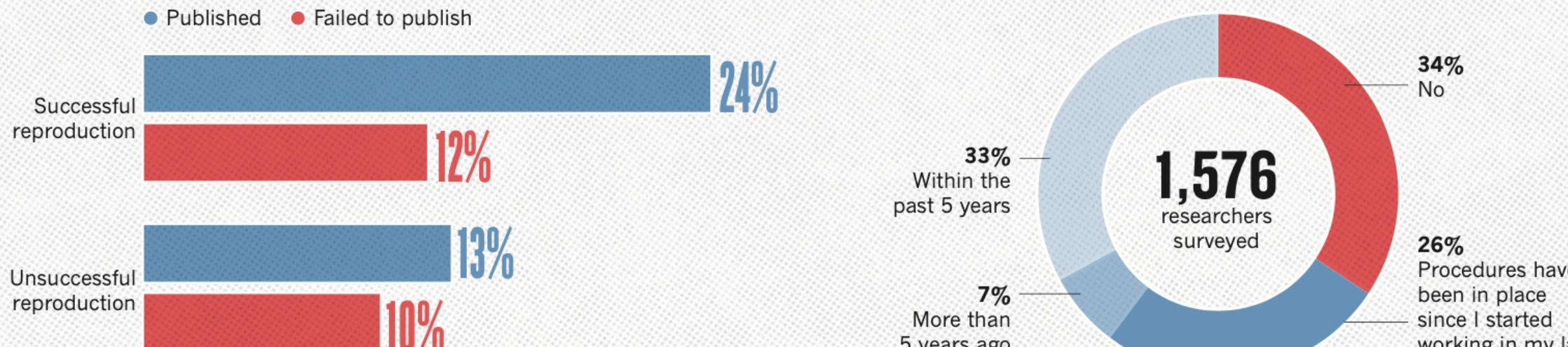
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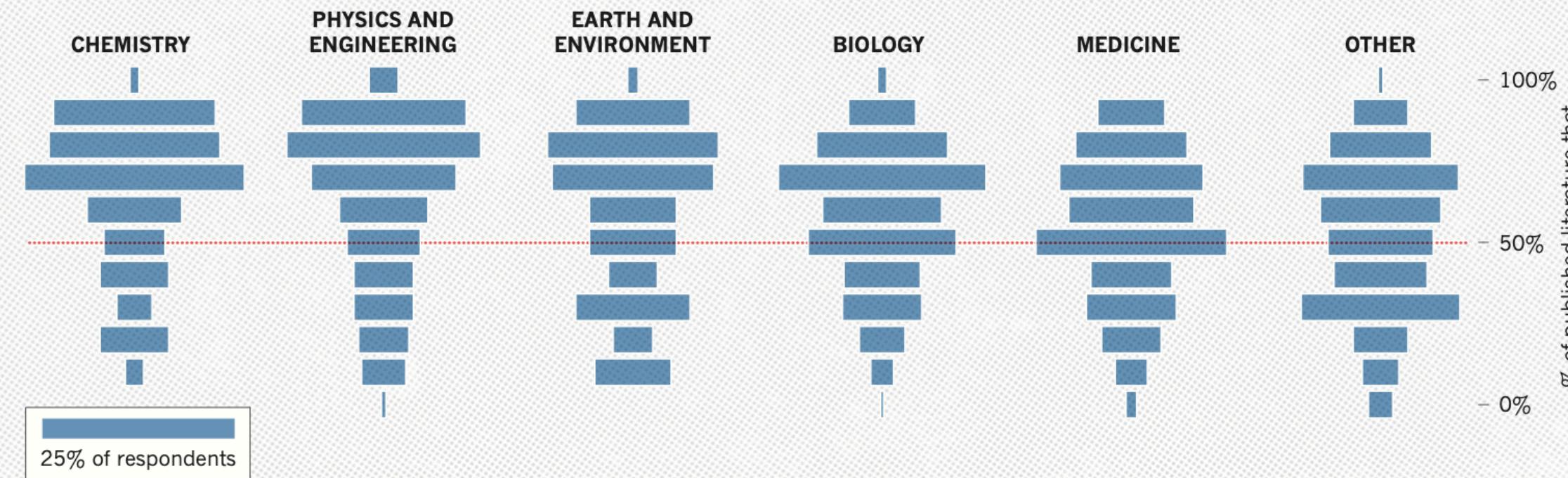
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What is reproducibility in scientific research?

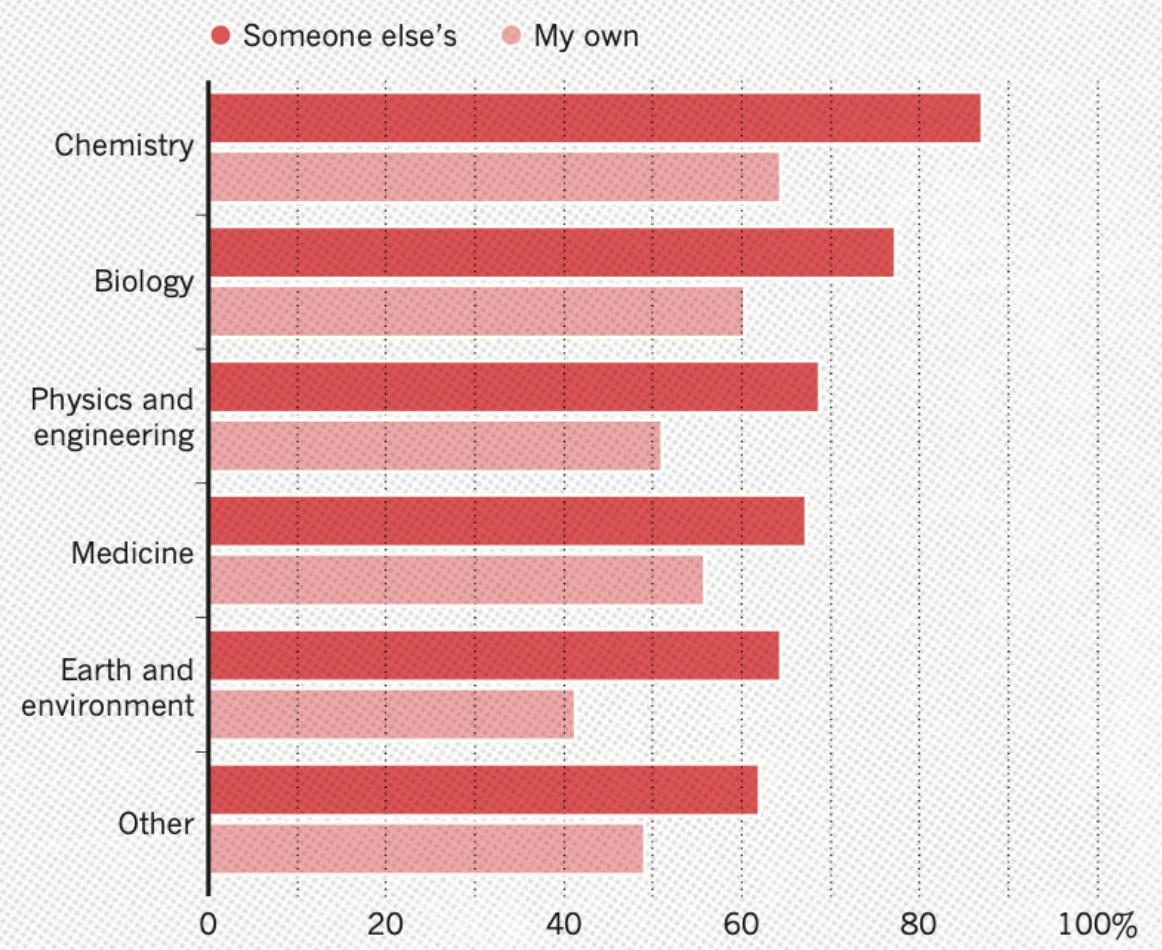
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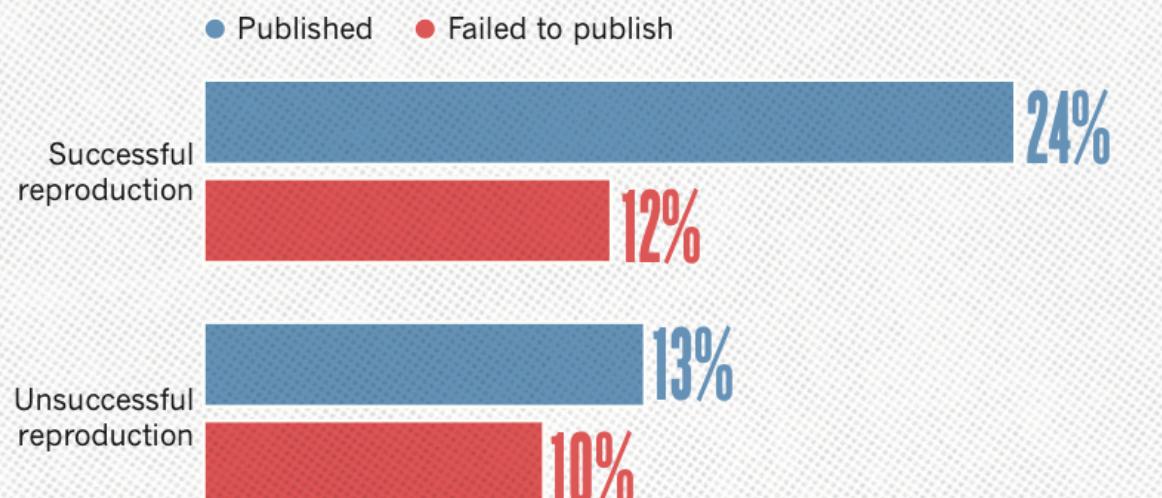
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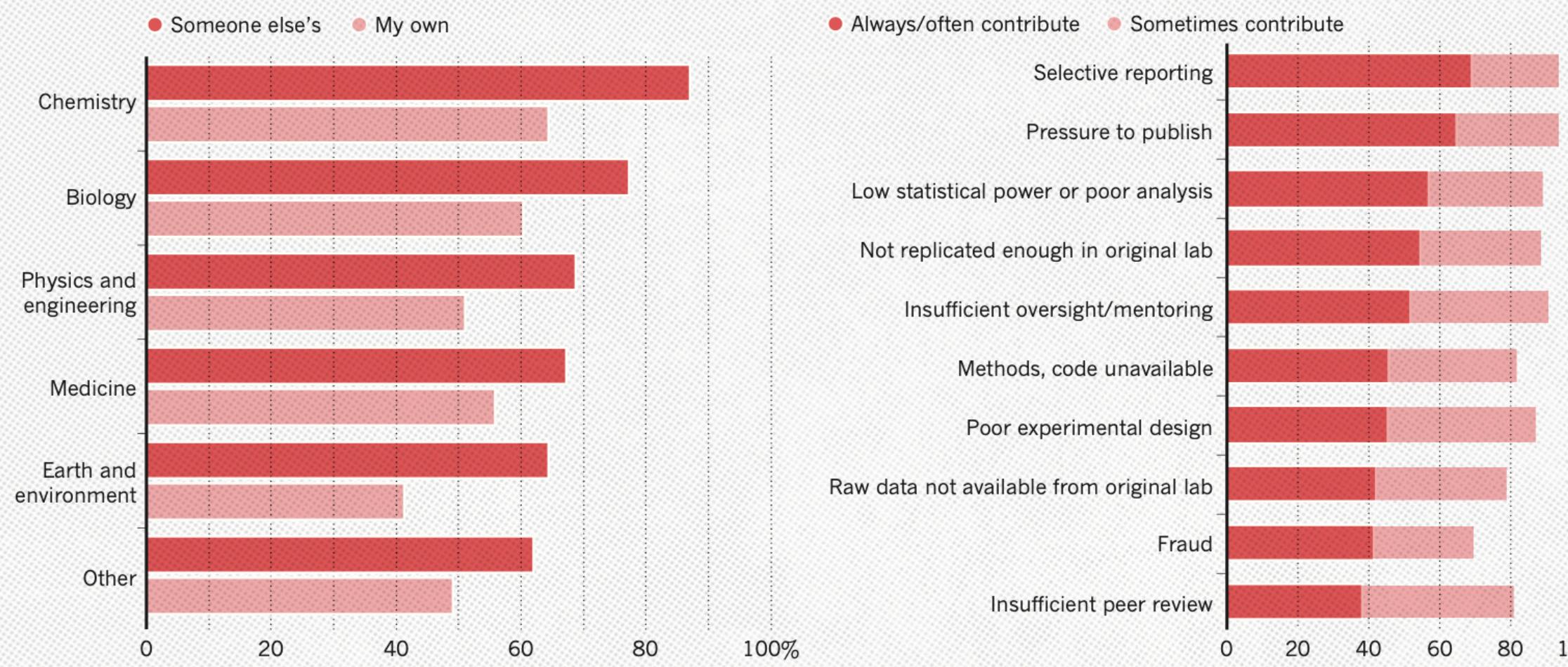
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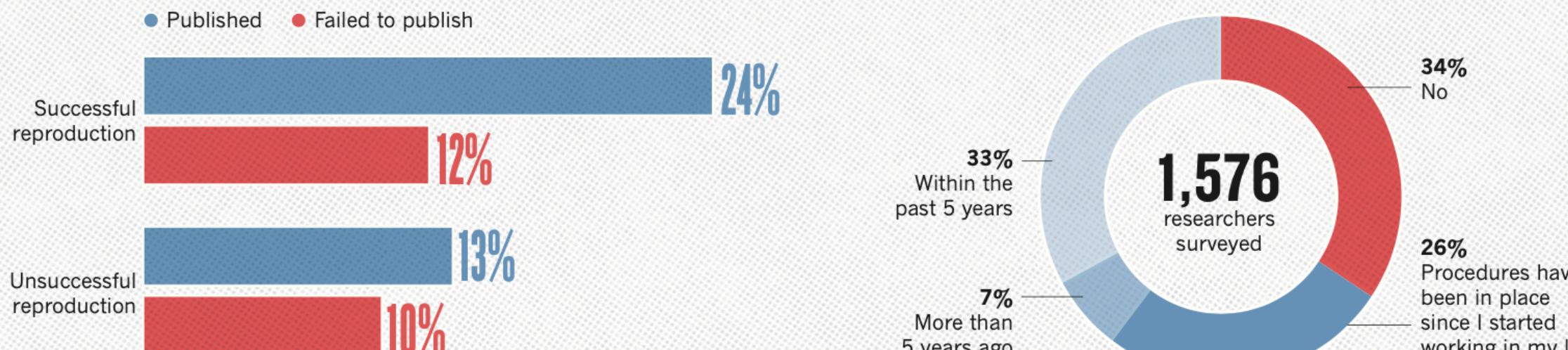
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I don't think we can define reproducibility across the board

Ferric Fang, University of Washington

Reproducibility is shorthand for a lot of problems

Jon Lorsch, National Institute of General Medical Sciences

**Repeatability,
Replicability,
Reproducibility**

**Repeatability,
Replicability,
Reproducibility,
Methods reproducibility,
Results reproducibility,
Inferential reproducibility,**

...

Association for Computing Machinery

Repeatability - Same team, same experimental setup

a researcher can reliably repeat her own computation

Replicability - Different team, same experimental setup

an independent group can obtain the same result using the author's own artifacts.

Reproducibility - Different team, different experimental setup

an independent group can obtain the same result using artifacts which they develop completely independently

Reproducibility - Different team, same experimental setup

as the ability to recompute data analytic results given an observed dataset and knowledge of the data analysis pipeline.

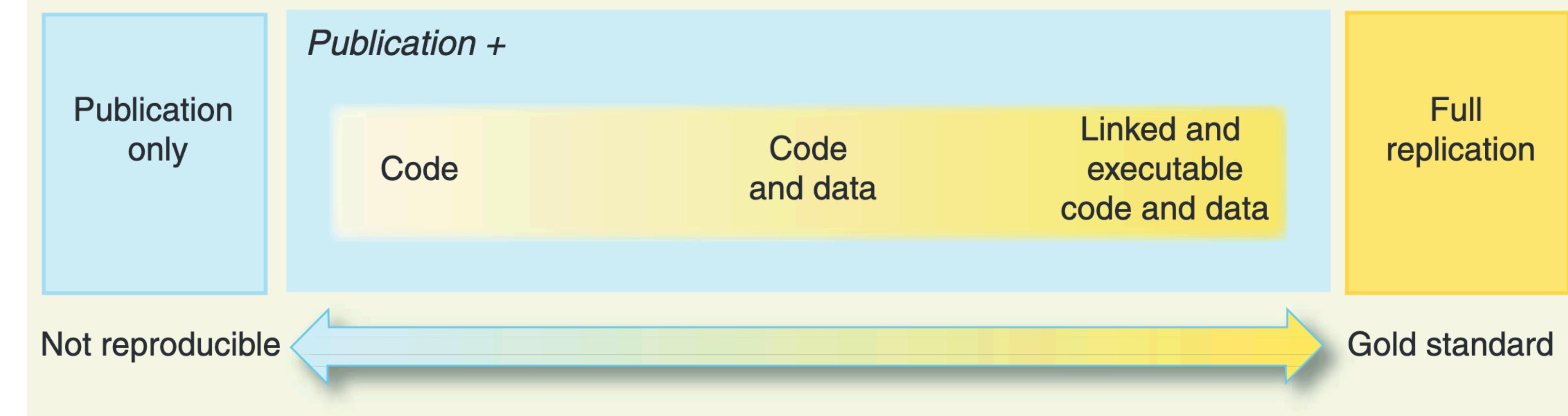
Replicability - Different team, different experimental setup

the chance that an independent experiment targeting the same scientific question will produce a consistent result

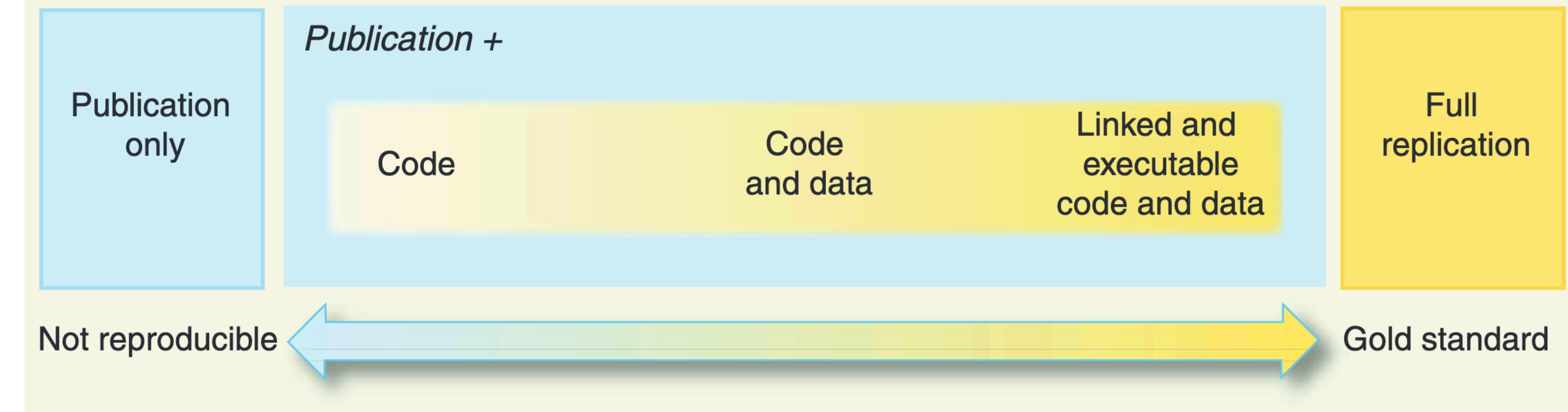
Ensuring Reproducibility in Scientific Research

Best Practices and Strategies

Reproducibility Spectrum

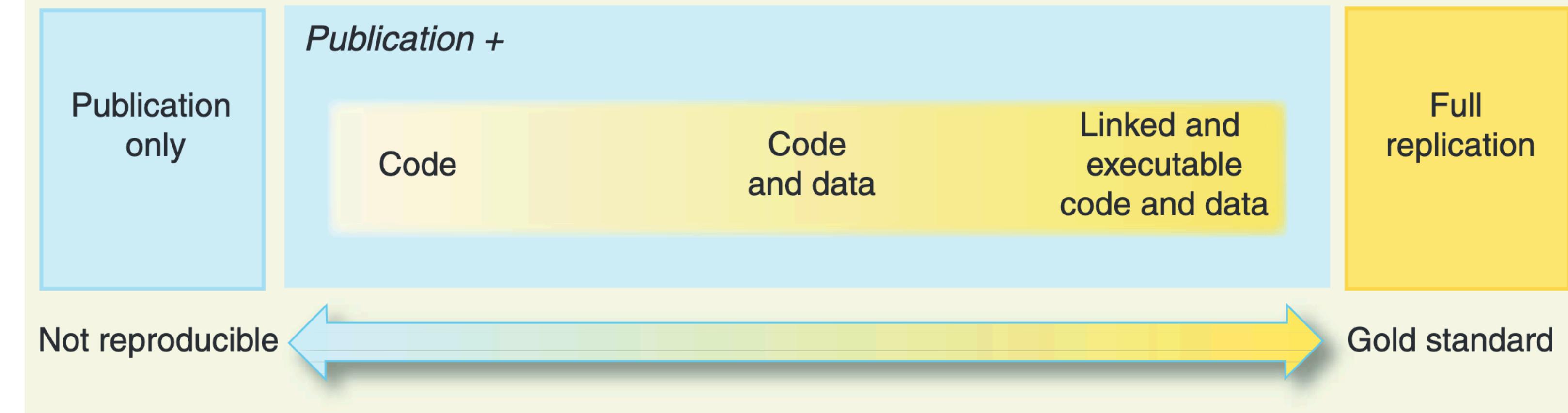


Reproducibility Spectrum



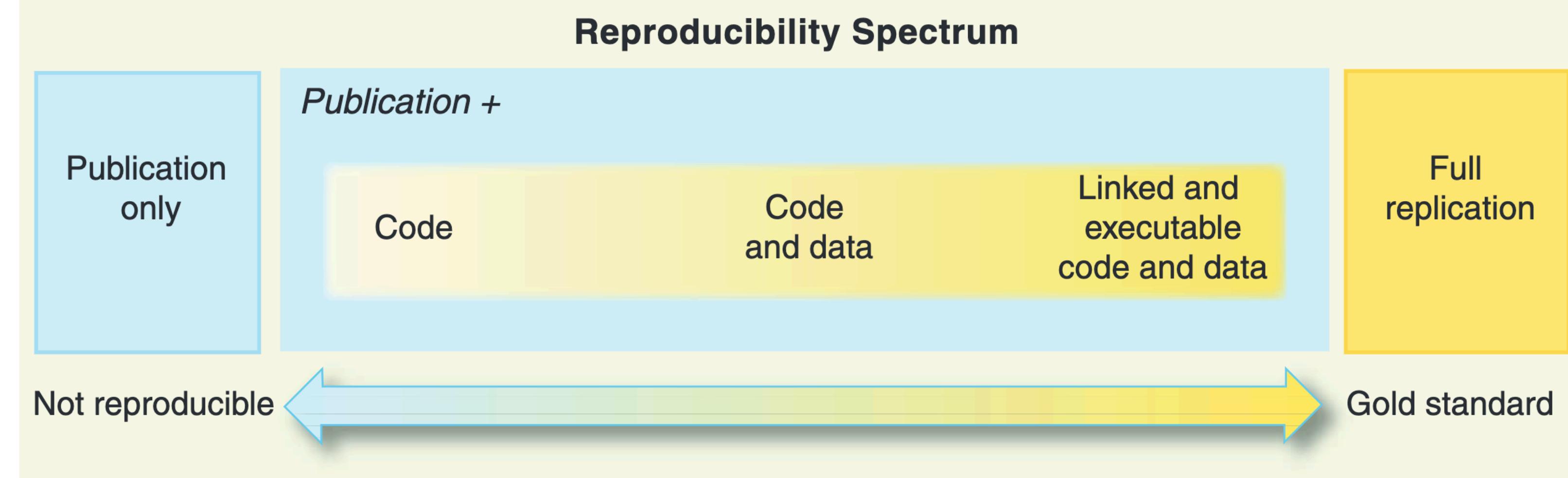
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Reproducibility Spectrum



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During analysis: best coding practices
code available and open for re-use



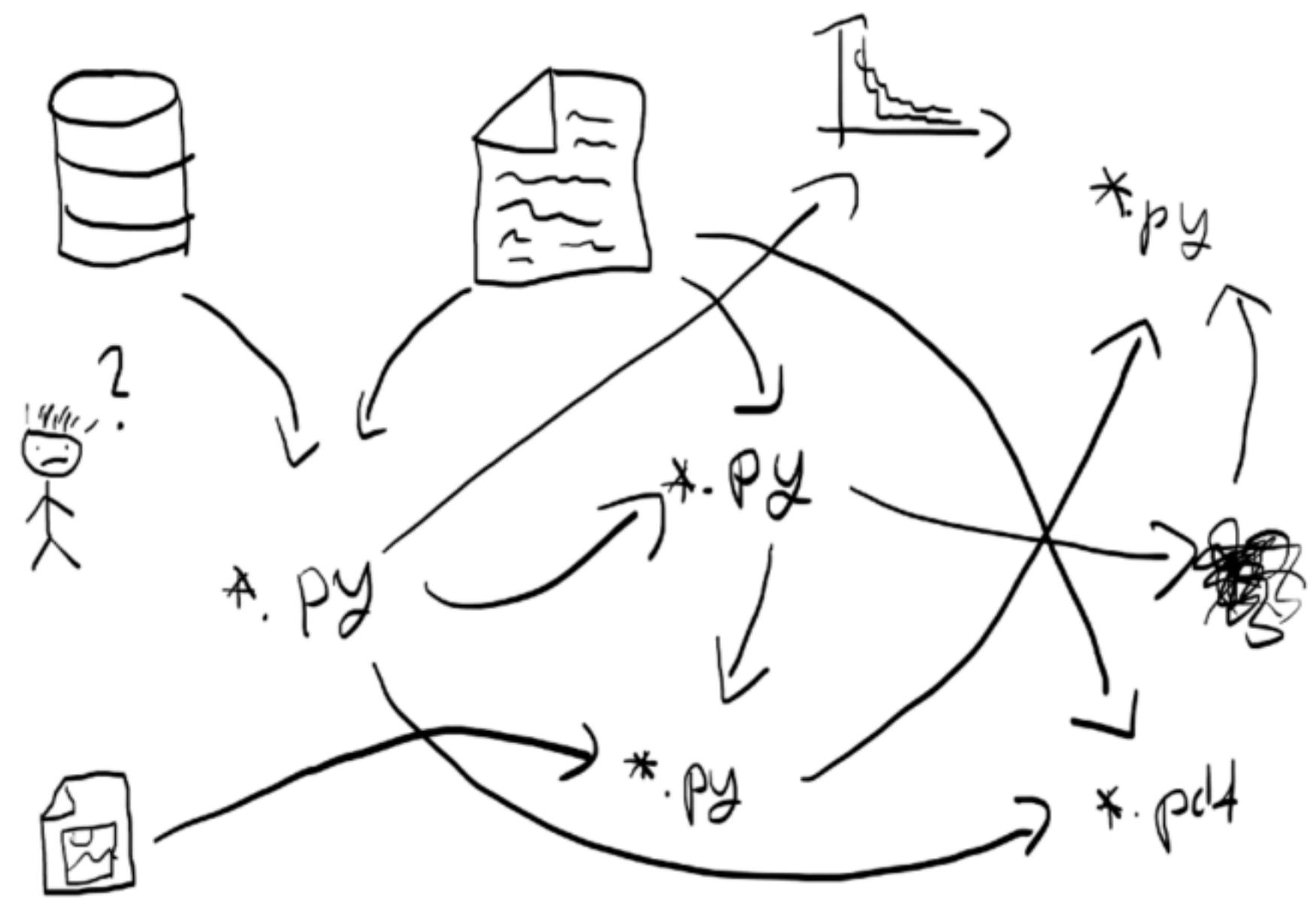
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During analysis: best coding practices
code available and open for re-use

After data analysis: finalizing results and sharing
data, code, software, and products of a research project must be accessible

Setting Up a Computational Research Project

Tips and Techniques for Success



Before data analysis: data storage and organization

- think twice about the data/file structure of your project
- **raw data is immutable**
- separate out its evolution
 - small projects get separate files
 - large projects get separate folders
- rename files
- keep your intermediate data organized (tidy data)
- finalized data should be clearly separated
- avoid **final_final_**

File structure

small project flat structure

```
PROJECT/
    └── figures/                                <- plots.m saves figures in here
    └── main.m                                  <- does something fancy, calls plots.m
    └── plots.m
    └── raw2wind.m                             <- script to clean .csv data to .mat
    └── readme.txt
    └── windSpeed/MITGreenBuilding.mat        <- cleaned data
    └── weatherStation/MITGreenBuilding_2019_07_01.csv <- raw data
    └── weatherStation/MITGreenBuilding_2019_07_02.csv
    └── weatherStation/MITGreenBuilding_2019_07_03.csv
    └── weatherStation/MITGreenBuilding_2019_07_04.csv
    └── weatherStation/MITGreenBuilding_2019_07_05.csv
    └── weatherStation/MITGreenBuilding_2019_07_06.csv
    └── weatherStation/MITGreenBuilding_2019_07_07.csv
```

File structure

medium project simple hierarchy

```
PROJECT/
├── bin/          <- compiled binaries.
├── data/
│   ├── raw/
│   └── clean/
├── figures/      <- figures used in place of a "results" folder.
├── scripts/
│   ├── process/  <- scripts to manipulate data between raw, cleaned, final stages.
│   └── plot/      <- intermediate plotting.
└── src
    ├── model1/
    ├── model2/
    └── model3/
    
└── LICENSE
└── Makefile
└── readme.md
```

File structure

large project
complex hierarchy

```
PROJECT/
├── LICENSE
├── Makefile           <- Makefile with commands like `make data` or `make train`
├── README.md          <- The top-level README for developers using this project.
├── data/
│   ├── external/       <- Data from third party sources.
│   ├── interim/        <- Intermediate data that has been transformed.
│   ├── processed/      <- The final, canonical data sets for modeling.
│   └── raw/            <- The original, immutable data dump.
├── docs/              <- A default Sphinx project; see sphinx-doc.org for details
├── models/             <- Trained and serialized models, model predictions, or model summaries
├── notebooks/          <- Jupyter notebooks. Naming convention is a number (for ordering),
                           the creator's initials, and a short '-' delimited description, e.g.
                           `1.0-jqp-initial-data-exploration`.
├── references/         <- Data dictionaries, manuals, and all other explanatory materials.
├── reports/
│   └── figures/         <- Generated graphics and figures to be used in reporting
├── requirements.txt    <- The requirements file for reproducing the analysis environment, e.g.
                           generated with `pip freeze > requirements.txt`
├── setup.py            <- Make this project pip installable with `pip install -e`
└── src/
    ├── __init__.py       <- Source code for use in this project.
    ├── data/              <- Scripts to download or generate data
    │   └── make_dataset.py
    ├── features/          <- Scripts to turn raw data into features for modeling
    │   └── build_features.py
    ├── models/            <- Scripts to train models and then use trained models to make
                           predictions
    │   ├── predict_model.py
    │   └── train_model.py
    └── visualization/     <- Scripts to create exploratory and results oriented visualizations
        └── visualize.py
tox.ini                <- tox file with settings for running tox; see tox.testrun.org
```

During analysis: best coding practices

- use version control system and make it available
 - git, mercurial, svn
- use scripts, or even better a workflow management system
 - nextflow, snakemake
- use environments and make them available and documented
 - conda, docker, singularity
- provide code samples and test data

After data analysis: finalizing results and sharing

- data and code archiving in public repositories (DOI)
 - zenodo, figshare, dryad, OSF
- prepare in advance data submission
- depending on the size of the project create **research compendiums**
 - data, code, software, and products of a research project are archived together

Git Version Control for Scientific Computing

Managing Code and Collaborating Effectively



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- It **provides a way to collaborate with others** and maintain a **complete history of all changes** made to a project over time
- Git is widely used in software development, but can be used for **any type of file-based project**

- Git **is not** GitHub

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genomewalker / **FunData** Public

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main 2 branches 0 tags Go to file Add file <> Code

Your main branch isn't protected Protect this branch

genomewalker Minor ba7a838 13 hours ago 16 commits

File/Folder	Commit Message	Time
data	Added wrapper wf	14 hours ago
day1	Renamed folders	17 hours ago
day2	Minor	13 hours ago
.gitignore	Initial commit	yesterday
LICENSE	Create LICENSE	13 hours ago
README.md	Minor	13 hours ago

README.md

Fundamentals in Computational Analysis of Large-Scale Datasets

Welcome to the GitHub repository for Reproducible data analysis and workflows module of the "Fundamentals in Computational Analysis of Large-Scale Datasets" course. This repository contains all the materials needed for the course, including two days of tasks and a wiki with detailed explanations and examples.

About

A repository for the Fundamentals Data Analysis course

Readme

MIT license

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No releases published

Create a new release

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Publish your first package

Languages

Python 54.0% Shell 46.0%

- Git **is not** GitHub

Home

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 - [Introduction to Git](#)
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 - [Task 2: Writing a More Complex BASH script](#)
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Introduction to BASH Scripting

Automating Tasks and Streamlining Workflows



- can **automate repetitive tasks** in scientific research, such as **data preprocessing, analysis, and visualization**



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- can also be used to **create reproducible research workflows**, by documenting the steps taken and the commands executed in a script.
- is a **valuable skill** for researchers in fields such as bioinformatics, neuroscience, and physics, where data processing and analysis are essential

Hands-on session

<https://github.com/GeoGenetics/data-analysis-2024/reproducible-data-analysis>