SCHOOL OF DATA ANALYSIS

Reproducible Machine Learning for Humans

Nikita Kazeev on behalf on the Everware and REP teams

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Yandex School of Data Analysis

A noncommercial private university https://yandexdataschool.com

- Education:
  - Strong courses in Data & Computer Science
  - Free tuition
  - No employment obligations on part of the students (yet many go to Yandex)
  - 450+ students graduated since 2007
- Research
  - Organizes a Machine Learning Conference
  - Interest in interdisciplinary research (eScience) — from Information Retrieval to Particle Physics
  - A full member of the LHCb experiment at CERN

Me

- A data scientist
- MSc in Physics
- Work for the LHCb collaboration at CERN
  - Data storage optimization
  - A search engine for physics data
  - An automated anomaly detection systAem
- Taught machine learning at Machine Learning in High Energy Physics Summer Schools

Plan

- The problem of research irreproducibility
- Our tools for computational experiments
  - Everware
  - Reproducible Experiment Platform (REP)
- Demo

Irreproducibility indicators

- ‘Which version of my code I used to generate figure 13?’
- ‘The new student wants to reuse that model I published three years ago but he can’t reproduce the figures’
- ‘I thought I’ve used the same parameters but I’m getting different results...’
- ‘Which dataset exactly did I use for algorithm comparison?‘
- ‘Why did I do that?!’
- ‘It worked yesterday!!’

Cases in point: Medical science

Amgen (a commercial company) in 2012

- 53 landmark papers in cancer drug development
- Scientific findings confirmed only in 6 (11%) cases

Bayer (a commercial company) in 2011

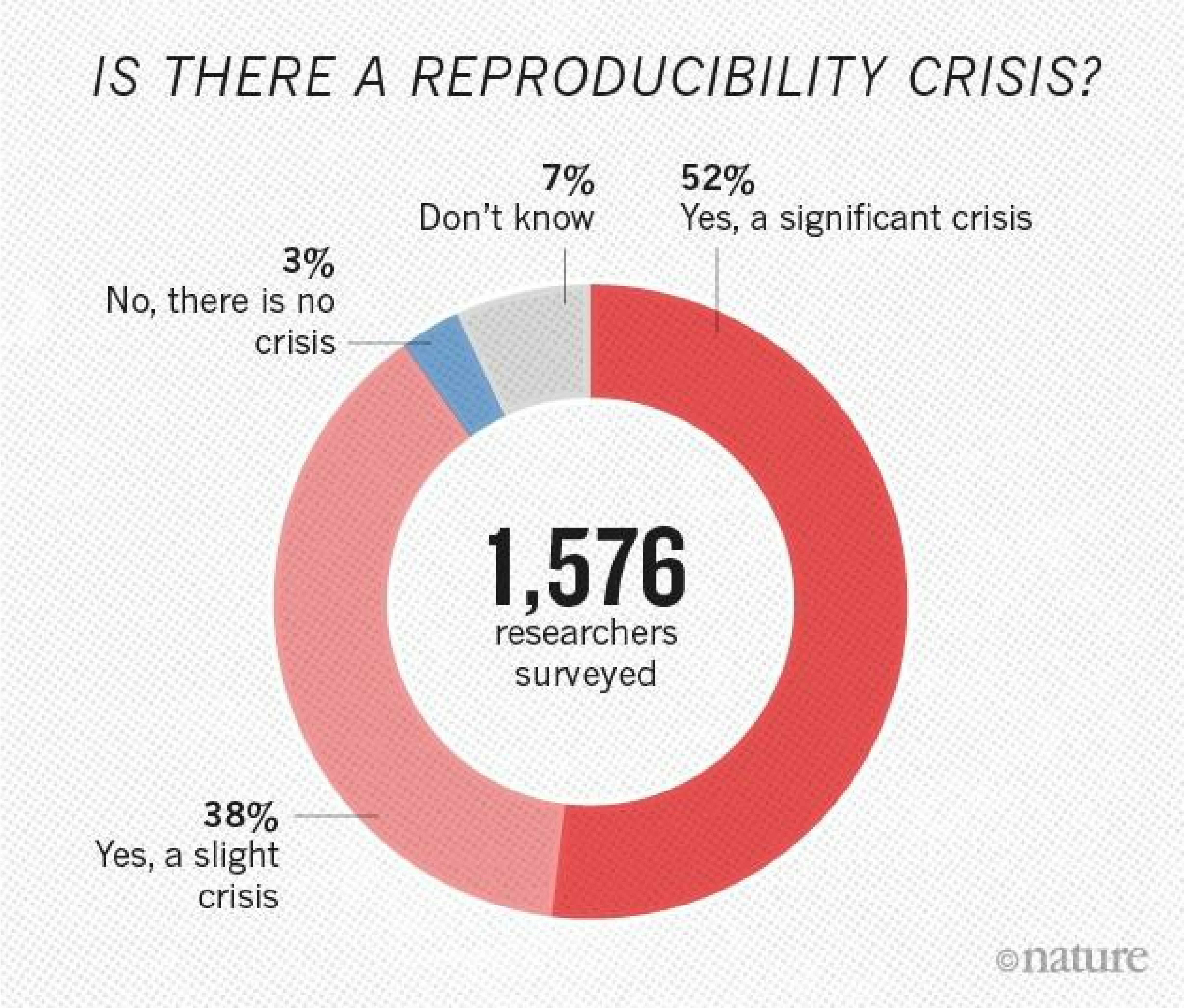
- 67 projects
- Results confirmed in 20-25% cases

A new study is under way and to be completed in 2017

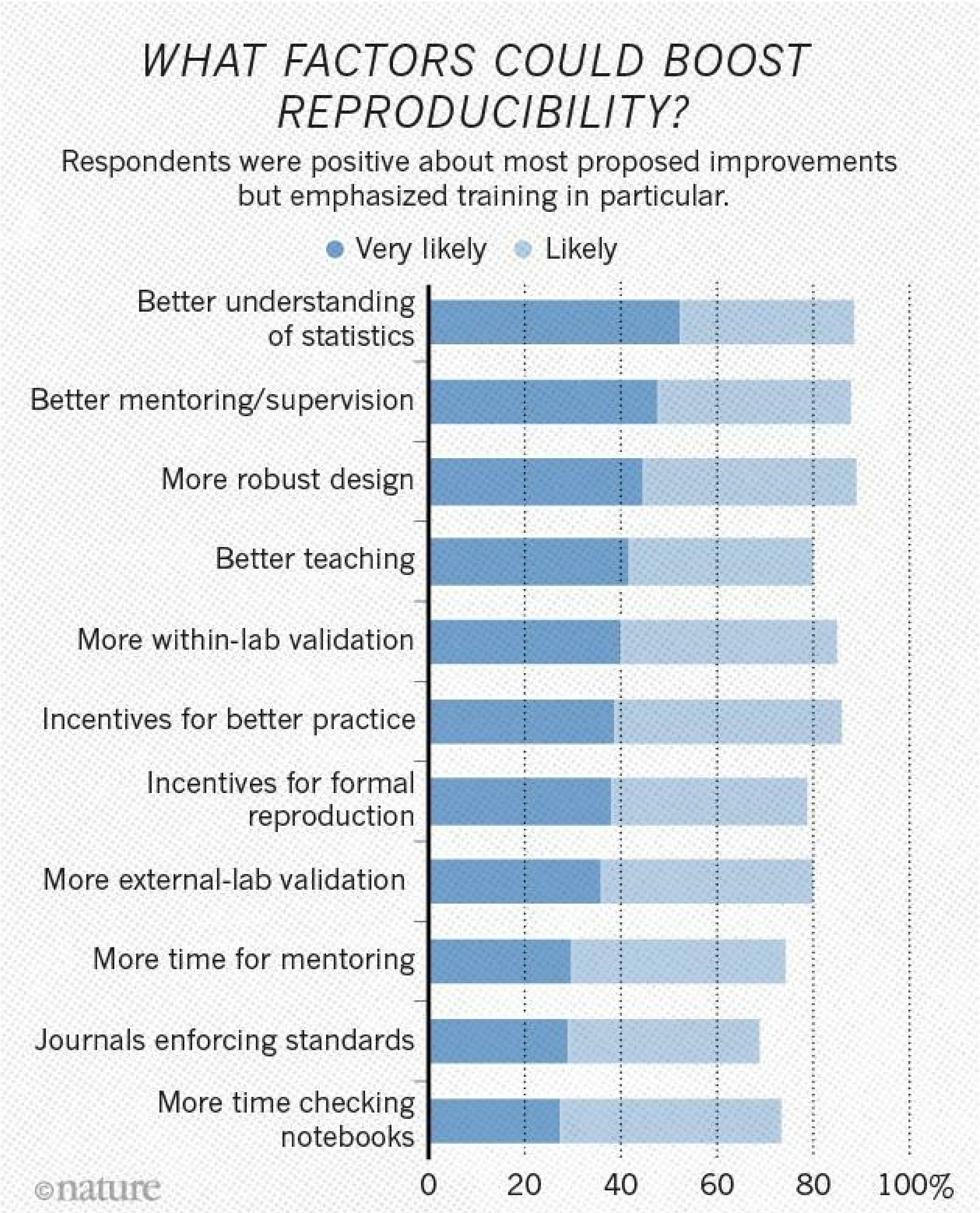
- https://osf.io/e81xl/wiki/home/

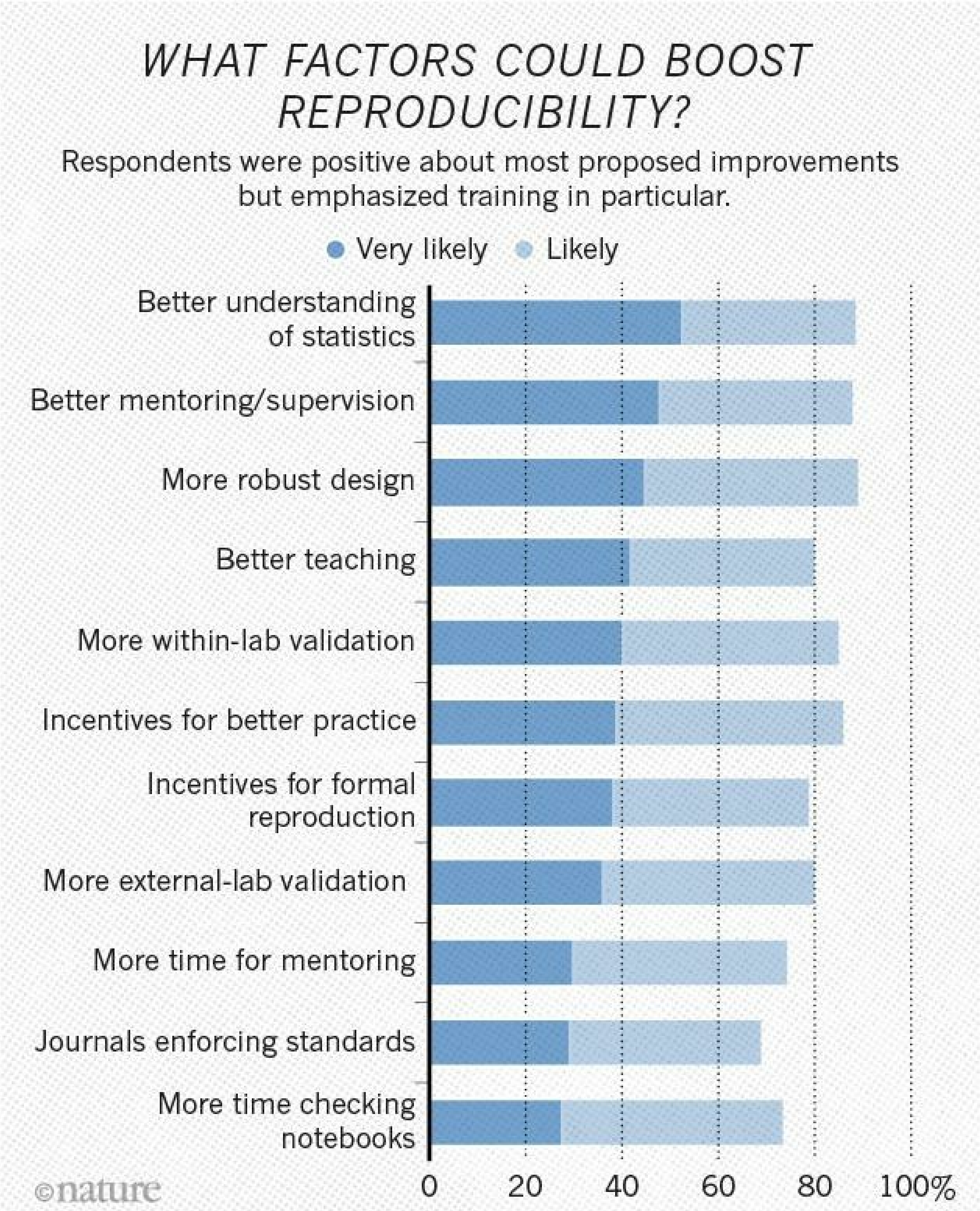
- http://www.nature.com/nature/journal/v483/n7391/full/483531a.html
- http://www.nature.com/news/cancer-reproducibility-project-scales-back-ambitions-1.18938
- http://www.nature.com/nrd/journal/v10/n9/full/nrd3439-c1.html

Nature's Reproducibility Survey



- Nature: 1,500 scientists lift the lid on reproducibility by Monya Baker
- raw survey data (link)


WHAT FACTORS COULD BOOST REPRODUCIBILITY?
Respondents were positive about most proposed improvements but emphasized training in particular.
● Very likely
● Likely
Better understanding of statistics
Better mentoring/supervision
More robust design
Better teaching
More within-lab validation
Incentives for better practice
Incentives for formal reproduction
More external-lab validation
More time for mentoring
Journals enforcing standards
More time checking notebooks
0
20
40
60
80
100%
©nature



***Computational experiment* is a significant part of an experiment, that starts after the data is collected.**

Possible rffects of reproducible computation:

- Practical
  - better mentoring/supervision
  - more within-lab validation
  - simplified external-lab validation
  - incentive for better practice
  - robust design
- Educational
  - wider access to the best practices
  - better teaching

High Energy Physics

- **data** storage
  - shared storage (XROOTD, AFS, EOS, CERNBOX)
- standardized **environment**
  - software: ROOT, minuit, experiments software stacks , ...
  - computational cluster (e.g. `lxplus`)
- **code** versioning repository (gitlab)
- advanced analysis approaches
  - blind analysis
  - reviews, cross-checks within group, inter-group collaboration
- collaborative culture
  - q&a groups, experts
  - publishing workflow

Reproducible computational study key components

- Basic assumptions (vocabulary)
- Data
- Environment + Resources (CPU / GPU)
- Code
- Workflow
- Automated intermediate results checks
- Final results (datasets, publications)

Common environment

Enter Reproducible Experiment Platform (**REP**)

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- Open-source, Apache 2.0: https://github.com/yandex/rep
- Well-documented, supported by Yandex, http://yandex.github.io/rep/

A reproducible study example

https://github.com/everware/everware-dimuon-example

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- **data**: CERNBOX

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Steps to run:

- install Docker
  - https://docs.docker.com/engine/installation/
- clone the repository
  - `git clone https://github.com/everware/everware-dimuon-example.git`
- build the Docker image (will need to download ~500 Mb)
  - `docker build . -t dimuon`
- run Docker with the repository folder mounted and Jupyter port forwarded
  - `docker run -it -p 127.0.0.1:8888:8888 -v $(pwd):/notebooks dimuon bash`
- insider run Jupyter
  - `cd /notebooks && jupyter notebook --no-browser`
- with the browser go to 127.0.0.1:8888

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Or you can use *Everware* - just click.

Everware is ...

... about re-useable science, it allows people to jump right into your research code. Lets you launch *Jupyter* notebooks from a git repository with a click of a button.

- https://github.com/everware - Code
- https://everware.rep.school.yandex.net - Yandex instance

More examples:

- Comparison of ML algorithms; R, Everware, CircleCI https://github.com/openml/study_example
- Gravitational waves identification (LIGO experiment); REP, Everware https://github.com/anaderi/GW150914
- Search for particle traces (COMET experiment); Everware, TravisCI https://github.com/yandexdataschool/comet-example-ci

Under the hood of Everware

- an extension for *JupyterHub*:
  - a spawner for building and running custom *Docker* images
- integrated with:
  - Docker Hub (for getting Docker images)
  - GitHub (for authentication and repository interaction)

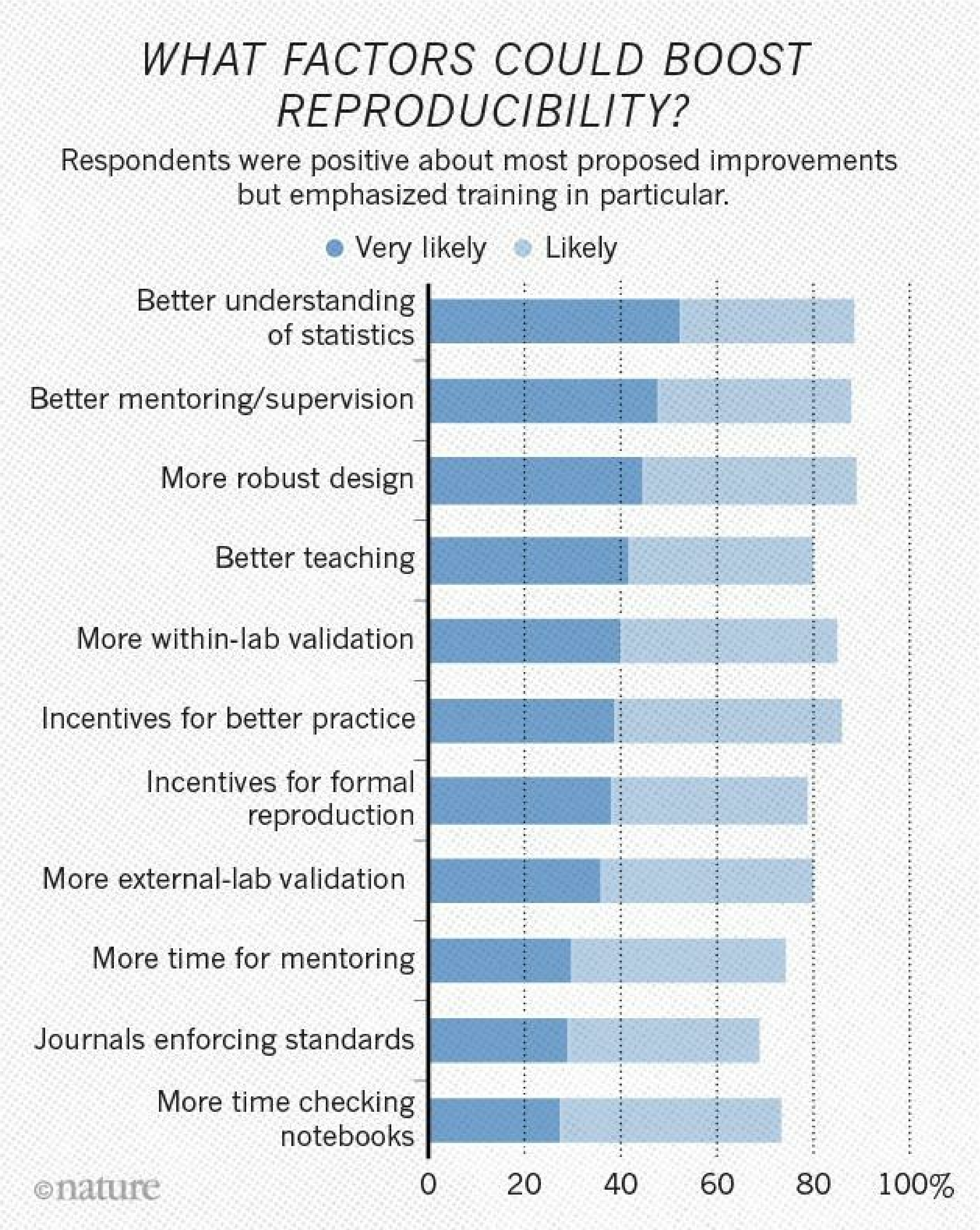
Pros & cons

Pros

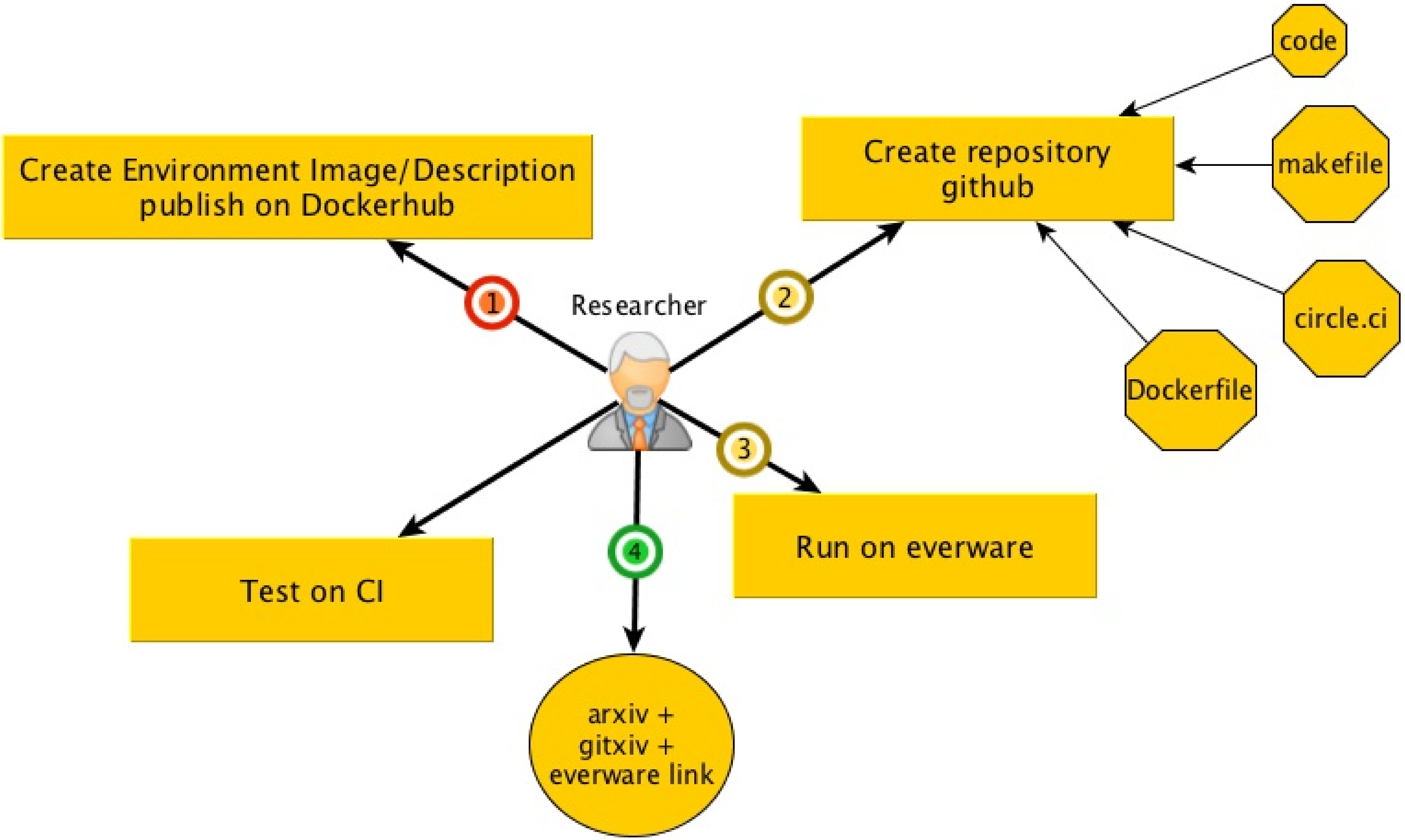
- easier supervision / mentoring
- easier within-lab validation
- wider access to the best practices
- simplified cross-lab validation
- good incentive for formal reproduction

Cons

- learning a bit of open-source technology
- re-organize internal research process
- inner barrier for openness
- higher incentive for mindless *borrowing*
- promotes users to create unique environments

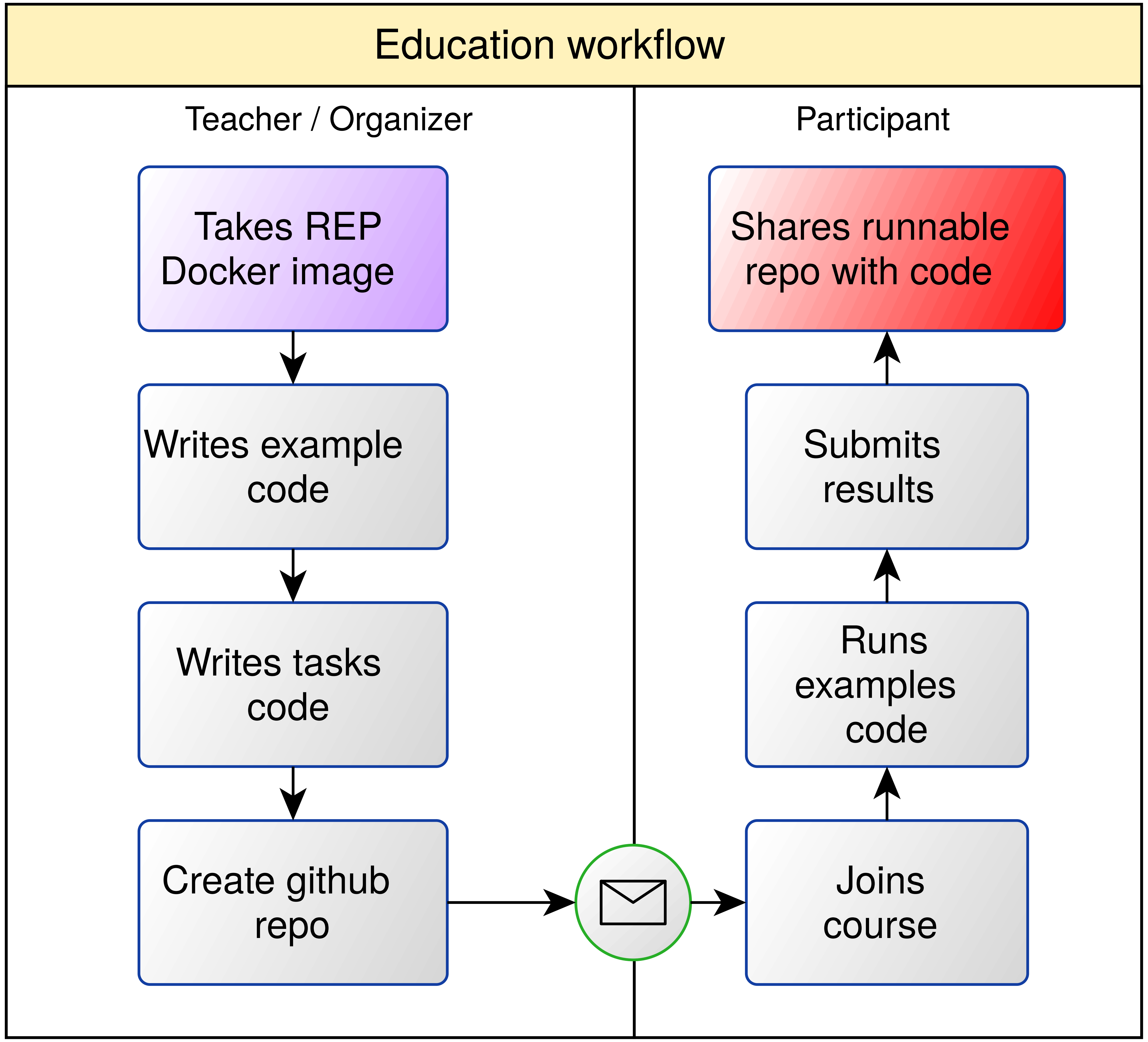


Research workflow with everware



https://github.com/everware/everware/wiki/How-to-embed-everware-into-research-use-cases

Education workflow with everware



- Python course at YSDA 2015
- Machine Learning in High Energy Physics summer school 2016
- YSDA course on Machine learning at Imperial College London 2016
- Kaggle competitions 2016
- Machine learning course at University of Eindhoven
- LHCb open data masterclass

Roadmap

- Integrate with data sharing resources (zotero, figshare, etc)
- Automatic capture of environment (integrate with repro-zip)
- Integration with publishing resources (gitxiv, re-science, openml)
- Not only jupyter-based computations
- Bring your own resources computational model

Conclusion

- Reproducibility depends on humans
  - Can be helped with human-facing technology;
- *Everware works* for research and education;
  - easy to try;
  - WIP, https://github.com/everware
    - feature requests are welcome
    - pull requests are most welcome
- REP might work as a common environment for your ML study
  - it also has nice tools to ease the routine

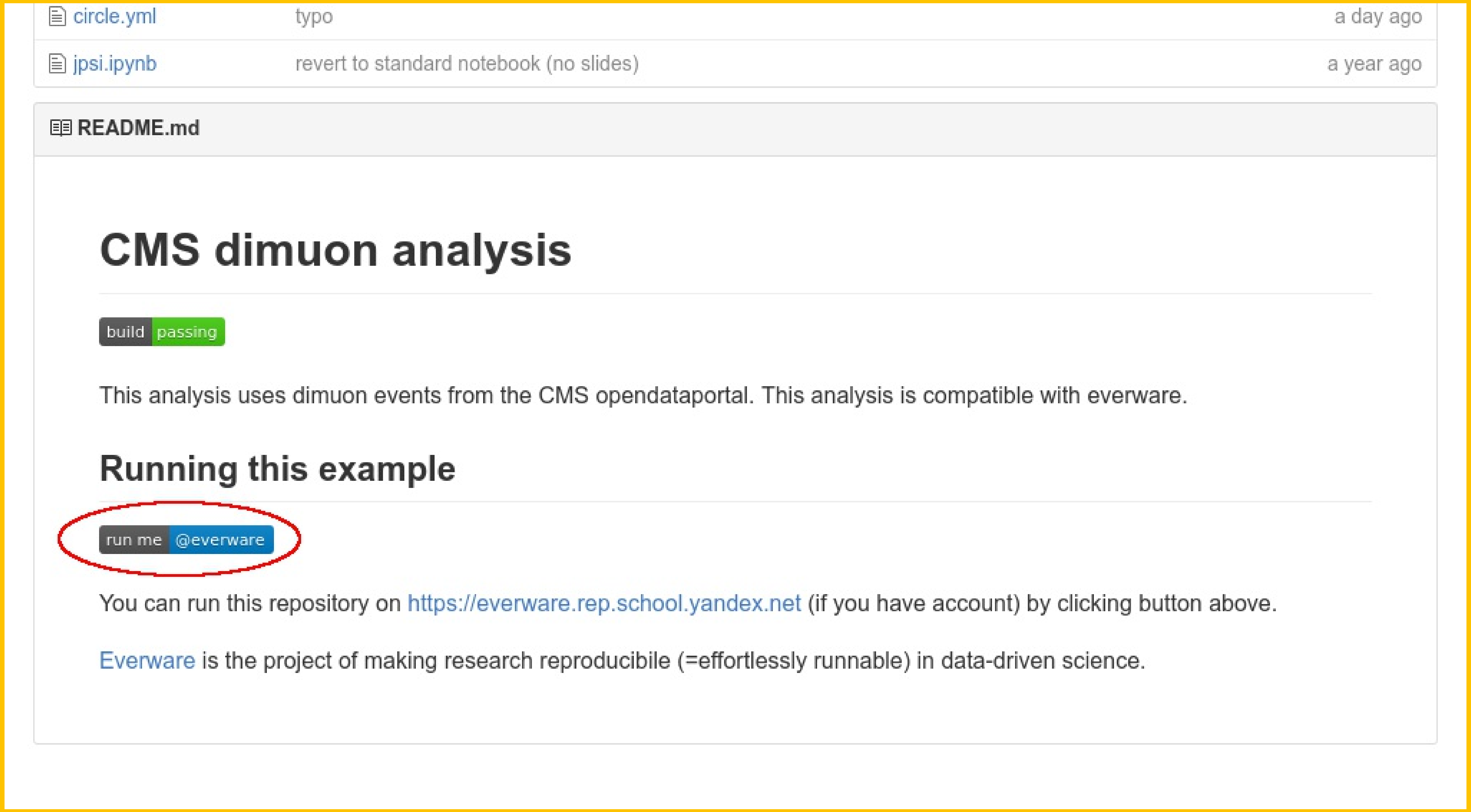
Thank you!

Backup

Everware demo

Running https://github.com/everware/everware-dimuon-example

Sorry, printed version doesn't support animation.



circle.yml	typo	a day ago
jpsi.ipynb	revert to standard notebook (no slides)	a year ago

README.md

CMS dimuon analysis

This analysis uses dimuon events from the CMS opendataportal. This analysis is compatible with everware.

Running this example

You can run this repository on https://everware.rep.school.yandex.net (if you have account) by clicking button above.

Everware is the project of making research reproducibile (=effortlessly runnable) in data-driven science.

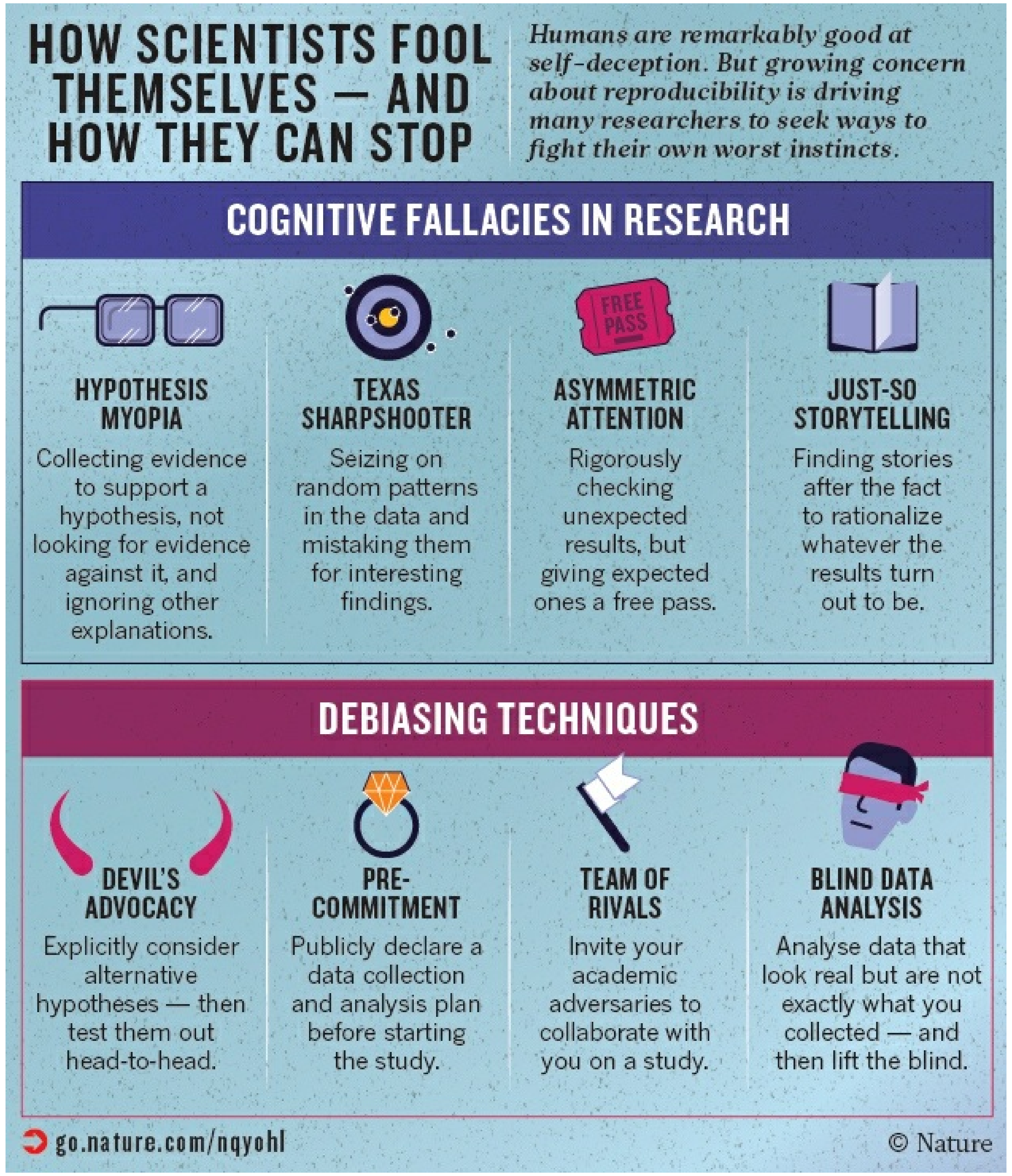
Yandex services landscape (est 1997)

- Web search
- Image search
- Speech recognition
- Car traffic prediction
- Mail and spam filtering
- Natural language translation
- Market (shopwindow for internet shops)
- Yandex Data Factory (https://yandexdatafactory.com)
- Yandex School of Data Analysis
  - (full member of LHCb since Dec'15)

References

- http://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970
- https://rescience.github.io/read/
- http://push.cwcon.org/
- https://openml.org
- https://figshare.com/
- https://gitlab.cern.ch/lhcb-bandq-exotics/Lb2LcD0K
- https://osf.io/ezcuj/wiki/home/
- https://osf.io/e81xl/wiki/home/
- Center for open science, https://cos.io/
- IPFS, https://github.com/ipfs/
- Nature, keyword: reproducibility, http://www.nature.com/news/reproducibility-1.17552

Dealing with cognitive bias



HOW SCIENTISTS FOOL THEMSELVES — AND HOW THEY CAN STOP

Humans are remarkably good at self-deception. But growing concern about reproducibility is driving many researchers to seek ways to fight their own worst instincts.

COGNITIVE FALLACIES IN RESEARCH

HYPOTHESIS MYOPIA
Collecting evidence to support a hypothesis, not looking for evidence against it, and ignoring other explanations.

TEXAS SHARPSHOOTER
Seizing on random patterns in the data and mistaking them for interesting findings.

ASYMMETRIC ATTENTION
Rigorously checking unexpected results, but giving expected ones a free pass.

JUST-SO STORYTELLING
Finding stories after the fact to rationalize whatever the results turn out to be.

DEBIASING TECHNIQUES

DEVIL'S ADVOCACY
Explicitly consider alternative hypotheses — then test them out head-to-head.

PRE-COMMITMENT
Publicly declare a data collection and analysis plan before starting the study.

TEAM OF RIVALS
Invite your academic adversaries to collaborate with you on a study.

BLIND DATA ANALYSIS
Analyse data that look real but are not exactly what you collected — and then lift the blind.

go.nature.com/nqyohl

http://go.nature.com/nqyohl