Reproducible Machine Learning for Humans

Nikita Kazeev on behalf on the Everware and REP teams

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2016-10-13, 4th National eScience Symposium, Amsterdam, the Netherlands

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

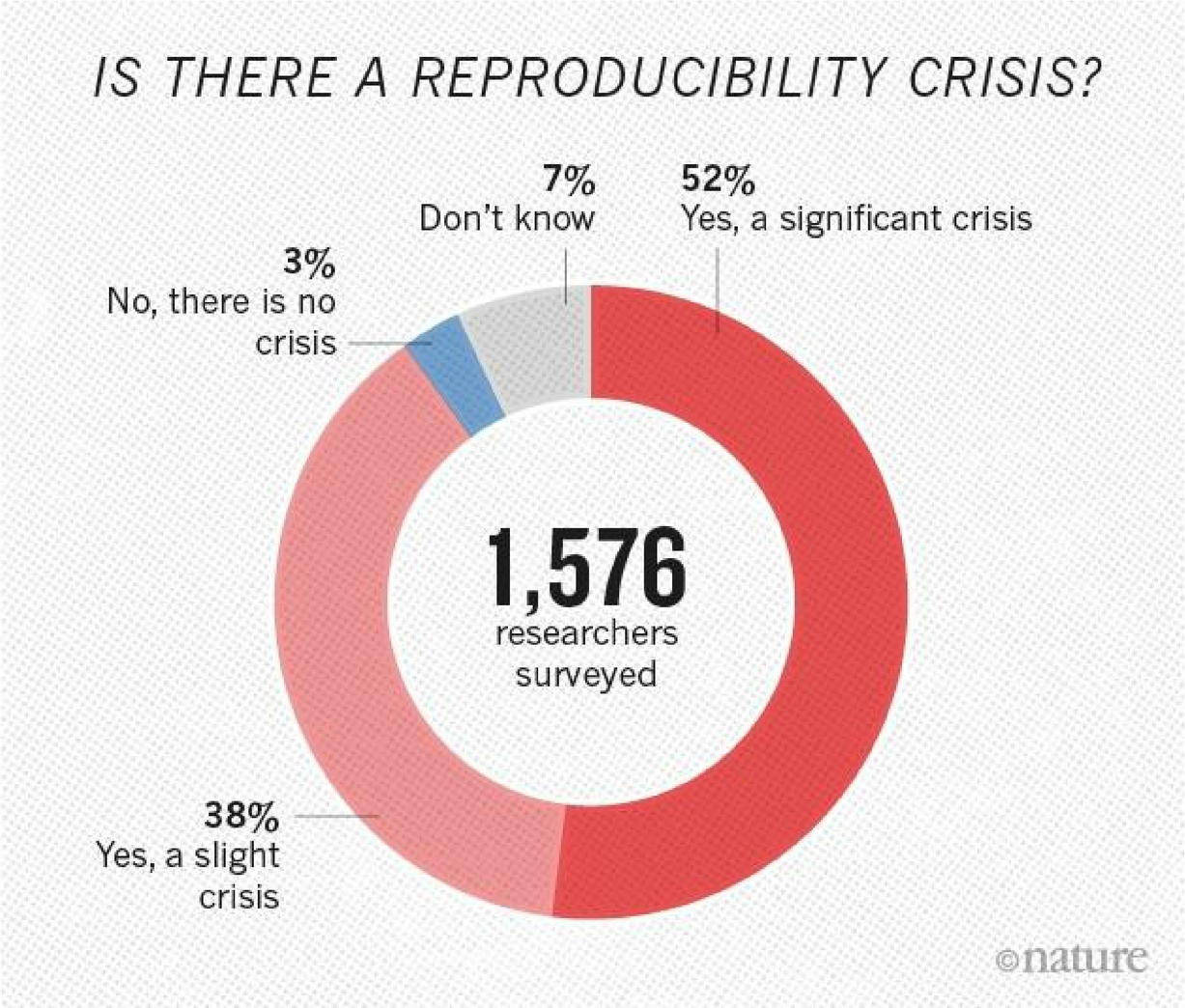
- 67 projects
- Results confirmed in 20-25% cases

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

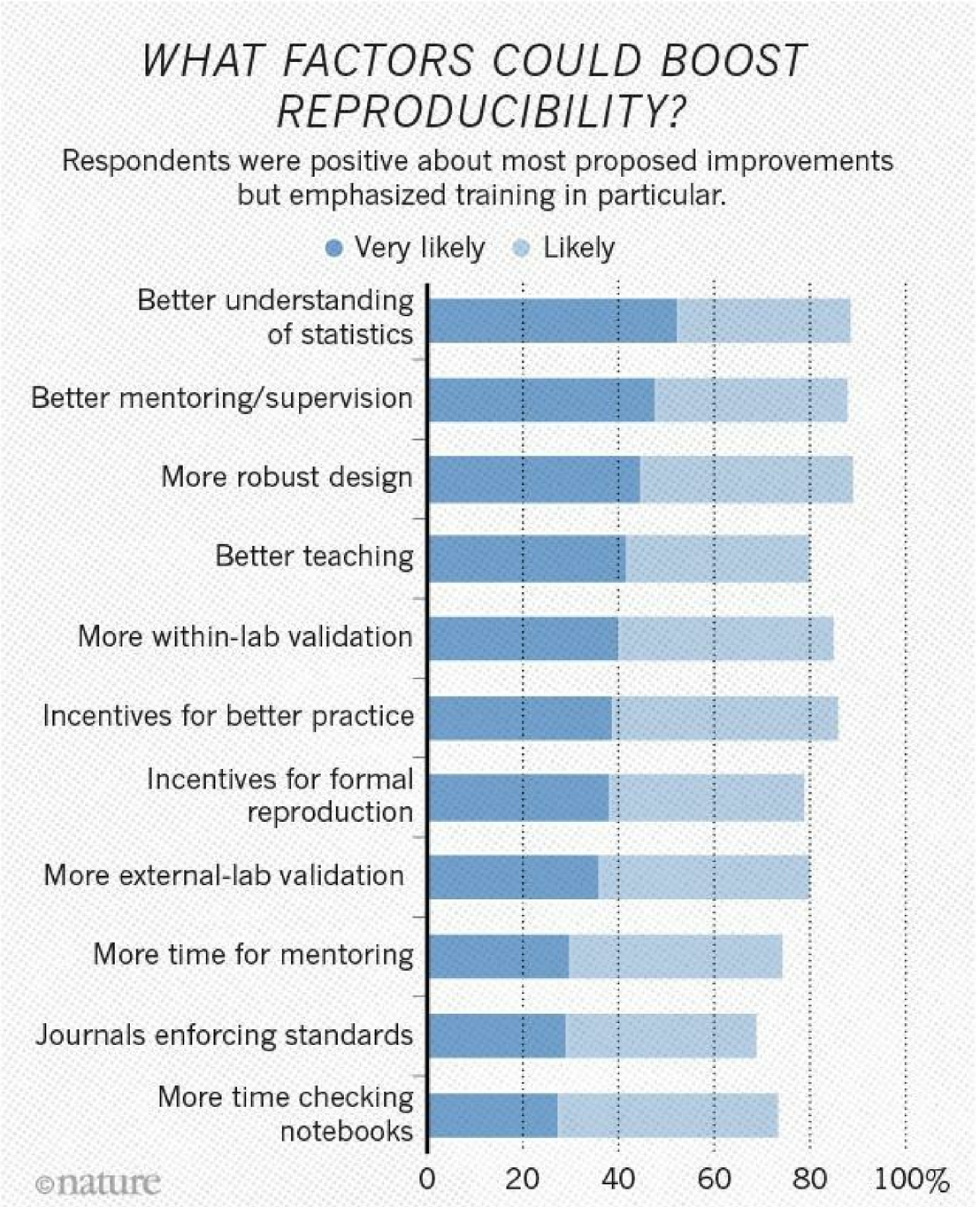
- https://osf.io/e81xl/wiki/home/

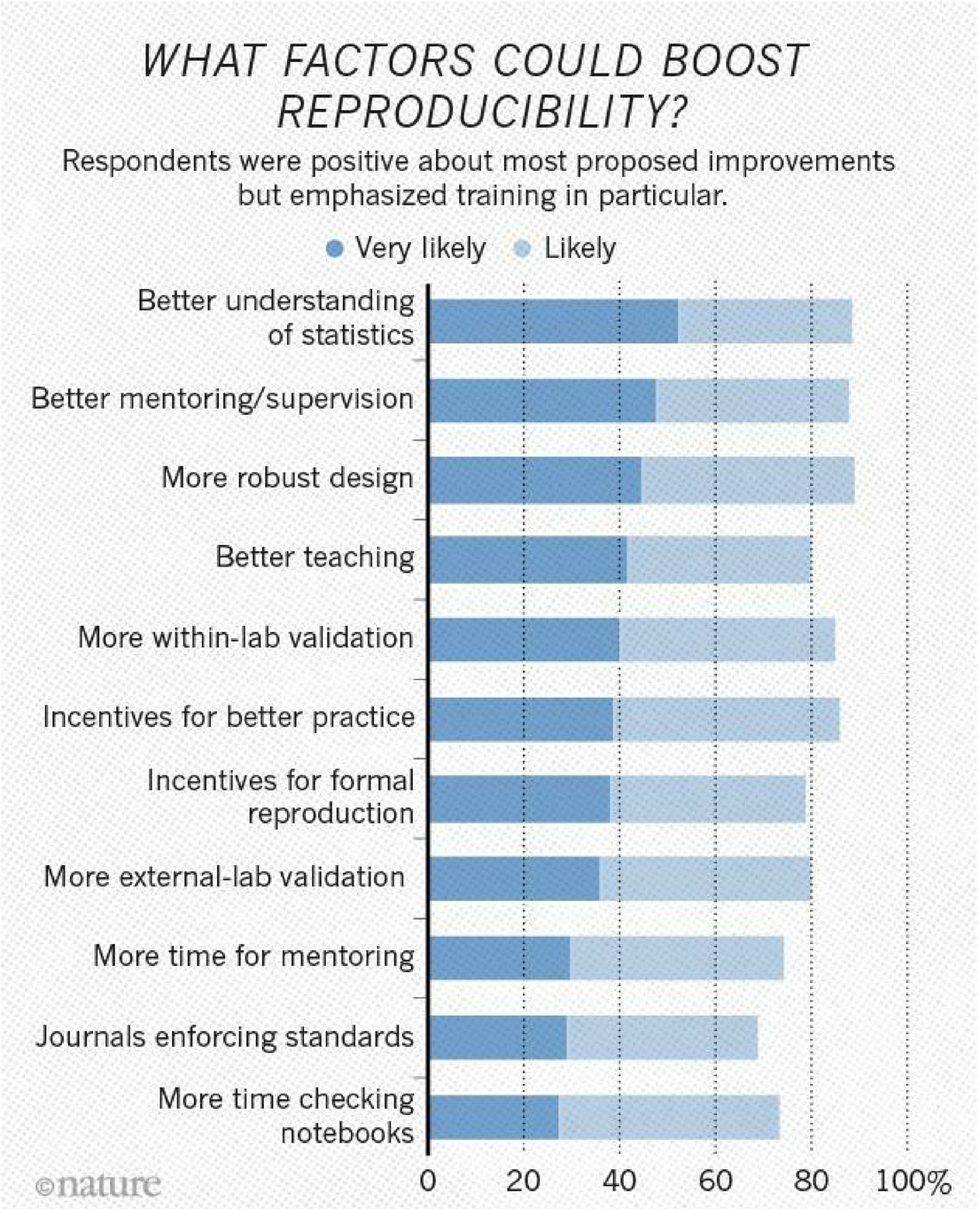
- http://www.nature.com/nature/journal/v483/n7391/full/483531a.html
- http://www.nature.com/news/cancer-reproducibility-project-scales-back-ambitions-1.18938
- http://www.nature.com/nrd/journal/v10/n9/full/nrd3439-c1.html

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

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- Pluggable quality metrics

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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:

- algorithm meta-analysis, https://github.com/openml/study_example
- gravitational waves, https://github.com/anaderi/GW150914
- COMET, https://github.com/yandexdataschool/comet-example-ci

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Under the hood of Everware

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

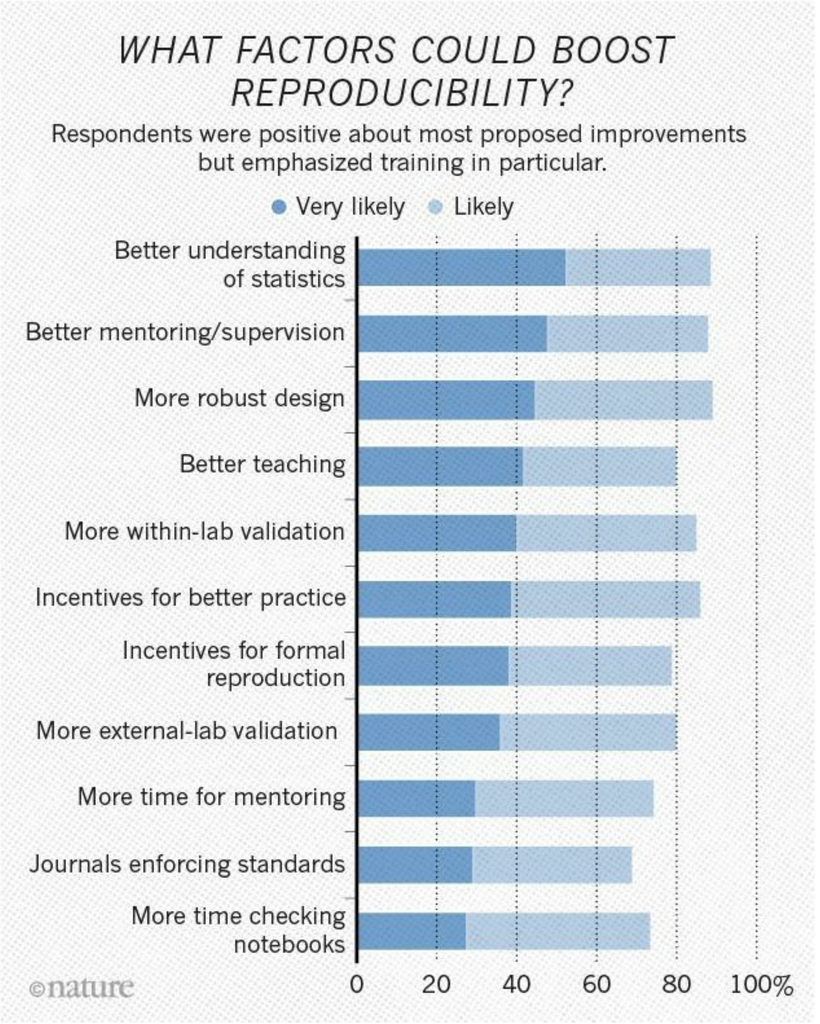
Pros & cons

Pros

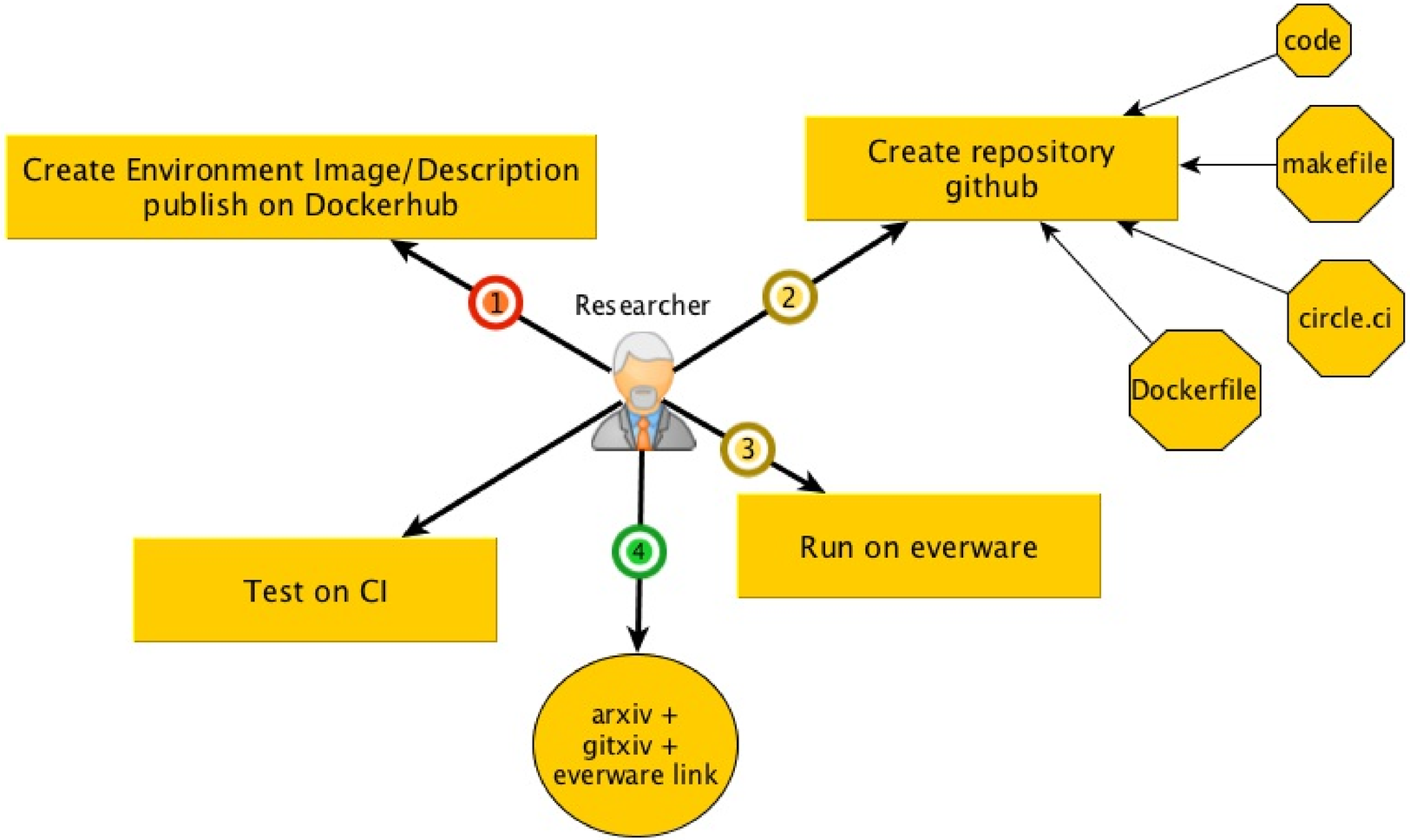
- easier supervision/mentoring
- easier within-lab validation
- wider access to the best practices
- simplified cross-lab validation
- good incentive for formal reproduction
- *good thing for industry career track development*
- access to wider set of practices

Cons

- learning a bit of open-source technology
- re-organize internal research process
- inner barrier for openness
- higher incentive for mindless *borrowing*
- environments divergence

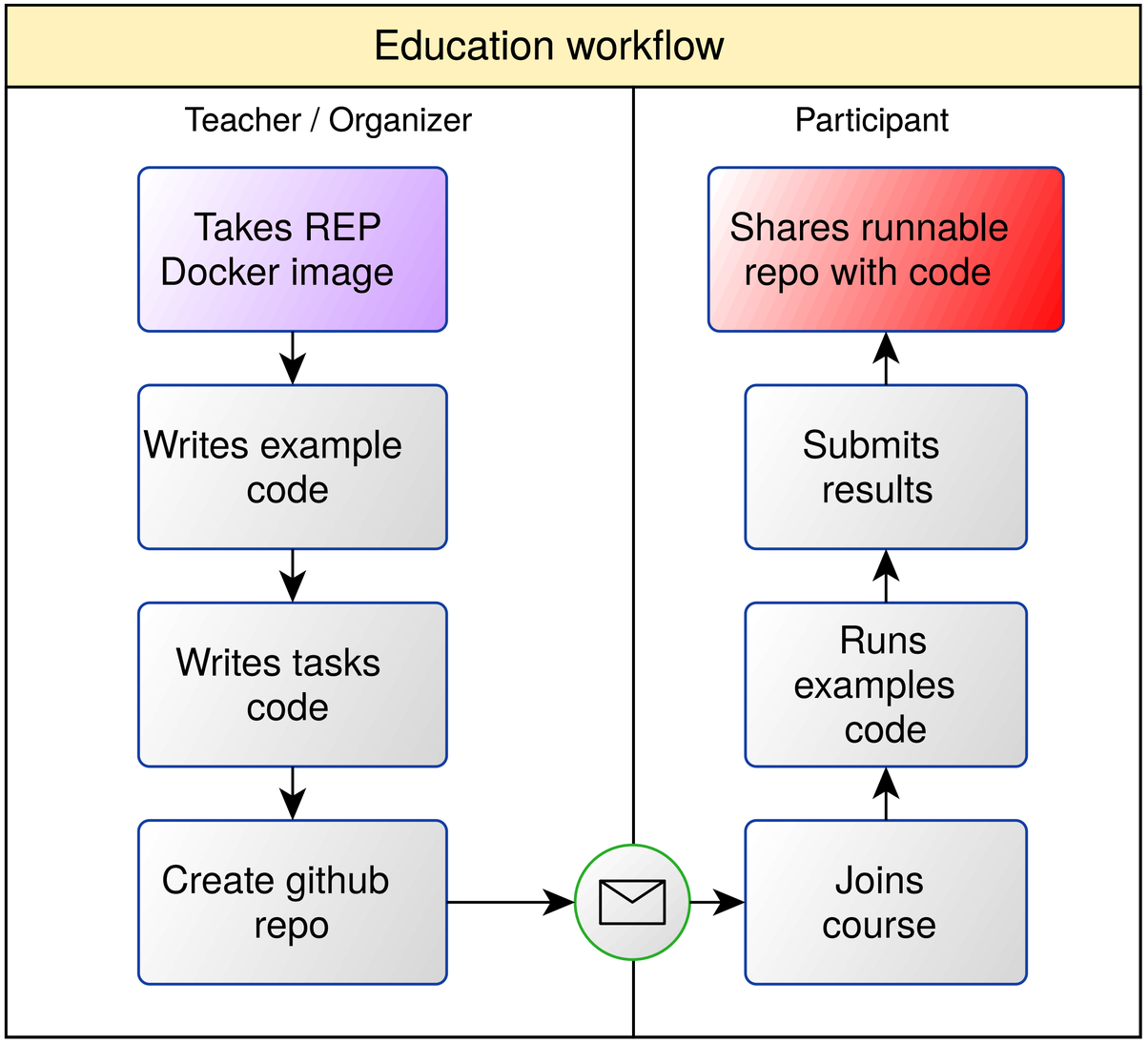


Research workflow with everware



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

Education workflow with everware



- Python course at YSDA 2015
- MLHEP Machine Learning summer schools 2015 and 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

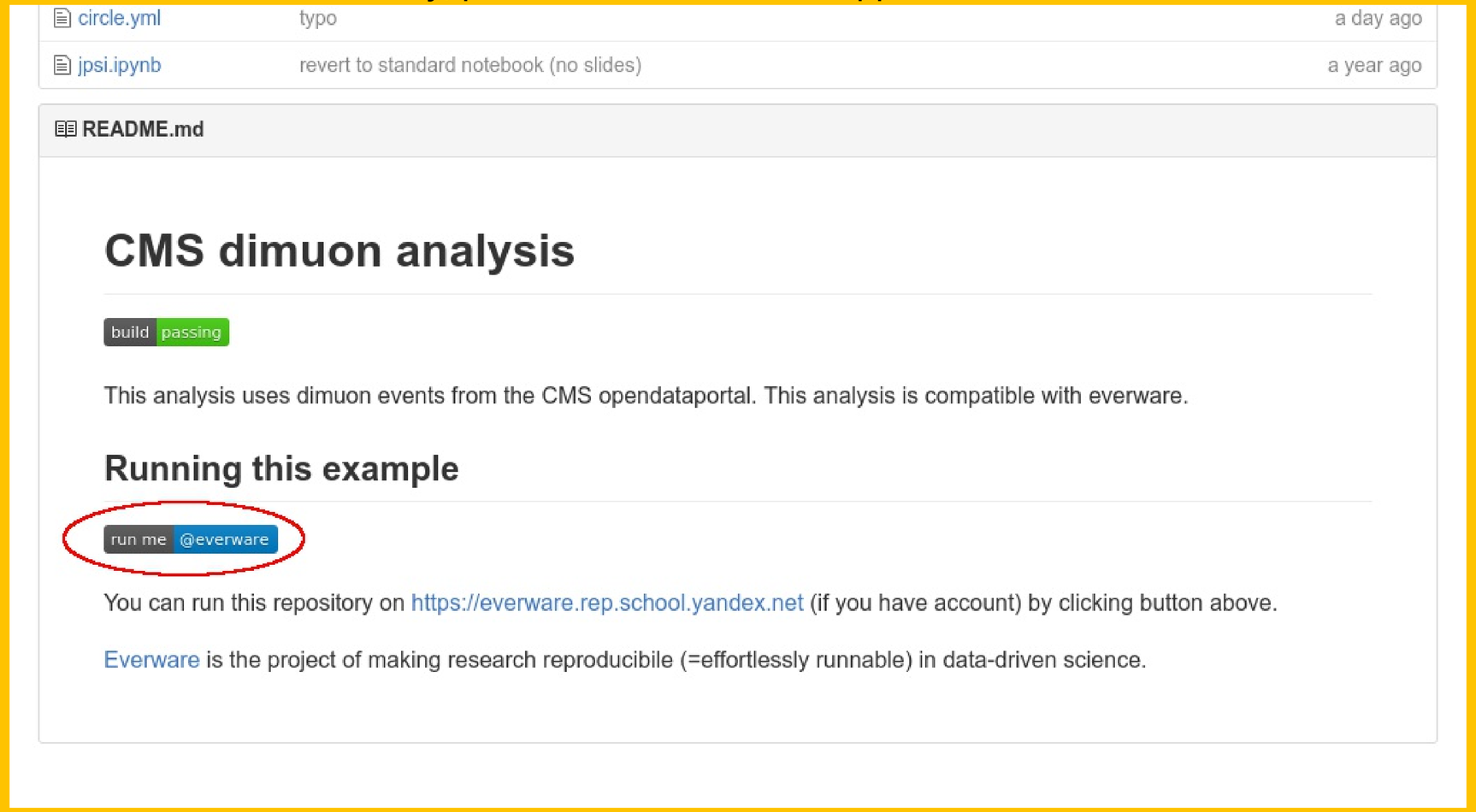
Thank you!

Backup

Everware demo

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

Sorry, printed version doesn't support animation.



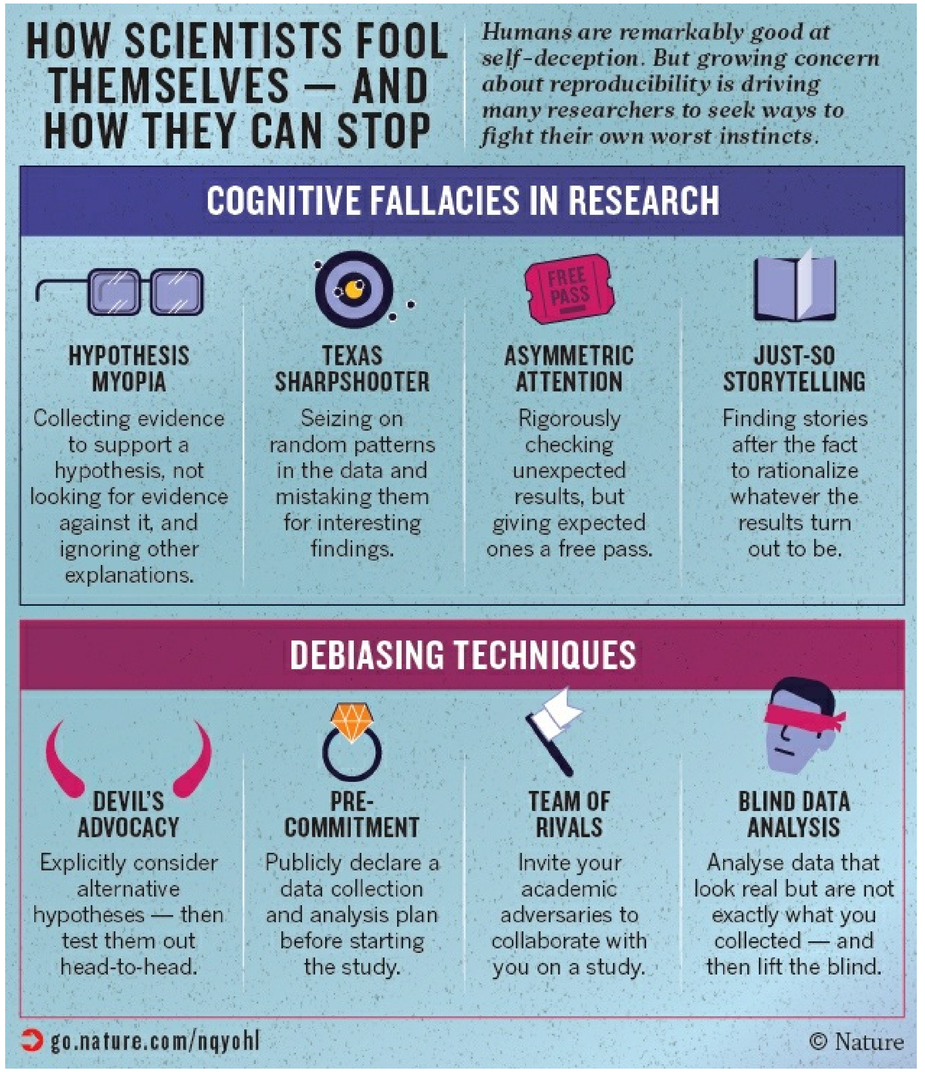
Yandex services landscape (est 1997)

- 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



http://go.nature.com/nqyohl