Everware toolkit

supporting reproducible science and challenge-driven education

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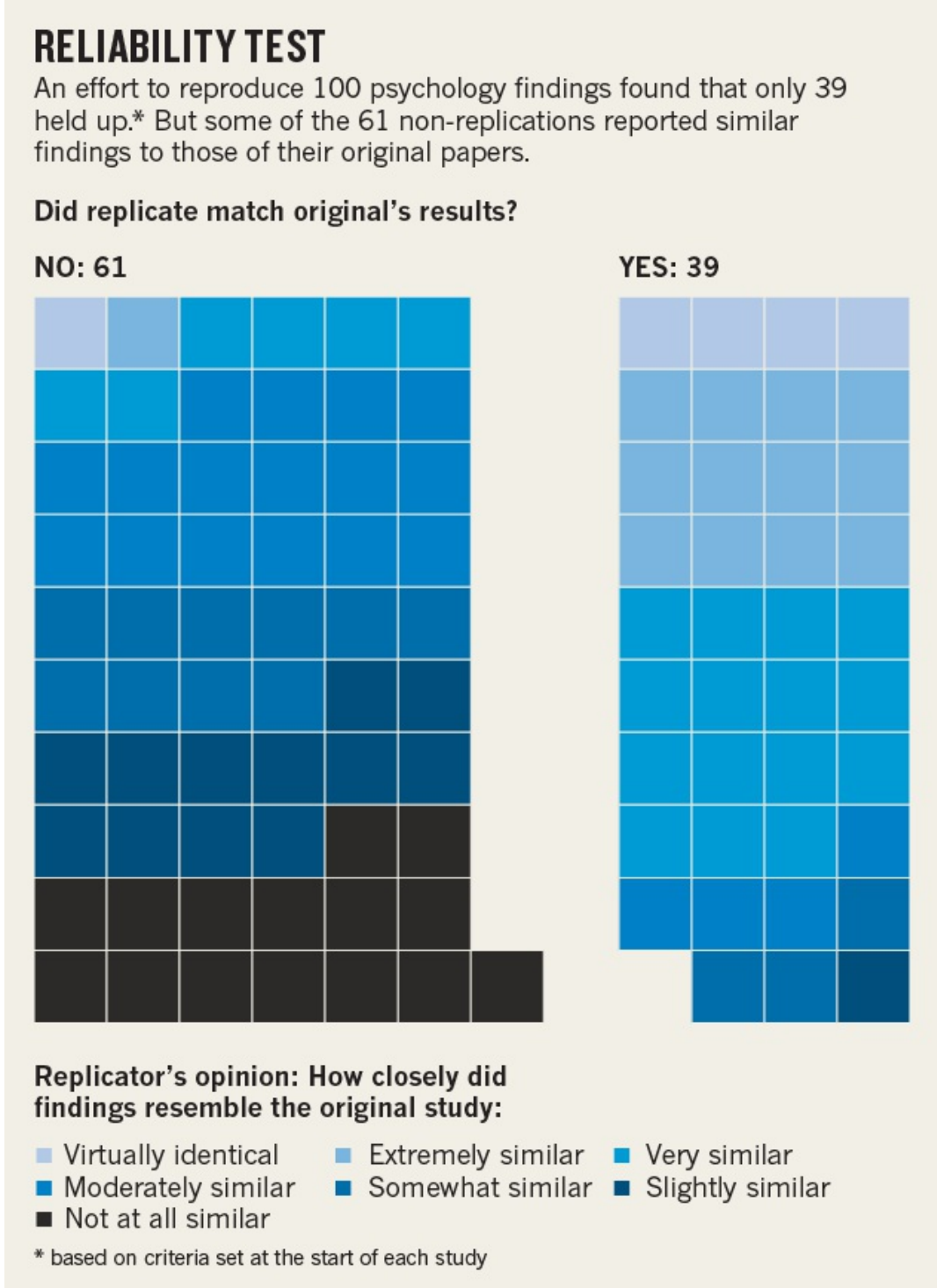
Irreproducibility indicators

- ‘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...’
- ‘On what dataset have I compared algorithms exactly?’
- ‘Why did I do that?!’
- ‘It worked yesterday!!’

Reproducibility concern: psychology

- 2011
- 250 scientists headed by Brian Nosek (Center of Open Science)
- 100 papers published in 2008 in three leading psychology journals
- https://osf.io/ezcuj/wiki/home/
- "only 39 could be reproduced"



http://www.nature.com/news/first-results-from-psychology-s-largest-reproducibility-test-1.17433

Reproducibility concern: biology

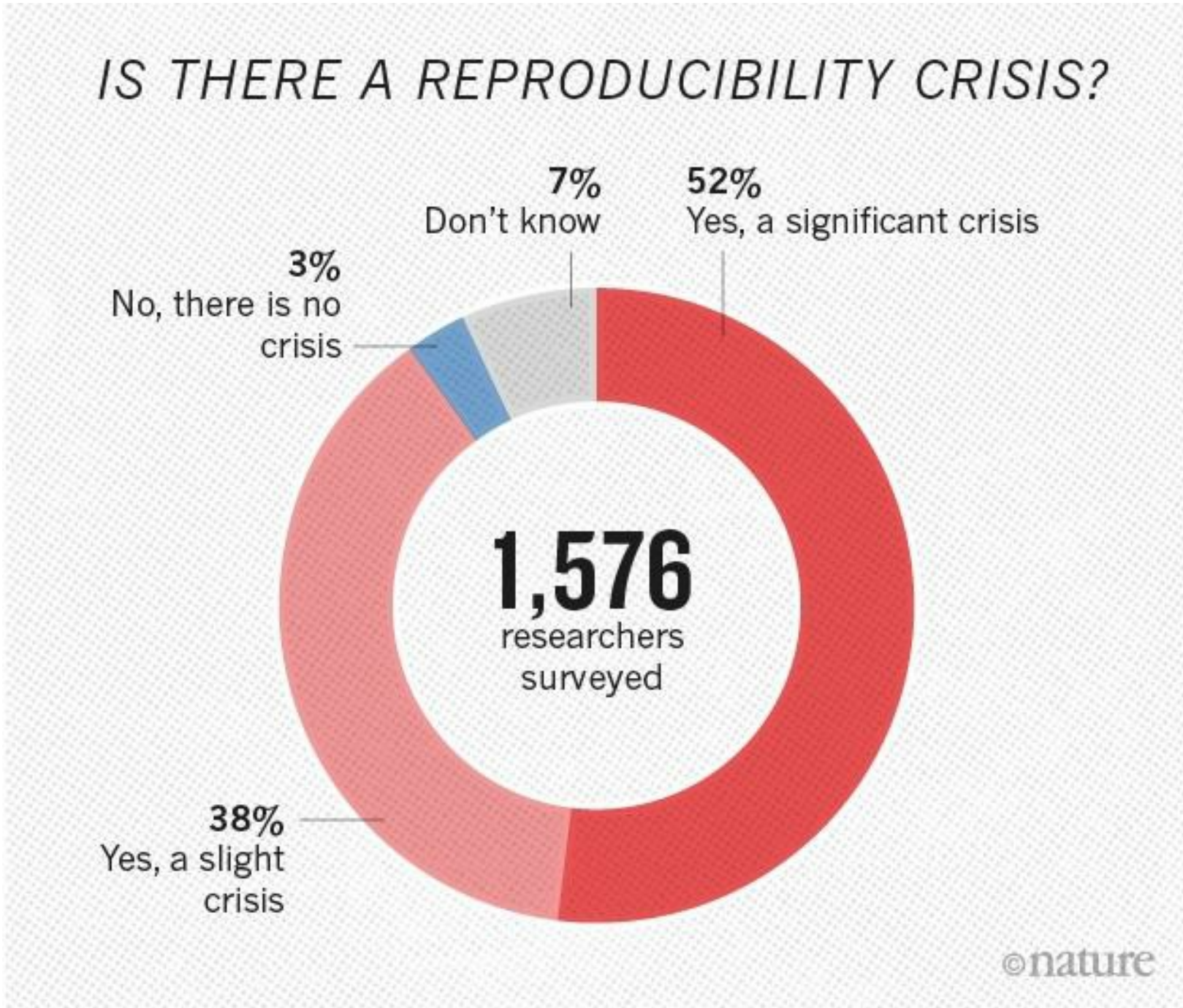
- 53 'landmark' papers in drug discovery
- 2012 by Amgen (US company)
- "confirmed in only 6 (11%) cases"

- 54 papers in cancer biology 2010-2012
- 2013
- US$1.6 million
- results, spreadsheet
- https://osf.io/e81xl/wiki/home/
- to be completed by 2017

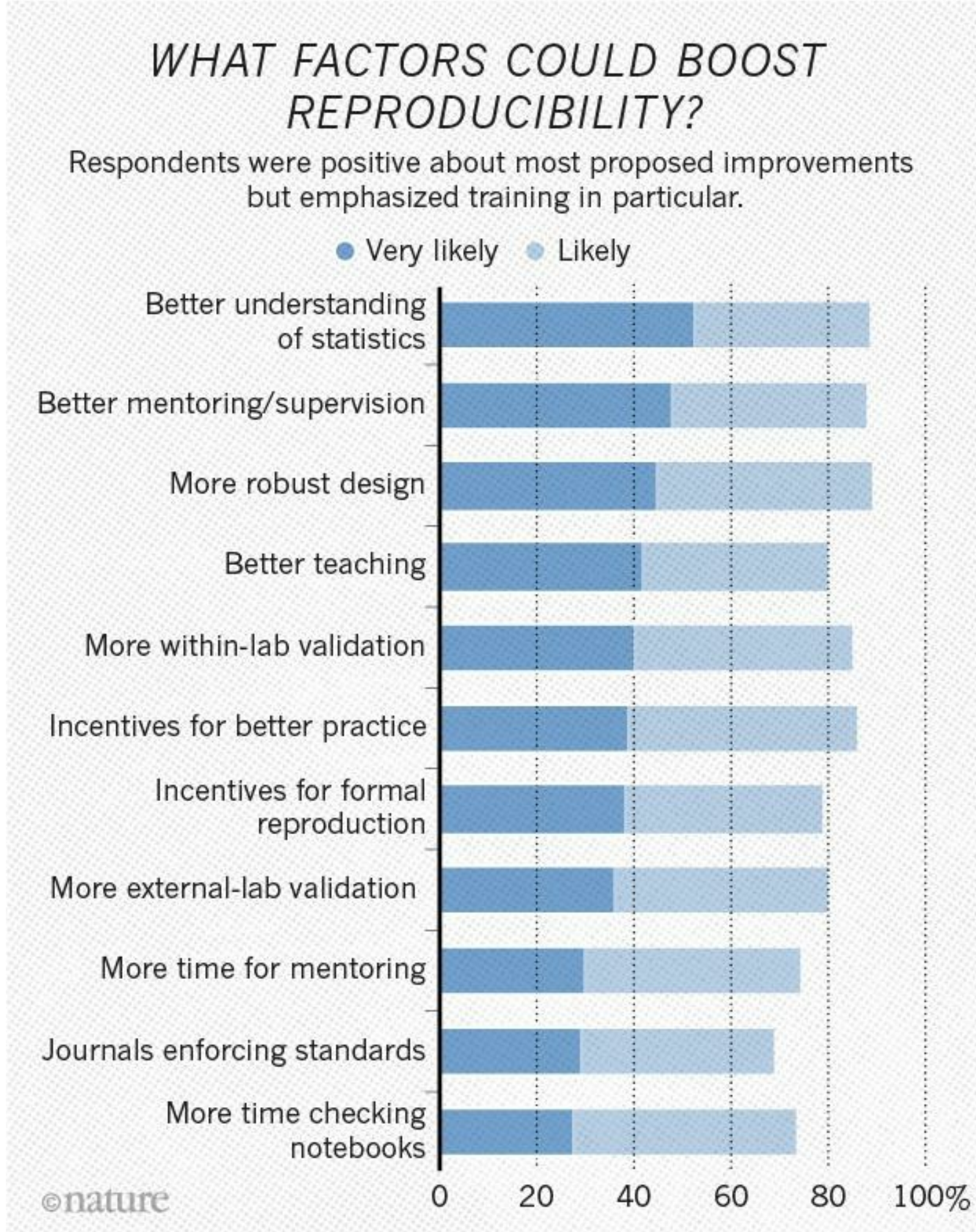
http://www.nature.com/nature/journal/v483/n7391/full/483531a.html

http://www.nature.com/news/cancer-reproducibility-project-scales-back-ambitions-1.18938

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

Rise of challenge-driven education

Learning by solving real-world problems in interdisciplinary & international projects.

- Imagine Cup, http://imaginecup.com/
- Hackathons, e.g., http://webfest.web.cern.ch/
- Open data days, http://opendataday.org/
- Guide to Challenge Driven Education, https://www.kth.se/social/group/guide-to-challenge-d/

Platforms (with plenty of examples):

- Kaggle, https://www.kaggle.com/
- Codalab, https://competitions.codalab.org/
- ...

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Complication and boost factors are similar to research reproducibility.

...part of the story

***Computational experiment* is a significant part of the experiment, that starts as data collected. Reproducibility of that part being just a partial answer can be aided technologically.**

Possible effects (see previous slide):

- 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

HEP way

- **data** storage
  - shared storage (XROOTD, AFS, EOS, CERNBOX)
- standardized **environment**
  - software: ROOT, minuit, RooFit, experiment-stack, ...
  - 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
- double experiment-checks

Reproducibility meta-practices

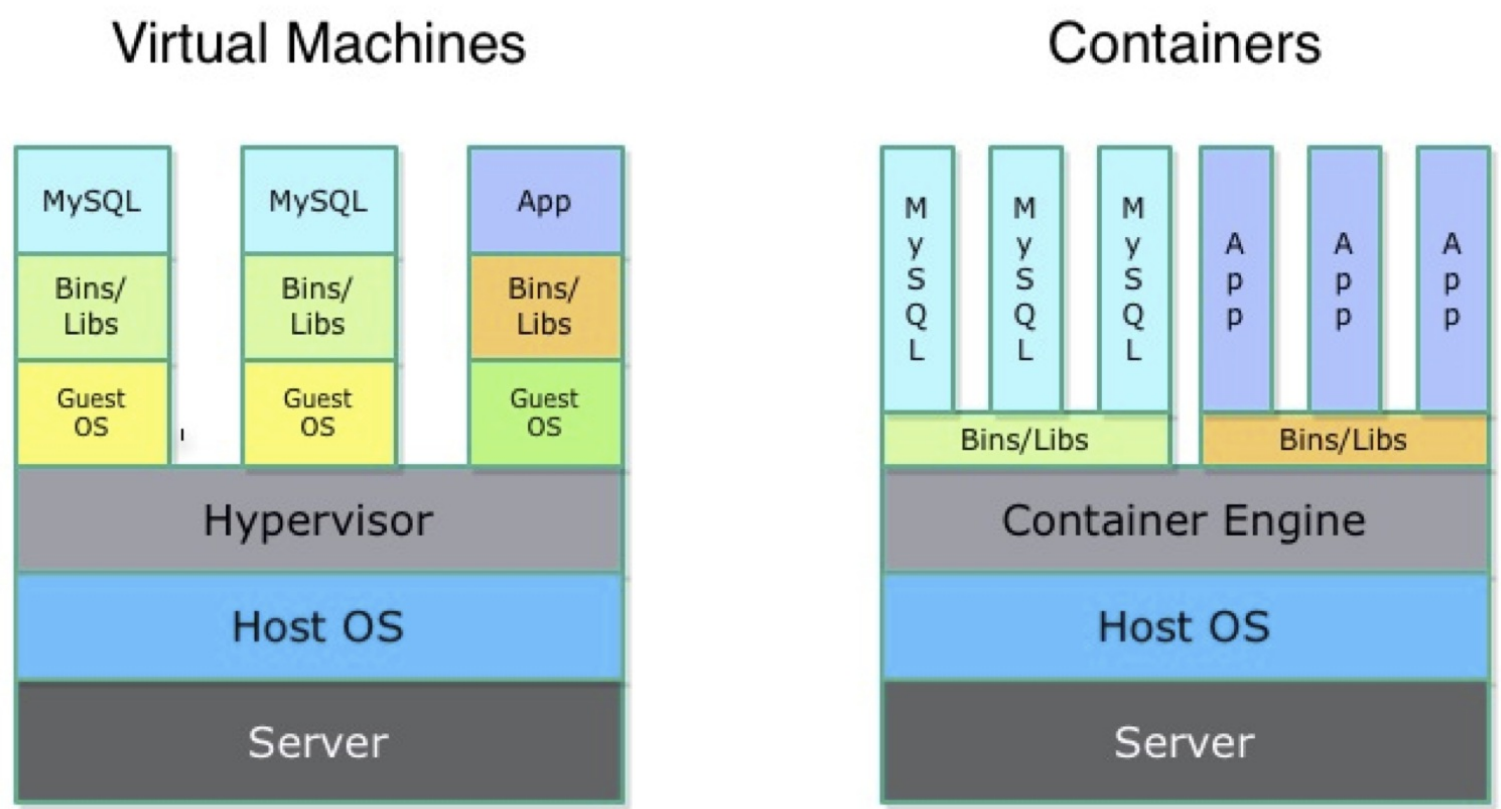
- early planning, pre-registering study
- literate programming
- open research/study

Reproducibility key components

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

Key missing part: environment version control

- language and OS agnostic,
- capture and restore environment configuration,
- run configurations



would enable:

- workflow automation
- automated results re-validation

Example

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

Sorry, printed version doesn't support animation.
https://github.com/everware/everware-dimuon-example

How it works

- **resources**: wherever *everware* is installed (Yandex)
- **data**: CERNBOX

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- **everware**: to rule them all (just a bunch of wrappers!)

Everware is ...

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

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

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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Think of transition from procedural coding approach to object-oriented.

Everware toolkit

- set of command-line tools for basic environment hacking (docker)
- extension for *JupyterHub*:
  - spawner for building and running custom *docker* images
- integrated with:
  - dockerhub
  - github (for authentication and repository interaction)
- similar to *mybinder.org* but with focus on scientific research
- guidelines

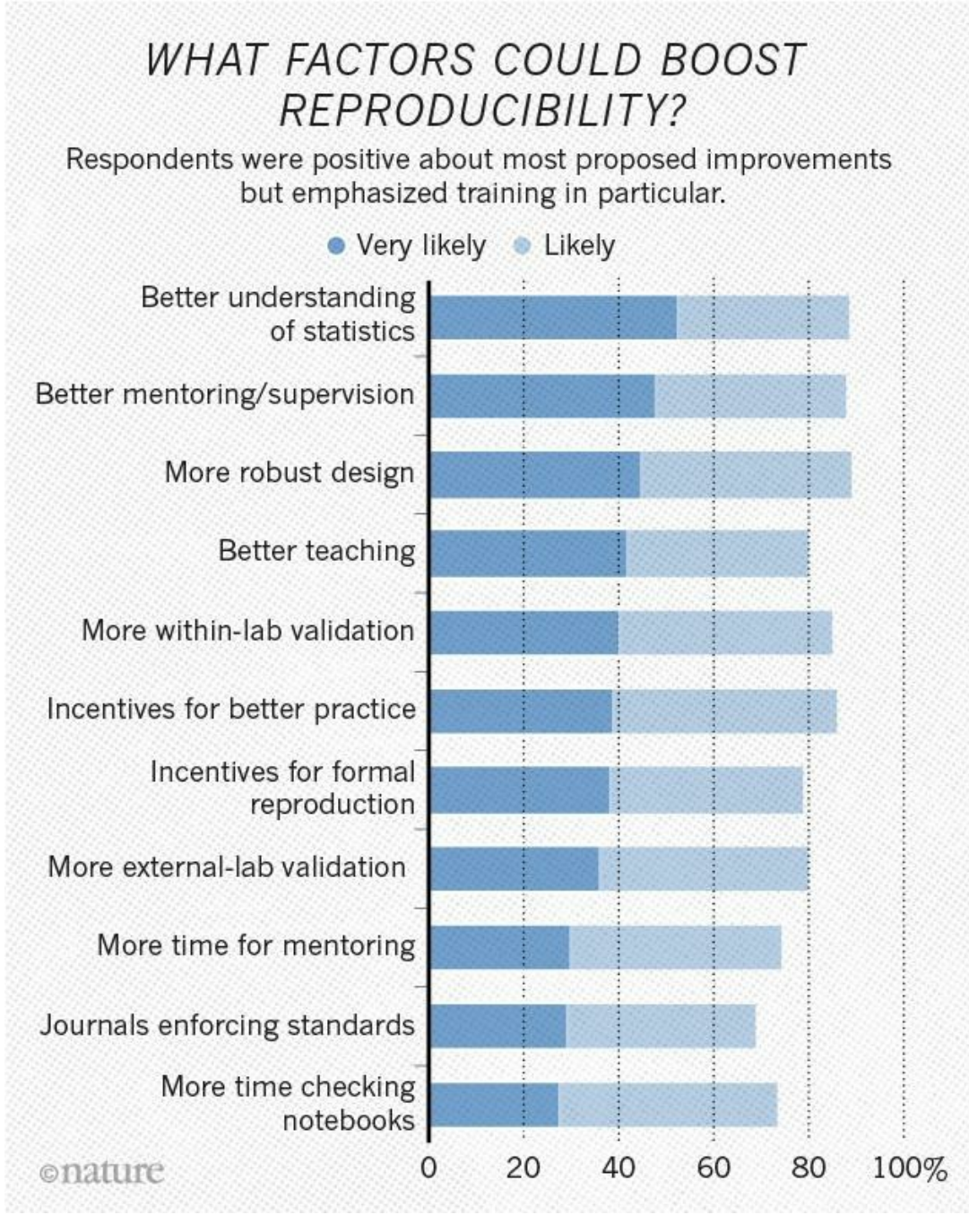
Pros & cons

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-sourced) technology
- re-organize internal research process
- inner barrier for openness
- higher incentive for mindless *borrowing*
- divergence/potential learning curves

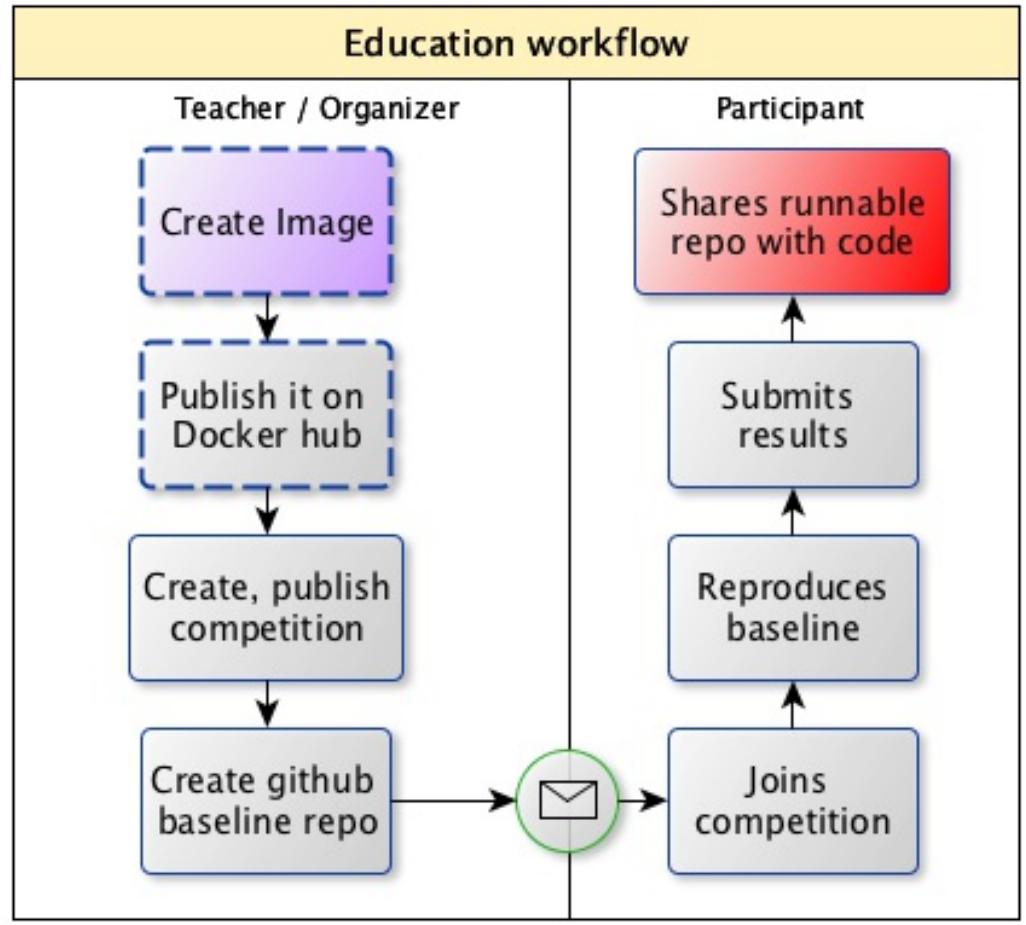


Research workflow with everware

- User creates a git repository for his project
- User creates some code, notebooks, figures out what libraries he needs
- User creates `Dockerfile` where he writes all the dependencies for his code (use `everware-cli`)
- User creates `Makefile` that simplifies start one of the targets in `Makefile` passes through all the essential steps of analysis
- (optional) User tests that his analysis is runnable by one of the CI systems (e.g. on travis, adding, `.travis.yml`)
- User tests that analysis is also runnable by everware
- User completes his research and checks that he/she can reproduce all the figures/tables supporting his hypothesis by running corresponding notebooks (or automates cascade of notebooks execution by single `Makefile` target)
- User publishes paper, filling-in special form link to his git repository and to everware that any member of the researcher community can pick-up from to improve his research

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

Education workflow with everware



Tested on (some examples):

- Python course at YSDA 2015
- HEP Machine Learning summer school 2015-2016
- 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 is not easy;
  - ...but is not that scary,
  - ...with a bit of openness,
  - and technology;
- *everware works* for research and education (no people were harmed during testing);
  - easy to try;
  - WIP, https://github.com/everware (open-source, care to join?);
  - See talk on LHCb open data masterclass for an extensive example.

Thank you!

Andrey Ustyuzhanin, anaderiru @ twitter

Slideshow created using remark

Backup slides

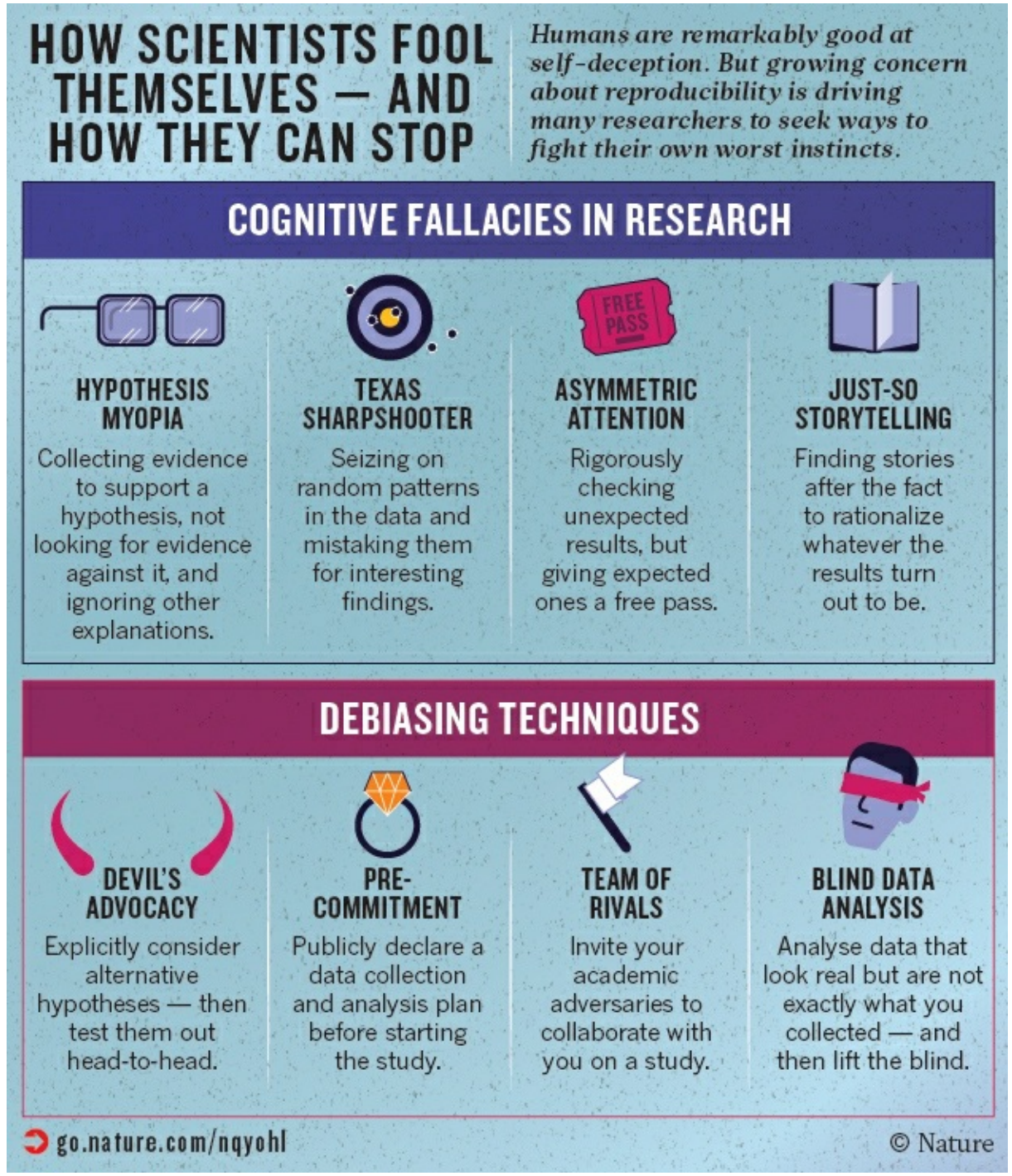
Yandex School of Data Analysis is

- non commercial private university https://yandexdataschool.com (separate from Yandex)
- 450+ students graduated since 2007
- Graduate students receive strong education in Data & Computer Science (main supply of Yandex employees)
- Interest in interdisciplinary research — Data Science methods to Information Retrieval and Fundamental Sciences
- organizes bi-yearly international Machine Learning Conference, YAC https://yandexdataschool.com/conference/
- 25% of our students have background in Physics
- full member of LHCb since 2015, associate member during 2014-2015

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