

# Build your own Virtual Research Environment for Reproducible Research

Georgios Kaklamanos 17.07.2017

Gesellschaft für wissenschaftliche Datenverarbeitung Göttingen Georg-August-Universität Göttingen



# REPRODUCIBLE RESEARCH

# "Hypothetical" Scenarios



- Submitted a paper
  - Review process takes months
  - Requests to modify parameters / figures
  - Need to run / modify code from 6 months ago
- Found a paper which could help significantly in your research
  - No source code
  - No data

# "Hypothetical" Scenarios



- Received a zip archive with files and code from a previous student at your lab
  - Student has left
  - Code doesn't compile
  - No documentation
  - Program is critical to continue the project...
- These are global reproducibility problems



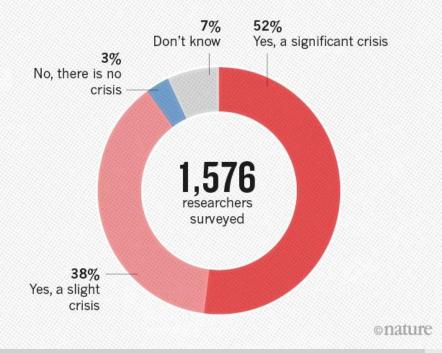


#### Nature Survey denotes a reproducibility crisis

- 70% of researchers
  - failed to reproduce other scientists experiments

- 50% of researchers
  - failed to reproduce own experiments

#### IS THERE A REPRODUCIBILITY CRISIS?



Source: [1]





#### How does it look across the fields?

- Phycology, 2006 study [2]
  - 249 data sets from American Psychology Association (APA) empirical articles
  - 73% of contacted authors did not respond with their data over a 6-month period.
- Cancer Research, 2012 study [3]
  - 47 out of 53 medical research papers were irreproducible (90%)
- Applied Computer Science, 2014 study [4]
  - 613 papers
  - 102 had code that could build and run



# How did we get here? Novelty Researcher!= Inventor



# "Nullius in Verba"

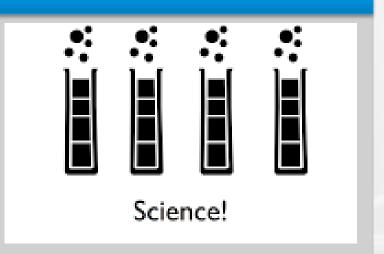
"It is an expression of the determination of Fellows to withstand the domination of authority and to verify all statements by an appeal to facts determined by experiment."

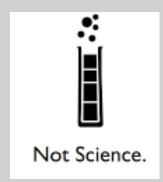
**Royal Society** 

# What is Replication



- Ultimate Standard for scientific evidence
- Ability to:
  - reproduce findings and conduct studies
  - with independent
    - Investigators
    - Data
    - Analytical methods
    - Laboratories
    - Instruments





Img source: <a href="http://blog.abegong.com/2013/12/replication-is-only-hope-for-science.html">http://blog.abegong.com/2013/12/replication-is-only-hope-for-science.html</a>

# **Replication Problems**



- Not all studies can be easily replicated
- Unique Cases
  - AstronomicObservations
- Time Constrains
  - Studies that span decades
- Infrastructure
  - Big Data / HPC access
- Costs

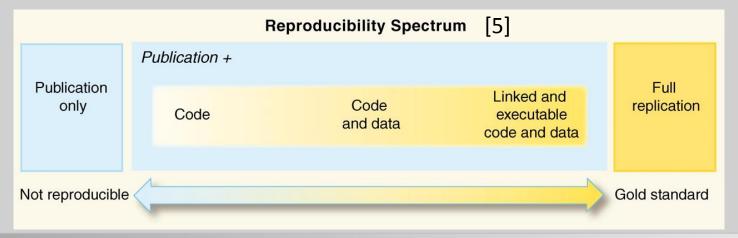






11

- Bridges the gap between replication and stand-alone study
- Uses same code / data / methodology
  - Validate findings



## Replication VS Reproducibility



- Focus:
  - Validity of Scientific Claim
- Asks:
  - "Is the claim true?"
- Reproduce results:
  - new investigators
  - New data, methods,
- Ultimate Standard for strengthening scientific evidence

- Focus:
  - Validity of data analysis
- Asks:
  - Can we trust this analysis?
- Reproduce Results
  - New investigators
  - Same data, methods,
- A minimum standard for any scientific work





#### **Among others**

- Individuals
  - Easier to Reproduce your Research
  - Easier to onboard new researchers on the group
  - Easier to share research with other researcher





#### Among others

- Community
  - Easier to disseminate results
  - Increase public trust in science
  - Able to assess the procedure of the analysis, not only the final outcome

# Reproducibility Facets



- We can make our research reproducible by focusing on these aspects:
  - Documentation
  - Organization
  - Automation
  - Dissemination



# INTRODUCTION TO JUPYTER

# Connecting to VMs



- All of you should have gotten information about how to connect to your VMs
  - Username
  - Password
  - -IP
- Windows Users: Putty
- Linux / MacOS Users: Terminal

# Workshop Repository



 The material of the workshop is stored in GitHub and served under this website

https://gwdg.github.io/ssgoe2017/

## **Gitter**



- A messaging platform
- **III**GITTER
- Focused on developers using GitHub
- There is a room for the workshop repository
- You can access from Gitter button on the workshop website

# **Etherpad**



To share notes during the workshop

https://etherpad.gwdg.de/p/ssgoe2017

## Q & A





Copyright note: Some slides in this presentation includes figures, trademarks, logos which are properties of third parties. Rights are reserved to the corresponding rights owners.

### References



#### References

- [1]: Monya Baker, 1.500 scientists lift the lid on reproducibility, Nature, https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970
- [2]: The poor availability of psychological research data for reanalysis. Wicherts, Jelte M.; Borsboom, Denny; Kats, Judith; Molenaar, Dylan American Psychologist, Vol 61(7), Oct 2006, 726-728. <a href="http://dx.doi.org/10.1037/0003-066X.61.7.726">http://dx.doi.org/10.1037/0003-066X.61.7.726</a>
- [3]: Drug development: Raise standards for preclinical cancer research,
   C. Glenn Begley & Lee M. Ellis, Nature 483, 531–533 (29 March 2012)
   doi:10.1038/483531a
- [4]: Collberg, Christian, et al. "Measuring reproducibility in computer systems research." Department of Computer Science, University of Arizona, Tech. Rep (2014).
- [5]: Roger D. Peng, Reproducible Research in Computational Science, Science 02 Dec 2011: Vol. 334, Issue 6060, pp. 1226-1227 DOI: 10.1126/science.1213847