Moore / Sloan Data Science Environment

Working Group on Reproducibility and Open Science

Randy LeVeque
David Beck
Joe Hellerstein
Bill Howe
Dan Halperin
Stephanie Wright
Many others... You??

http://escience.washington.edu/reproducible http://uwescience.github.io/reproducible

Ability to determine exactly how scientific results were obtained.

- Basis of scientific method.
- Required for confidently building on past results.
- Critical for accountability in engineering analysis / decision making.

Ability to determine exactly how scientific results were obtained.

- Basis of scientific method.
- Required for confidently building on past results.
- Critical for accountability in engineering analysis / decision making.

Standards and best practices in computational/data science are not yet well codified.

Ability to determine exactly how scientific results were obtained.

- Basis of scientific method.
- Required for confidently building on past results.
- Critical for accountability in engineering analysis / decision making.

Standards and best practices in computational/data science are not yet well codified.

 Experimental science: Lab notebooks, methodology section of publications, etc.

Ability to determine exactly how scientific results were obtained.

- · Basis of scientific method.
- Required for confidently building on past results.
- Critical for accountability in engineering analysis / decision making.

Standards and best practices in computational/data science are not yet well codified.

- Experimental science: Lab notebooks, methodology section of publications, etc.
- Mathematics: Proofs are required in publications.

Quote from Reproducible Research: A Cautionary Tale

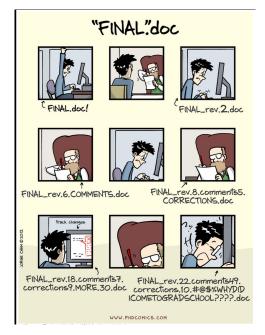
By David Crotty, March 26, 2014 on the scholarly kitchen blog

If your experiment consists of running numerical data through an algorithm, then releasing your data and your code allows others to quickly verify that you've done what you've said you've done. But when it comes to other types of research, wet bench experiments or observational work for example, reproduction is not quite so simple. Quote from Reproducible Research: A Cautionary Tale

By David Crotty, March 26, 2014 on the scholarly kitchen blog

If your experiment consists of running numerical data through an algorithm, then releasing your data and your code allows others to quickly verify that you've done what you've said you've done. But when it comes to other types of research, wet bench experiments or observational work for example, reproduction is not quite so simple.

If only it were so easy in computational/data science!



Private reproducibility...

Use scripts, not GUIs, for data analysis and visualization.

Use version control / provenance tracking tools.

Archive code and data used for published results.

Private reproducibility...

Use scripts, not GUIs, for data analysis and visualization.

Use version control / provenance tracking tools.

Archive code and data used for published results.

Why?

- Ability to check results in prior publication,
- Ability to build on your own past research of your own (or students / collaborators).
- Easily modify tables/figures to satisfy referees, etc.

Private reproducibility...

Use scripts, not GUIs, for data analysis and visualization.

Use version control / provenance tracking tools.

Archive code and data used for published results.

Why?

- Ability to check results in prior publication,
- Ability to build on your own past research of your own (or students / collaborators).
- Easily modify tables/figures to satisfy referees, etc.

Auditable Research: Even if code and data are not shared, there should be a permanent record that can be checked.

Analogous to lab notebooks.

Public Reproducibility...

Allowing others to reproduce your results. (Readers, referees, researchers down the hall...)

Public Reproducibility...

Allowing others to reproduce your results. (Readers, referees, researchers down the hall...)

Why?

- Verifying scientific integrity of results.
- Aids in understanding ideas, implementing methods
- Increases impact of work.

What does it mean that others can reproduce your results?

What does it mean that others can reproduce your results?

Possible answers...

 Download the code and type make plots, see identical plots appear.

What does it mean that others can reproduce your results?

Possible answers...

- Download the code and type make plots, see identical plots appear.
- Be able to implement the algorithm from description in paper and other archived sources, and get essentially the same results.

What does it mean that others can reproduce your results?

Possible answers...

- Download the code and type make plots, see identical plots appear.
- Be able to implement the algorithm from description in paper and other archived sources, and get essentially the same results.
- · Various things in between.

What does it mean that others can reproduce your results?

Possible answers...

- Download the code and type make plots, see identical plots appear.
- Be able to implement the algorithm from description in paper and other archived sources, and get essentially the same results.
- Various things in between.

Terms such as replicable or repeatable are sometimes used in addition to reproducible.

Science Code Manifesto

Manifesto Discussion Endorse Resources About

Software is a cornerstone of science. Without software, twenty-first century science would be impossible. Without better software, science cannot progress.

But the culture and institutions of science have not yet adjusted to this reality. We need to reform them to address this challenge, by adopting these five principles:

Code All source code written specifically to process data for a published paper must

be available to the reviewers and readers of the paper.

Copyright The copyright ownership and license of any released source code must be

clearly stated.

Citation Researchers who use or adapt science source code in their research must

credit the code's creators in resulting publications.

Credit Software contributions must be included in systems of scientific assessment,

credit, and recognition.

Curation Source code must remain available, linked to related materials, for the useful

lifetime of the publication.

Version control systems (VCS)
 CVS, Subversion (server-client),
 Git, Mercurial, Bazaar, etc. (distributed).

- Version control systems (VCS)
 CVS, Subversion (server-client),
 Git, Mercurial, Bazaar, etc. (distributed).
- Public hosting sites for VCS repositories
 Github, Bitbucket, Google code, sourceforge, etc.

Collaboration on open source projects, Archiving code used for publications.

- Version control systems (VCS)
 CVS, Subversion (server-client),
 Git, Mercurial, Bazaar, etc. (distributed).
- Public hosting sites for VCS repositories
 Github, Bitbucket, Google code, sourceforge, etc.

Collaboration on open source projects, Archiving code used for publications.

Other archives with stable URLs, DOIs
 Institutional or public data repositories, journal supplementary materials, figshare.com

Workflow Management Systems

VisTrails, Madagascar, Sumatra, Taverna, Galaxy, etc.

Capture the workflow used to generate figures, tables, etc.

Facilitate tracking the provinance of individual results. Data, code, compilers, graphics tools, etc.

Often work together with VCS for source code.

• Literate Programming tools

CWEB, Doxygen, Sphinx, Sweave, etc.

- Literate Programming tools
 CWEB, Doxygen, Sphinx, Sweave, etc.
- Notebooks / Publishing tools
 Mathematica, Maple, Matlab,
 Sage, IPython, knitr, RStudio, etc.

Virtualization

Package code along with complete environment (OS, compilers, graphics tools, etc.)

E.g., VirtualBox, VMware, etc.

Virtualization

Package code along with complete environment (OS, compilers, graphics tools, etc.)

E.g., VirtualBox, VMware, etc.

Cloud computing

E.g., Amazon EC2, Windows Azure, etc. + VM

Virtualization

Package code along with complete environment (OS, compilers, graphics tools, etc.)

E.g., VirtualBox, VMware, etc.

Cloud computing

E.g., Amazon EC2, Windows Azure, etc. + VM

Web platforms for running code

E.g., RunMyCode.org, wakari.io, cloud.sagemath.com

Policy Issues

Should journals require data/code sharing?

Policy Issues

Should journals require data/code sharing?

Some already do, e.g. Science:

Data and materials availability.

All data necessary to understand, assess, and extend the conclusions of the manuscript must be available to any reader of Science.

All computer codes involved in the creation or analysis of data must also be available to any reader of Science.

After publication, all reasonable requests for data and materials must be fulfilled.

http://www.sciencemag.org/site/feature/contribinfo/prep/

Certification of reproduciblity?

Stamp of reproducibility on journal papers.

E.g. Biostatistics awards "kite marks",

- D for data availability,
- C for code availability,
- R for full reproduciblity

Checked by "reproducibility editor".

Certification of reproduciblity?

Stamp of reproducibility on journal papers.

E.g. Biostatistics awards "kite marks",

- D for data availability,
- C for code availability,
- R for full reproduciblity

Checked by "reproducibility editor".

Campus-wide certification of labs or research groups following "best practices?" (What are these?)

Reward structure

What are the rewards / penalties for attempting to do reproducible research?

Often much more to be gained by moving on to next project than cleaning up and posting code.

Little recognition available vs. many potential downsides of sharing.

Reward structure

What are the rewards / penalties for attempting to do reproducible research?

Often much more to be gained by moving on to next project than cleaning up and posting code.

Little recognition available vs. many potential downsides of sharing.

How can we encourage more recognition and better support?

Concerns for young researchers in particular.

Reward structure

What are the rewards / penalties for attempting to do reproducible research?

Often much more to be gained by moving on to next project than cleaning up and posting code.

Little recognition available vs. many potential downsides of sharing.

How can we encourage more recognition and better support?

Concerns for young researchers in particular.

Altmetrics: Measuring contributions other than traditional journal publications, e.g., ImpactStory.org

Guidelines for Reproducibility & Open Science

See: http://uwescience.github.io/reproducible

Goals:

- To achieve greater scientific validity and integrity by making it easier to verify published results.
- To increase productivity of current and future researchers on funded projects.
- To increase the impact of the research performed, software developed, and papers published.
- To help promote data and code as first class research products.
- To increase access to and usability of research products by other researchers.
- To use the DSE as a test bed for developing and promoting tools and cultural changes across a broad spectrum of academic disciplines.