Scientific Reproducibility and Software

Victoria Stodden
Information Society Project @ Yale Law School
<vcs@stanford.edu>

Institute for Computational Engineering and Sciences
The University of Texas at Austin
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Agenda

1. Error Control: V, V, & EQ
2. Hypothesis: Increased Reproducibility Needed to comply with the Scientific Method
3. Survey: Barriers to Open Code/Data
4. Untangling Intellectual Property Issues
5. Barriers in like software lockin and idea evolution (Gaussian) Software needs: analog to digital so need to track (survey)
Controlling Error is Central to Scientific Progress

“The scientific method’s central motivation is the ubiquity of error - the awareness that mistakes and self-delusion can creep in absolutely anywhere and that the scientist’s effort is primarily expended in recognizing and rooting out error.” David Donoho et al. (2009)
Software Verification

• Accuracy with which a computational model delivers the results of the underlying mathematical model:
  - *Solution verification*: does the discretization error approach zero as we approach the continuous model?
  - *Code verification*: test suites: problems with known solutions, known rates of convergence..
Model Validation

- Accuracy of a computational model with respect to observed data:
  - Model error: misspecification
  - Observation error, measurement error
Uncertainty Quantification

- Numerical accuracy of estimates,
- Sensitivity of given results to boundary conditions,
- Model calibration metrics,
- Parameter estimation, confidence intervals.
Controlling Error is Central to the Scientific Method

In stochastic modeling “the possibility of erroneous decisions cannot be eliminated, and the best one can do is to seek methods of making decisions that, in a sense, minimize the risk of mistakes.” Jerzy Neyman, “Statistics - Servant of All Sciences,” *Science*, 1955, p. 401
Hypothesis

- Verification, Validation, & Error Quantification are necessary but not sufficient for the practice of the scientific method.

- Error control is not insular, but also involves community vetting.
Reproducibility

- Computational science: researcher works with code or data in generating published results.
- Reproducibility: the ability of other to recreate and verify computational results, given appropriate software and computing resources.
Reproducibility: Hypothesis

- Facts are established through social acceptance (Latour), through independent replication through open inspection.

- Reproducibility of results is essential for computational science to conform with the scientific method.
Science is Changing

- A transformation of the scientific enterprise through massive computation, in scale, scope, and pervasiveness, is currently underway.

- JASA June 1996: 9 of 20 articles computational
- JASA June 2006: 33 of 35 articles computational
Example: Community Climate System Model (CCSM)

- Collaborative system simulation
- Code available by permission
- Data output files by permission
Example: High Energy Physics

- 4 LHC experiments at CERN: 15 petabytes produced annually
- Data shared through grid to mobilize computing power
- Director of CERN (Heuer): “Ten or 20 years ago we might have been able to repeat an experiment. They were simpler, cheaper and on a smaller scale. Today that is not the case. So if we need to re-evaluate the data we collect to test a new theory, or adjust it to a new development, we are going to have to be able reuse it. That means we are going to need to save it as open data....” Computer Weekly, August 6, 2008
Example: Astrophysics Simulation Collaboratory

- Data and code sharing within community
- Interface for dynamic simulation
- mid 1930’s: calculate the motion of cosmic rays in Earth’s magnetic field
Example: Proofs

- Mathematical proof via simulation, not deduction
- Breakdown point: \( \frac{1}{\sqrt{2\log(p)}} \)

- A valid proof?
- A contribution to the field of mathematics?
The Third Branch of the Scientific Method

- Branch 1: *Deductive/Theory*: e.g. mathematics; logic
- Branch 2: *Inductive/Empirical*: e.g. the machinery of hypothesis testing; statistical analysis of controlled experiments
- Branch 3: Large scale extrapolation and prediction: Knowledge from computation or tools for established branches?
Contention About 3rd Branch

- Anderson: The End of Theory. (Wired, June 2008)
- Hillis Rebuttal: We are looking for patterns first then create hypotheses as we always have.. (The Edge, June 2008)
- Weinstein: Simulation underlies existing branches
  1. Tools to build intuition (branch 1)
  2. Hypotheses to test (branch 2)
Emerging Credibility Crisis in Computational Science

- Typical scientific communication doesn’t include code, data, test suites.
- Much published computational science near impossible to replicate.

- Accession to 3rd branch of the scientific method involves the production of *routinely verifiable knowledge*. 
Potential Solution:
Really Reproducible Research

Pioneered by Jon Claerbout

“An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.”

(quote from David Donoho, “Wavelab and Reproducible Research,” 1995)
Barriers to Sharing: Survey

Hypotheses:

1. Scientists are primarily motivated by personal gain or loss.

2. Scientists are primarily worried about being scooped.
Survey of Computational Scientists

- **Subfield**: Machine Learning
- **Sample**: American academics registered at top Machine Learning conference (NIPS).
- **Respondents**: 134 responses from 638 requests.
Reported Sharing Habits

- 81% claim to reveal some code and 84% claim to reveal some data.
- Visual inspection of their websites: 30% had some code posted, 20% had some data posted.
## Top Reasons Not to Share

<table>
<thead>
<tr>
<th>Code</th>
<th>Reason</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>77%</td>
<td>Time to document and clean up</td>
<td>54%</td>
</tr>
<tr>
<td>44%</td>
<td>Not receiving attribution</td>
<td>42%</td>
</tr>
<tr>
<td>40%</td>
<td>Possibility of patents</td>
<td>-</td>
</tr>
<tr>
<td>34%</td>
<td>Legal barriers (ie. copyright)</td>
<td>41%</td>
</tr>
<tr>
<td>-</td>
<td>Time to verify release with admin</td>
<td>38%</td>
</tr>
<tr>
<td>30%</td>
<td>Potential loss of future publications</td>
<td>35%</td>
</tr>
<tr>
<td>52%</td>
<td>Dealing with questions from users</td>
<td>34%</td>
</tr>
<tr>
<td>30%</td>
<td>Competitors may get an advantage</td>
<td>33%</td>
</tr>
<tr>
<td>20%</td>
<td>Web/Disk space limitations</td>
<td>29%</td>
</tr>
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For example..

"Behind one door is tenure - behind the other is flipping burgers at McDonald's."
# Top Reasons to Share

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<tbody>
<tr>
<td>91%</td>
<td>Encourage scientific advancement</td>
<td>81%</td>
</tr>
<tr>
<td>90%</td>
<td>Encourage sharing in others</td>
<td>79%</td>
</tr>
<tr>
<td>86%</td>
<td>Be a good community member</td>
<td>79%</td>
</tr>
<tr>
<td>82%</td>
<td>Set a standard for the field</td>
<td>76%</td>
</tr>
<tr>
<td>85%</td>
<td>Improve the caliber of research</td>
<td>74%</td>
</tr>
<tr>
<td>81%</td>
<td>Get others to work on the problem</td>
<td>79%</td>
</tr>
<tr>
<td>85%</td>
<td>Increase in publicity</td>
<td>73%</td>
</tr>
<tr>
<td>78%</td>
<td>Opportunity for feedback</td>
<td>71%</td>
</tr>
<tr>
<td>71%</td>
<td>Finding collaborators</td>
<td>71%</td>
</tr>
</tbody>
</table>
**Have you been scooped?**

<table>
<thead>
<tr>
<th>Idea Theft</th>
<th>Count</th>
<th>Proportion</th>
</tr>
</thead>
<tbody>
<tr>
<td>At least one publication scooped</td>
<td>53</td>
<td>0.51</td>
</tr>
<tr>
<td>2 or more scooped</td>
<td>31</td>
<td>0.30</td>
</tr>
<tr>
<td>No ideas stolen</td>
<td>50</td>
<td>0.49</td>
</tr>
</tbody>
</table>
Preliminary Findings

- *Surprise*: Motivated to share by communitarian ideals.
- *Not surprising*: Reasons for not revealing reflect private incentives.
- *Surprise*: Scientists not that worried about being scooped.
- *Surprise*: Scientists quite worried about IP issues.
Legal Barriers to Reproducibility

- Original expression of ideas falls under copyright by default (written expression, code, figures, tables..)

- Copyright creates exclusive rights vested in the author to:
  - reproduce the work
  - prepare derivative works based upon the original
  - Exceptions and limitations: Fair Use, Academic purposes
Creative Commons

- Founded by Larry Lessig to make it easier for artists to share and use creative works
- A suite of licenses that allows the author to determine terms of use attached to works
Creative Commons Licenses

• A notice posted by the author removing the default rights conferred by copyright and adding a selection of:
  • BY: if you use the work attribution must be provided,
  • NC: work cannot be used for commercial purposes,
  • ND: derivative works not permitted,
  • SA: derivative works must carry the same license as the original work.
Open Source Software Licensing

- Creative Commons follows the licensing approach used for open source software, but adapted for creative works

- Code licenses:
  - BSD license: attribution
  - GNU GPL: attribution and share alike
  - Hundreds of software licenses..
Apply to Scientific Work?

• Remove copyright’s block to fully reproducible research
• Attach a license with an attribution component to all elements of the research compendium (including code, data), encouraging full release.

Solution: Reproducible Research Standard
Reproducible Research Standard

Realignment of legal framework with scientific norms:

- Release media components (text, figures) under CC BY.
- Release code components under Modified BSD or similar.
- Both licenses free the scientific work of copying and reuse restrictions and have an attribution component.
“ShareAlike” Inappropriate

• “ShareAlike”: licensing provision that requires identical licensing of downstream libraries,
• Issue 1: Control of independent scientists’ work,
• Issue 2: Incompatibility of differing licenses with this provisions.
• GPL not suitable for scientific code.
Releasing Data?

• Raw facts not copyrightable.

• Original “selection and arrangement” of these facts is copyrightable. (Feist Publ’ns Inc. v. Rural Tel. Serv. Co., 499 U.S. 340 (1991))
Benefits of RRS

- Focus becomes release of the entire research compendium
- Hook for funders, journals, universities
- Standardization avoids license incompatibilities
- Clarity of rights (beyond Fair Use)
- IP framework supports scientific norms
- Facilitation of research, thus citation, discovery...
Reproducibility is an Open Problem (and scale matters)

- Simple case: open data and small scripts. Suits simple definition.
- Hard case: Inscrutable code, organic programming.
- Harder case: massive computing platforms, streaming data.
- Can we have reproducibility in the hard cases?
Solutions for Harder Cases

- Tools for reproducibility:
  - Standardized testbeds
  - Open code for continuous data processing, flags for “continuous verifiability”
  - Standards and platforms for data sharing
  - Provenance and workflow tracking tools (Mesirov)

- Tools for attribution:
  - Generalized contribution tracking
  - Legal attribution/license tracking tracking and search (RDFa)
Case Study: mloss.org

- Machine Learning Open Source Software
- Active code repository
- Code release at least as important as data release
- Open question: software support
Case Study: DANSE

- Neutron scattering
- Make new data available
- Unify software for analysis
Case Study: Wolfram|Alpha

- Obscure code - testbeds for verifiability
- Dataset construction methods opaque
- (claims copyright over outputs)
Openness and Taleb’s Criticism

- Open Access movement removes the notion of a scientific community

EVA: EVAluation of Automatic protein structure prediction

**Status:**
- four programs for secondary structure prediction tested every week

**Measuring accuracy:**
1. secondary structure prediction
2. comparative modelling

**Objectives**
CASP addresses the question 'how well can experts predict protein structure if given sufficient incentive to do so?'. In contrast, the questions addressed by EVA is 'how well could molecular biologists predict protein structure, if they simply take the output from the programs out there?'. Thus, the goals are:

- Provide a continuous, fully automated, and statistically significant analysis of structure prediction servers.
- As has been shown by many of us, predictions based on small numbers of samples are NOT representative. EVA running for a year could produce a fairly representative picture. Even running for a month EVA could produce more reliable estimates than CASP can do in 2 years (at least, for answering the particular, restricted — but important — question ‘how well do servers do’).
- EVA will NOT answer to requests of users!! It will NOT be a meta-server, rather it will simply sit there and evaluate servers based on known structures.
- EVA will NOT evaluate any server without the consent of the author. (Of course, the hope is that most of you to whom this message goes would co-operate.)
- We are seriously concerned about the ‘negative’ aspect of the freedom of the Web being that any newcomer can spend a day and hack out a program that predicts 3D structure, put it on the web, and it will be used.

**Technical aspects**
- Repeat: no use of EVA upon request, only for evaluation purposes.
- Targets: provided by the PDB pre-release, i.e. 20+ per week.
Real and Potential Wrinkles

- Reproducibility neither necessary nor sufficient for correctness, but essential for dispute resolution,
- Software “lock-in” and the evolution of scientific ideas (standards lock-in),
- Attribution in digital communication:
  - Legal attribution and academic citation not isomorphic
  - Contribution tracking (RDFa)
- RRS: Need for individual scientist to act,
- “progress depends on artificial aids becoming so familiar they are regarded as natural” I.J. Good, “How Much Science Can You Have at Your Fingertips”, 1958
Papers and Links

“Enabling Reproducible Research: Open Licensing for Scientific Innovation”

“15 Years of Reproducible Research in Computational Harmonic Analysis”

“The Legal Framework for Reproducible Research in the Sciences: Licensing and Copyright”

http://www.stanford.edu/~vcs
http://www.stanford.edu/~vcs/Conferences/RoundtableNov212009/
Appendix: Attribution

• Legal attribution and academic citation not isomorphhic.

• Minimize administrative burden
• Evolving norms / field specific norms / technology

• “keep intact all copyright notices for the Work and provide, reasonable to the medium or means You are utilizing…”