Reproducibility in High Performance Computing

Victoria Stodden
School of Information Sciences
University of Illinois at Urbana-Champaign

Invited Plenary - SC15
Austin, TX
November 18 2015

Agenda:
Sources of Irreproducibility and Solution Steps

1. Empirical Reproducibility
2. Computational Reproducibility:
    - Tools and Cyberinfrastructure
    - Community and Policy Responses
3. Statistical Reproducibility

Who am I?

- PhD in statistics and Law Degree from Stanford University.
- Associate Professor at the University of Illinois at Urbana-Champaign, School of Information Sciences.
- co-chair Advisory Committee, NSF Division of Advanced Cyberinfrastructure, member of the Advisory Committee for the NSF CISE Directorate.
- serves on the National Academies of Science committee on "Responsible Science: Ensuring the Integrity of the Research Process."

Credibility Crisis

Los Angeles Times | BUSINESS

LOCAL U.S. WORLD BUSINESS SPORTS ENTERTAINMENT HEALTH STYLE TRAV

Science has lost its way, at a big cost to humanity

Researchers are rewarded for splashy findings, not for double-checking accuracy. So many scientists looking for cures to diseases have been building on ideas that aren't even true.

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Home > Science Magazine > 17 January 2014 > McNutt, 343 (6168): 229

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Related Content

Science 17 January 2014:
Vol. 343 no. 6168 p. 229
DOI: 10.1126/science.1250475

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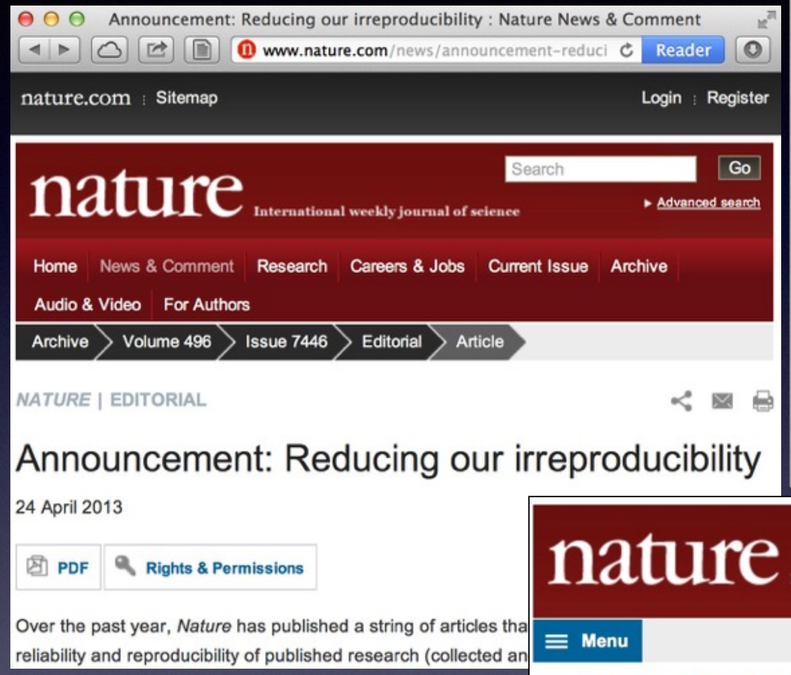
EDITORIAL

Reproducibility

Marcia McNutt

» Marcia McNutt is Editor-in-Chief of *Science*.

Science advances on a foundation of trusted di
approach that scientists use to gain confidence
community was shaken by reports that a troub
not reproducible. Because confidence in results
community, we are announcing new initiatives
Science. For preclinical studies (one of the targ
recommendations of the U.S. National Institute
increasing transparency.* Authors will indicate
handling (such as how to deal with outliers), wh
ensure a sufficient signal-to-noise ratio, wheth
experimenter was blind to the conduct of the e
guidelines.


Announcement: Reducing our irreproducibility : Nature News & Comment

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Archive > Volume 496 > Issue 7446 > Editorial > Article

NATURE | EDITORIAL

Announcement: Reducing our irreproducibility

24 April 2013

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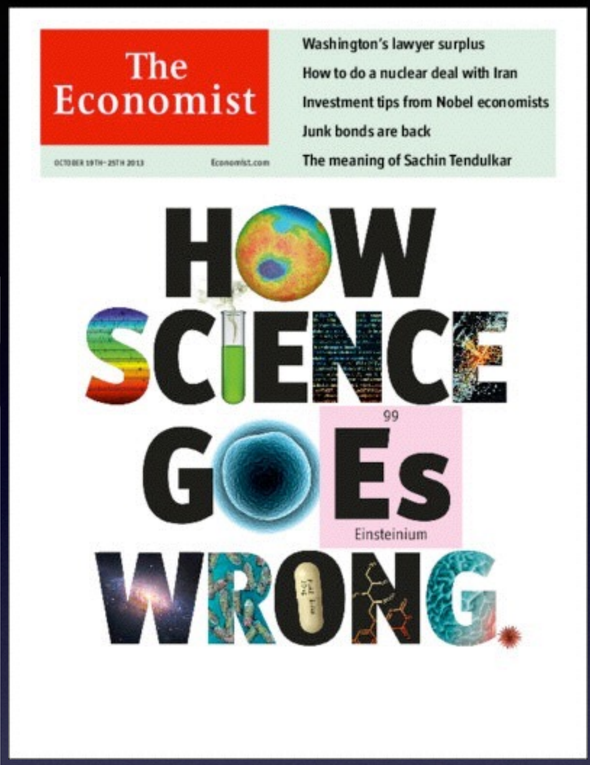
Over the past year, *Nature* has published a string of articles tha
reliability and reproducibility of published research (collected an


The Economist

Washington's lawyer surplus
How to do a nuclear deal with Iran
Investment tips from Nobel economists
Junk bonds are back
The meaning of Sachin Tendulkar

HOW SCIENCE GOES WRONG

99 Einsteinium

nature International weekly journal of science

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archive ▸ volume 483 ▸ issue 7391 ▸ editorials ▸ article

NATURE | EDITORIAL

Must try harder

Nature **483**, 509 (29 March 2012) | doi:10.1038/483509a
Published online 28 March 2012

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Too many sloppy mistakes are creeping into scientific papers. Lab heads must look more rigorously at the data — and at themselves.

TheScientist
EXPLORING LIFE. INSPIRING INNOVATION

NIH Tackles Irreproducibility

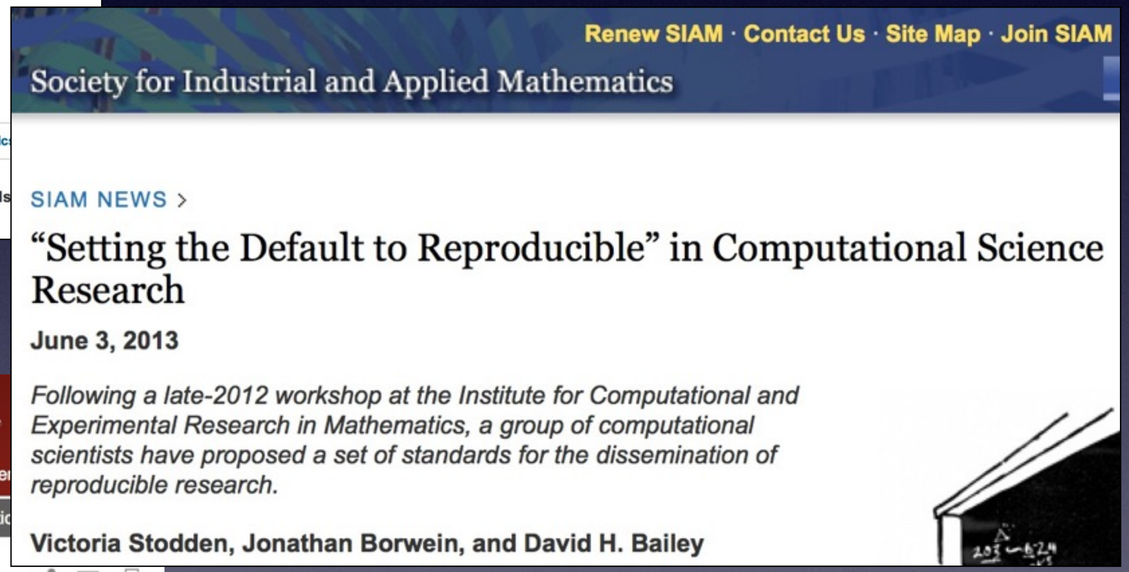
The federal agency speaks out about how to improve the quality of scientific research.

By Jef Akst | January 28, 2014

Unpacking "Reproducibility"

"Empirical Reproducibility"

"Computational Reproducibility"



"Statistical Reproducibility"

V. Stodden, IMS Bulletin (2013)

I. Empirical Reproducibility

Cell Reports
Commentary

Cell PRESS
Open ACCESS

Sorting Out the FACS: A Devil in the Details

William C. Hines,[1,5,*] Ying Su,[2,3,4,5,*] Irene Kuhn,[1] Kornelia Polyak,[2,3,4,5] and Mina J. Bissell[1,5]
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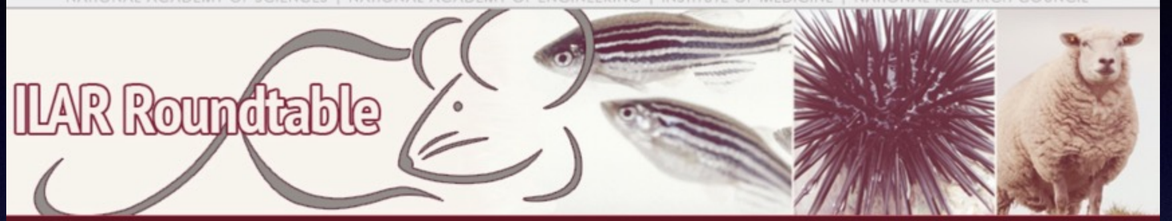
http://dx.doi.org/10.1016/j.celrep.2014.02.021

The reproduction of results is the cornerstone of science; yet, at times, reproducing the results of others can be a difficult challenge. Our two laboratories, one on the East and the other on the West Coast of the United States, decided to collaborate on a problem of mutual interest—namely, the heterogeneity of the human breast. Despite using seemingly identical methods, reagents, and specimens, our two laboratories quite reproducibly were unable to replicate each other's fluorescence-activated cell sorting (FACS) profiles of primary breast cells. Frustration of studying cells close to their context in vivo makes the exercise even more challenging.

Paired with in situ characterizations, FACS has emerged as the technology most suitable for distinguishing diversity among different cell populations in the mammary gland. Flow instruments have evolved from being able to detect only a few parameters to those now capable of measuring up to—and beyond—an astonishing 50 individual markers per cell (Cheung and Utz, 2011). As with any exponential increase in data complexity, breast reduction mammoplasties. Molecular analysis of separated fractions was to be performed in Boston (K.P.'s laboratory, Dana-Farber Cancer Institute, Harvard Medical School), whereas functional analysis of separated cell populations grown in 3D matrices was to take place in Berkeley (M.J.B.'s laboratory, Lawrence Berkeley National Lab, University of California, Berkeley). Both our laboratories have decades of experience and established protocols for isolating cells from primary normal breast tissues as well as the capabilities required for



Reproducibility Issues in Research with Animals and Animal Models

The missing "*R*": Reproducibility in a Changing Research Landscape

A workshop of the Roundtable on Science and Welfare in Laboratory Animal Use

National Academy of Sciences, NAS 125
2100 C Street NW, Washington DC
June 4-5, 2014

The ability to reproduce an experiment is one important approach that scientists use to gain confidence in their conclusions. Studies that show that a number of significant peer-reviewed studies are not reproducible has alarmed the scientific community. Research that uses animals and animal models seems to be one of the most susceptible to reproducibility issues.

Evidence indicates that there are many factors that may be contributing to scientific irreproducibility, including insufficient reporting of details pertaining to study design and planning; inappropriate interpretation of results; and author, reviewer, and editor abstracted reporting, assessing, and accepting studies for publication.

In this workshop, speakers from around the world will explore the many facets of the issue and potential pathways to reducing the problems. Audience participation portions of the workshop are designed to facilitate understanding of the issue.

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Upcoming Events
April 20-21, 2015
Design, Implementation, Monitoring and Sharing of Performance Standards

Past Events
September 3-4, 2014
Transportation of Laboratory Animals
• *Presentations and videos online*

June 4-5, 2014
Reproducibility Issues in Research with Animals and Animal Models
• *Presentations and videos online*

2. Computational Reproducibility

Traditionally two branches of the scientific method:

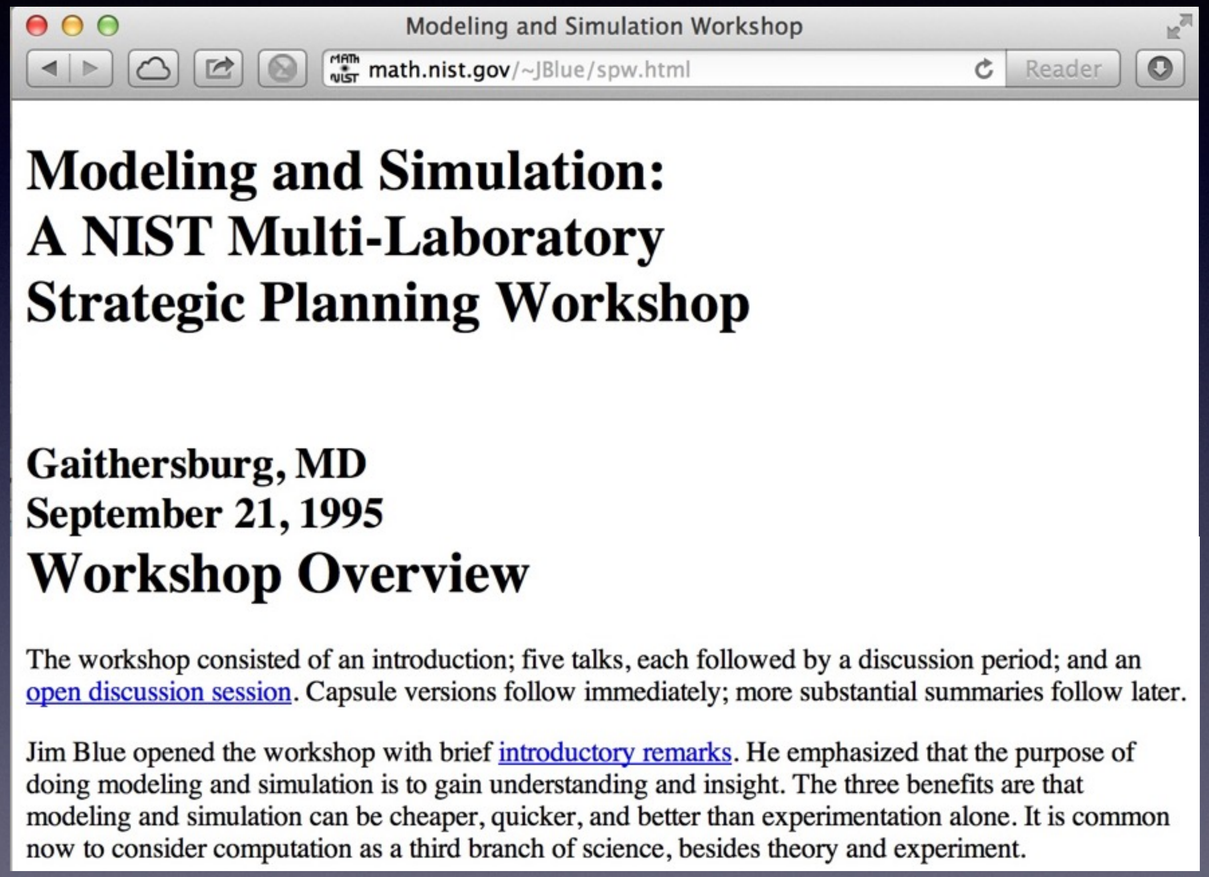
Branch 1 (deductive): mathematics, formal logic,

Branch 2 (empirical): statistical analysis of controlled experiments.

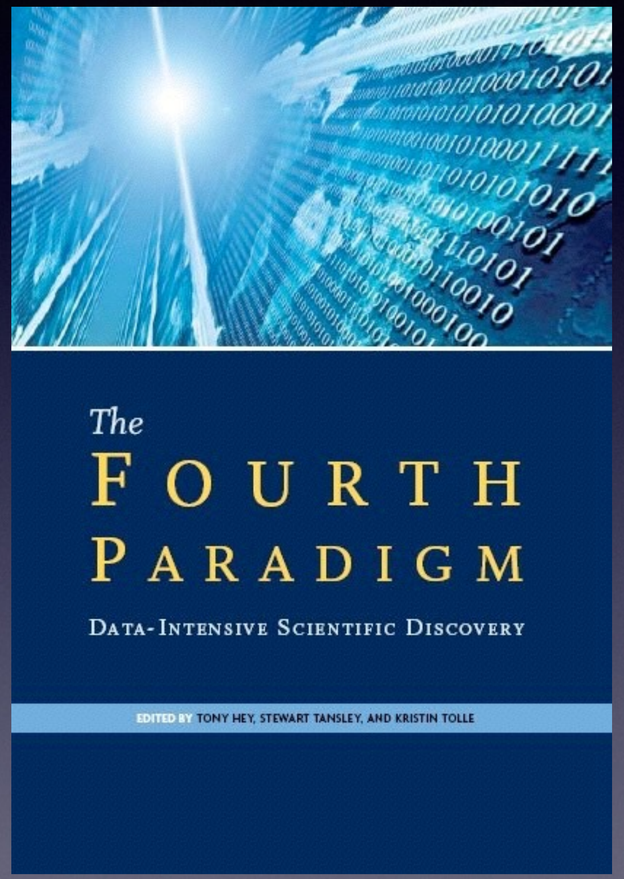
Many claim the emergence of new branches:

Branch 3,4? (computational): large scale simulations / data driven computational science.

Commonly believed...



"It is common now to consider computation as a third branch of science, besides theory and experiment."



"This book is about a new, fourth paradigm for science based on data-intensive computing."

The Impact of Technology

1. *Big Data / Data Driven Discovery*: high dimensional data, p >> n,

2. *Computational Power*: simulation of the complete evolution of a physical system, systematically varying parameters,

3. Deep intellectual contributions now encoded only in *software*.

CSHL Keynote; Dr. Lior Pachter, UC Berkeley

The software contains "ideas that enable biology..."
Stories from the Supplement, 2013.

The Ubiquity of Error

The central motivation for the scientific method is to root out error:

- Deductive branch: the well-defined concept of the proof,
- Empirical branch: the machinery of hypothesis testing, appropriate statistical methods, structured communication of methods and protocols.

Claim: Computation presents only a potential third/fourth branch of the scientific method (Donoho, Stodden, et al. 2009), until the development of comparable standards.

Really Reproducible Research

- "Really Reproducible Research" (1992) inspired by Stanford Professor Jon Claerbout:

  "The idea is: 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 ... set of instructions [and data] which generated the figures." David Donoho, 1998

- Reproducing the computational steps *vs* replicating the experiments independently including data collection and software implementation.

ICERM Workshop

ICERM

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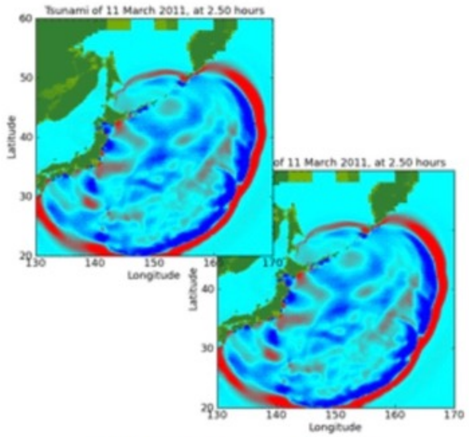
Reproducibility in Computational and Experimental Mathematics *(December 10-14, 2012)*

Description



Click for code to create this image.

In addition to advancing research and discovery in pure and applied mathematics, computation is pervasive across the sciences and now computational research results are more crucial than ever for public policy, risk management, and national security. Reproducibility of carefully documented experiments is a cornerstone of the scientific method, and yet is often lacking in computational mathematics, science, and engineering. Setting and achieving appropriate standards for reproducibility in computation poses a number of interesting technological and social challenges. The purpose of this workshop is to discuss aspects of reproducibility most relevant to the mathematical sciences among researchers from pure and applied mathematics from academics and other settings, together with interested parties from funding agencies, national laboratories, professional societies, and publishers. This will be a working workshop, with relatively few talks and dedicated time for breakout group discussions on the current state of the art and the tools, policies, and infrastructure that are needed to improve the situation. The groups will be charged with developing guides to current best practices and/or white papers on desirable advances.

Organizing Committee

- David H. Bailey (Lawrence Berkeley National Laboratory)
- Jon Borwein (Centre for Computer Assisted Research Mathematics and its Applications)
- Randall J. LeVeque (University of Washington)
- Bill Rider (Sandia National Laboratory)
- William Stein (University of Washington)
- Victoria Stodden (Columbia University)

ICERM Workshop Report

Setting the Default to Reproducible

Reproducibility in Computational and Experimental Mathematics

Developed collaboratively by the ICERM workshop participants[1]

Compiled and edited by the Organizers

V. Stodden, D. H. Bailey, J. Borwein, R. J. LeVeque, W. Rider, and W. Stein

Abstract

Science is built upon foundations of theory and experiment validated and improved through open, transparent communication. With the increasingly central role of computation in scientific discovery this means communicating all details of the computations needed for others to replicate the experiment, i.e. making available to others the associated data and code. The "reproducible research" movement recognizes that traditional scientific research and publication practices now fall short of this ideal, and encourages all those involved in the production of computational science – scientists who use computational methods and the institutions that employ them, journals and dissemination mechanisms, and funding agencies – to facilitate and practice really reproducible research.

Set the Default to "Open"

Reproducible Science in the Computer Age. Conventional wisdom sees computing as the "third leg" of science, complementing theory and experiment. That metaphor is outdated. Computing now pervades all of science. Massive computation is often required to reduce and analyze data; simulations are employed in fields as diverse as climate modeling and astrophysics. Unfortunately, scientific computing culture has not kept pace. Experimental researchers are taught early to keep notebooks or computer logs of every work detail: design, procedures, equipment, raw results, processing techniques, statistical methods of analysis, etc. In contrast, few computational experiments are performed with such care. Typically, there is no record of workflow, computer hardware and software configuration, or parameter settings. Often source code is lost. While crippling reproducibility of results, these practices ultimately impede the researcher's own productivity.

The State of Experimental and Computational Mathematics. Experimental mathematics[1]—application of high-performance computing technology to research questions in pure and applied mathematics, including

"It says it's sick of doing things like inventories and payrolls, and it wants to make some breakthroughs in astrophysics."

ScienceCartoonsPlus.com.

physicists, legal scholars, journal editors, and funding agency officials representing academia, government labs, industry research, and all points in between. While

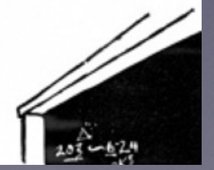
SIAM NEWS >

"Setting the Default to Reproducible" in Computational Science Research

June 3, 2013

Following a late-2012 workshop at the Institute for Computational and Experimental Research in Mathematics, a group of computational scientists have proposed a set of standards for the dissemination of reproducible research.

Victoria Stodden, Jonathan Borwein, and David H. Bailey



Criterion	Definition
Assertions (#1)	A precise statement of assertions to be made in the paper.
Comp. Approach (#2)	A statement of the computational approach, and why it constitutes a rigorous test of the hypothesized assertions.
Software Cited (#3 & 4)	Complete statements of, or references to, every algorithm employed, and salient details of auxiliary software (both research and commercial software) used in the computation.
Hardware Discussed (#5)	Salient details of the test environment, including hardware, system software and the number of processors utilized.
Analysis (#6)	Salient details of data reduction and statistical analysis methods.
Parameter Discussed (#7)	Discussion of the adequacy of parameters such as precision level and grid resolution.
Parameters Given (#7)	Were necessary run parameters given?
Results (#8)	Full statement (or at least a valid summary) of experimental results.
Available Code (#10)	Availability of computer code, input data and output data, with some reasonable level of documentation.
Functions Calls	Which precise functions were called, with what settings?
Comp. Instructions (#12)	Instructions for repeating computational experiments described in the paper.
Alternate Avenues (#14)	Avenues of exploration examined throughout development, including information about negative findings.
Citation (#15)	Proper citation of all code and data used, including that generated by the authors.

Submissions (pending)
Agenda (pending)
Final Report (pending)

Related Links:
XSEDE Home
XSEDE14 Annual Conference
Yale 2009 Roundtable

Organizing Committee

Lorena A. Barba
George Washington University

Eivind Hovig
University of Oslo

reproducibility@XSEDE: An XSEDE14 Workshop

Overview

The reproducibility@XSEDE workshop is a full-day event scheduled for **Monday, July 14, 2014 in Atlanta, GA**. The workshop will take place in conjunction with XSEDE14 (conferences.xsede.org), the annual conference of the Extreme Science and Engineering Discovery Environment (XSEDE), and will feature an interactive, open-ended, discussion-oriented agenda focused on reproducibility in large-scale computational science. Consistent with the overall XSEDE14 conference theme, we seek to engage participants from a broad range of backgrounds, including practitioners whose computational interests extend beyond traditional modeling and simulation as well as decision-makers and other professionals whose work informs and determines the direction of computation-enabled research. We hope to help

Supporting Computational Science

- Dissemination Platforms:

ResearchCompendia.org	IPOL	Madagascar
MLOSS.org	thedatahub.org	nanoHUB.org
Open Science Framework		RunMyCode.org

- Workflow Tracking and Research Environments:

VisTrails	Kepler	CDE	Chameleon
Galaxy	GenePattern	Jupyter / IPython Notebook	
Sumatra	Taverna	Pegasus	

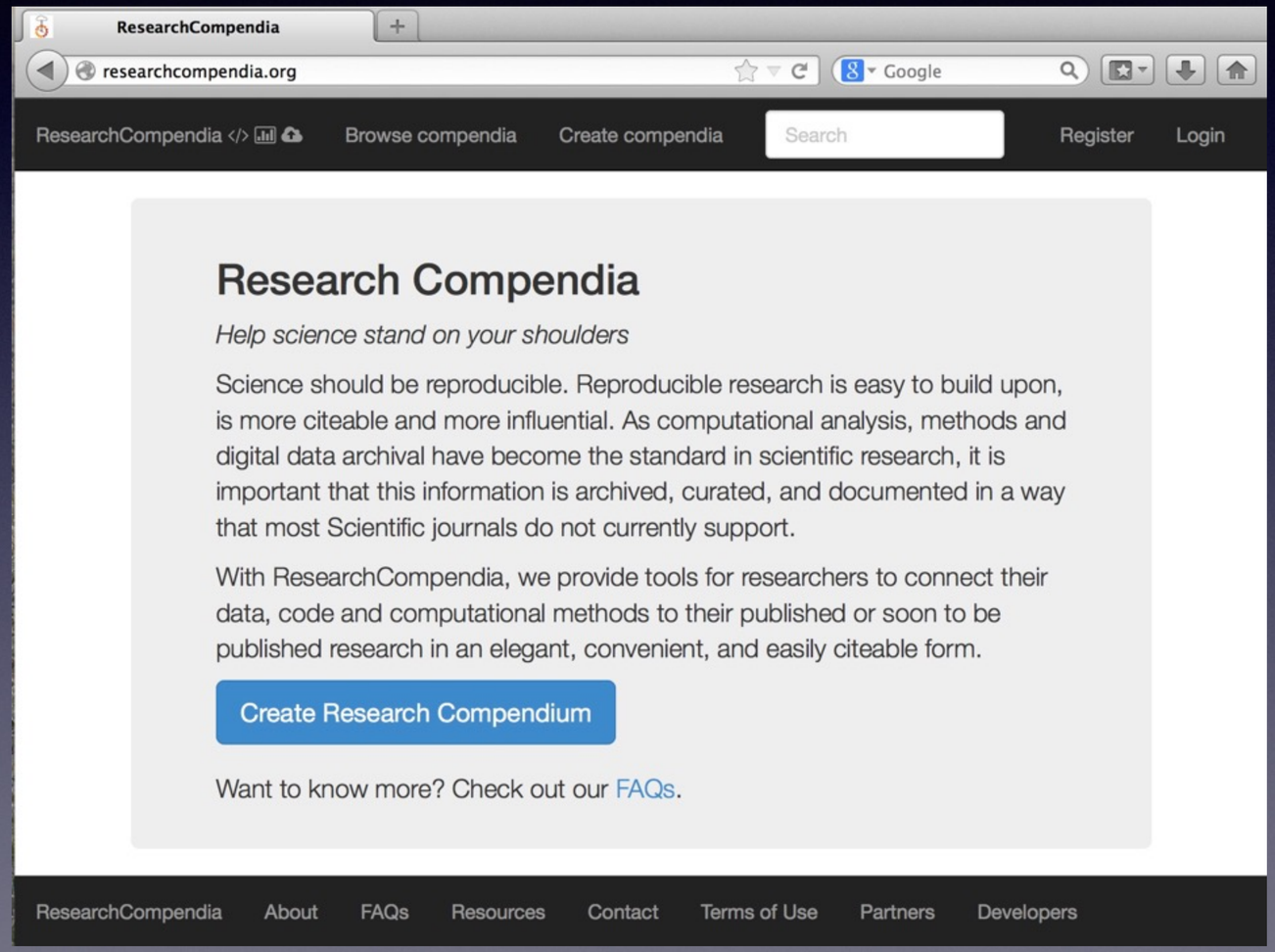
- Embedded Publishing:

Verifiable Computational Research	SOLE	knitR
Collage Authoring Environment	SHARE	Sweave

Research Compendia

Goal: improve understanding of reproducible computational science, trace sources of error.

- link data/code to published claims,
- enable re-use,
- sharing guide for researchers,
- certification of results,
- large scale validation of findings,
- stability, sensitivity checks.



Is “Huh?” a Universal Word? Conversational Infrastructure and the Convergent Evolution of Linguistic Items

Mark Dingemanse, Francisco Torreira, N. J. Enfield, Johan J. Bolhuis

Code and Data Abstract

A word like Huh?–used as a repair initiator when, for example, one has not clearly heard what someone just said–is found in roughly the same form and function in spoken languages across the globe. We investigate it in naturally occurring conversations in ten languages and present evidence and arguments for two distinct claims: that Huh? is universal, and that it is a word. In support of the first, we show that the similarities in form and function of this interjection across languages are much greater than expected by chance. In support of the second claim we show that it is a lexical, conventionalised form that has to be learnt, unlike grunts or emotional cries. We discuss possible reasons for the cross-linguistic similarity and propose an account in terms of convergent evolution. Huh? is a universal word not because it is innate but because it is shaped by selective pressures in an interactional environment that all languages share: that of other-initiated repair. Our proposal enhances evolutionary models of language change by suggesting that conversational infrastructure can drive the convergent cultural evolution of linguistic items.

</> code | data | article

Compendium Type:: article
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Random survival forests for high-dimensional data

Hemant Ishwaran, Udaya B. Kogalur, Xi Chen, Andy J. Minn

Code and Data Abstract

Minimal depth is a dimensionless order statistic that measures the predictiveness of a variable in a survival tree. It can be used to select variables in high-dimensional problems using Random Survival Forests (RSF), a new extension of Breiman's Random Forests (RF) to survival settings. We review this methodology and demonstrate its use in high-dimensional survival problems using a public domain R-language package randomSurvivalForest. We discuss effective ways to regularize forests and discuss how to properly tune the RF parameters 'nodesize' and 'mtry'. We also introduce new graphical ways of using minimal depth for exploring variable relationships.

</> code | data | Article | Verify

Hemant Ishwaran, Udaya B. Kogalur, Xi Chen, Andy J. Minn, et al. 2011. "Random survival forests for high-dimensional data." *Statistical Analysis and Data Mining*. 4 (1) 115–132. doi:10.1002/sam.10103. Retrieved 12/04/2014 from labs.researchcompendia.org/compendia/2014.8/

Code DOI: doi:10.7938/M1H41PBB.
Data DOI: doi:10.7938/M1CC0XMM.

Compendium Type: Journal or Magazine Articles
Primary Research Field: Computer and Information Sciences
Secondary Research Field: Mathematics
Content License: Public Domain Mark
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Verification

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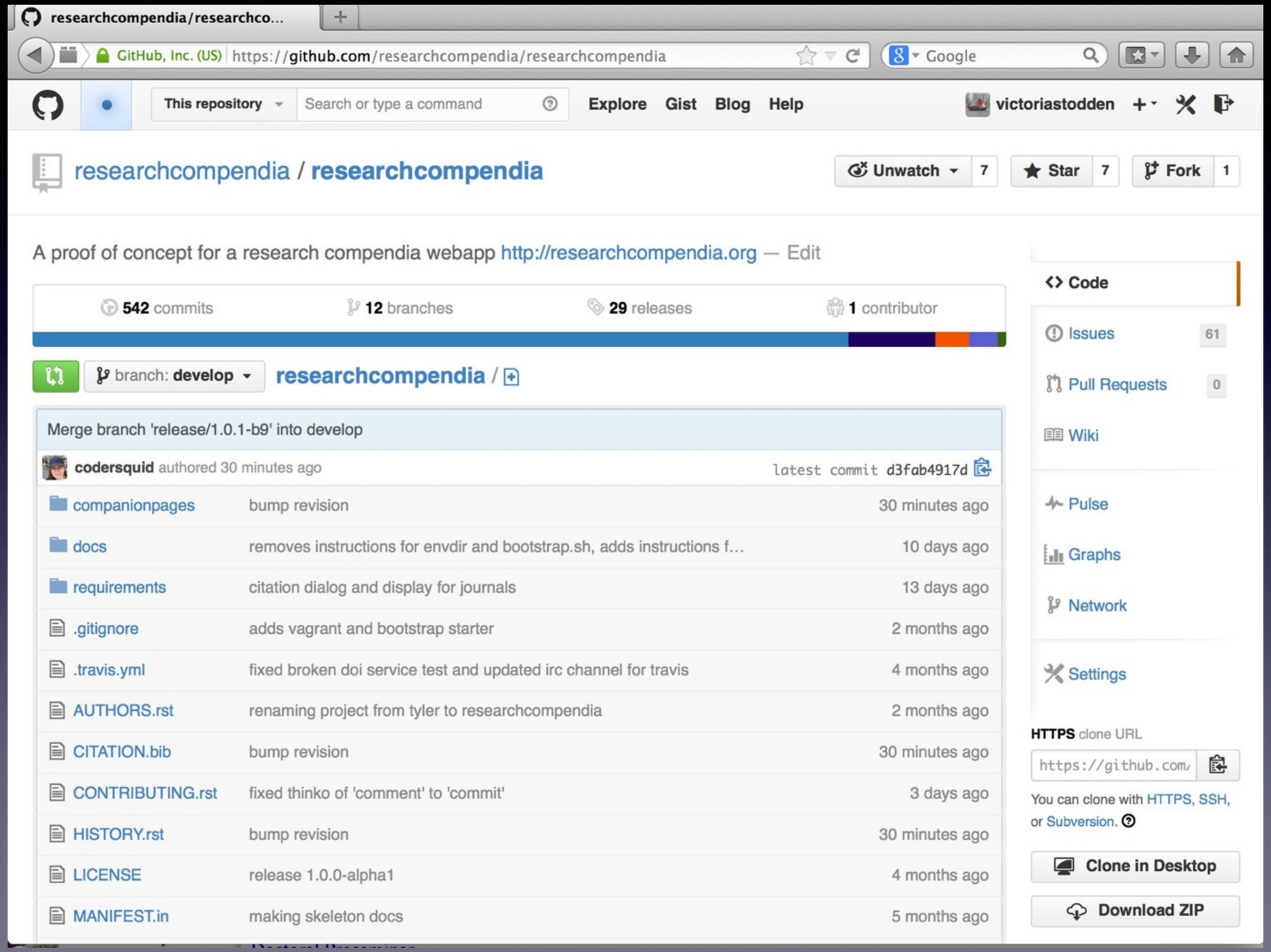
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542 commits
12 branches
29 releases
1 contributor
branch: develop
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Merge branch 'release/1.0.1-b9' into develop
codersquid authored 30 minutes ago
latest commit d3fab4917d
companionpages bump revision 30 minutes ago
docs removes instructions for envdir and bootstrap.sh, adds instructions f… 10 days ago
requirements citation dialog and display for journals 13 days ago
.gitignore adds vagrant and bootstrap starter 2 months ago
.travis.yml fixed broken doi service test and updated irc channel for travis 4 months ago
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HISTORY.rst bump revision 30 minutes ago
LICENSE release 1.0.0-alpha1 4 months ago
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Three sections:

1. Tools
2. Practices and Guidelines
3. Platforms

Chapters available for download:
https://osf.io/s9tya/wiki/

Data / Code Sharing Practices

Survey of the NIPS community:

- 1,758 NIPS registrants up to and including 2008,
- 1,008 registrants when restricted to .edu registration emails,
- After piloting, the final survey was sent to 638 registrants,
- 37 bounces, 5 away, and 3 in industry, gave a final response rate was 134 of 593 or 23%.
- Queried about reasons for sharing or not sharing data/code associated with their NIPS paper.

Sharing Incentives

Code		Data
91%	Encourage scientific advancement	81%
90%	Encourage sharing in others	79%
86%	Be a good community member	79%
82%	Set a standard for the field	76%
85%	Improve the calibre of research	74%
81%	Get others to work on the problem	79%
85%	Increase in publicity	73%
78%	Opportunity for feedback	71%
71%	Finding collaborators	71%

Survey of the Machine Learning Community, NIPS (Stodden 2010)

Barriers to Sharing

Code		Data
77%	Time to document and clean up	54%
52%	Dealing with questions from users	34%
44%	Not receiving attribution	42%
40%	Possibility of patents	-
34%	Legal Barriers (ie. copyright)	41%
-	Time to verify release with admin	38%
30%	Potential loss of future publications	35%
30%	Competitors may get an advantage	33%
20%	Web/disk space limitations	29%

Survey of the Machine Learning Community, NIPS (Stodden 2010)

Ownership of Research Codes

Patent and Copyright Agreement for Personnel at Stanford - SU18

I understand that, consistent with applicable laws and regulations, Stanford University is governed in the handling of intellectual property by its official policies titled Inventions, Patents and Licensing and Copyright Policy (both published in the Research Policy Handbook), and I agree to abide by the terms and conditions of those policies, as they may be amended from time to time.

Pursuant to those policies, and in consideration of my employment by Stanford, the receipt of remuneration from Stanford, participation in projects administered by Stanford, access to or use of facilities or resources provided by Stanford and/or other valuable consideration, I hereby agree as follows:

1. I will disclose to Stanford all potentially patentable inventions conceived or first reduced to practice in whole or in part in the course of my University responsibilities or with more than incidental use of University resources. I hereby assign to Stanford all my right, title and interest in such patentable inventions and to execute and deliver all documents and do any and all things necessary and proper on my part to effect such assignment.
   (See Inventions, Patents and Licensing for further clarification and discussion related to this paragraph.)
2. I am free to place my inventions in the public domain as long as in so doing neither I nor Stanford violates the terms of any agreements that governed the work done.
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   a. is a work-for-hire (and copyright therefore vests in the University under copyright law),
   b. is supported by a direct allocation of funds through the University for the pursuit of a specific project,
   c. is commissioned by the University,
   d. makes significant use of University resources or personnel, or
   e. is otherwise subject to contractual obligations.

I hereby assign or confirm in writing to Stanford all my right, title and interest, including associated copyright, in and to copyrightable materials falling under a) through e), above.

4. I am now under no consulting or other obligations to any third person, organization or corporation in respect to rights in inventions or copyrightable materials which are, or could be reasonably construed to be, in conflict with this agreement.

   NOTE: An alternative to this agreement may be appropriate for personnel with a prior existing and conflicting employment agreement that establishes a right to intellectual property in conflict with Stanford policies. Personnel in this situation should contact the Office of the Vice Provost and Dean of Research.

5. I will not enter into any agreement creating copyright or patent obligations in conflict with this agreement.
6. This agreement is effective on the later of July 1, 2011 (on the one hand) or my date of hire, enrollment, or participation in projects administered by Stanford (on the other hand), and is binding on me, my estate, heirs and assigns.

_____

Electronic Signature in AXESS
http://axess.stanford.edu

The signer should make a copy of this agreement for his or her own records, and hereby waives any objection to Stanford's use of an electronic version of this agreement as a substitute for the original for any legally recognized purpose.
July 2011

Provider: Office of the Vice Provost and Dean of Research, Stanford University
Contact: Assistant Dean of Research
Last updated: July 2011

Legal Barriers: Copyright

"To promote the Progress of Science and useful Arts, by securing for limited Times to Authors and Inventors the exclusive Right to their respective Writings and Discoveries." (U.S. Const. art. I, §8, cl. 8)

- Original expression of ideas falls under copyright *by default* (papers, code, figures, tables..)
- Copyright secures exclusive rights vested in the author to:
  - reproduce the work
  - prepare derivative works based upon the original

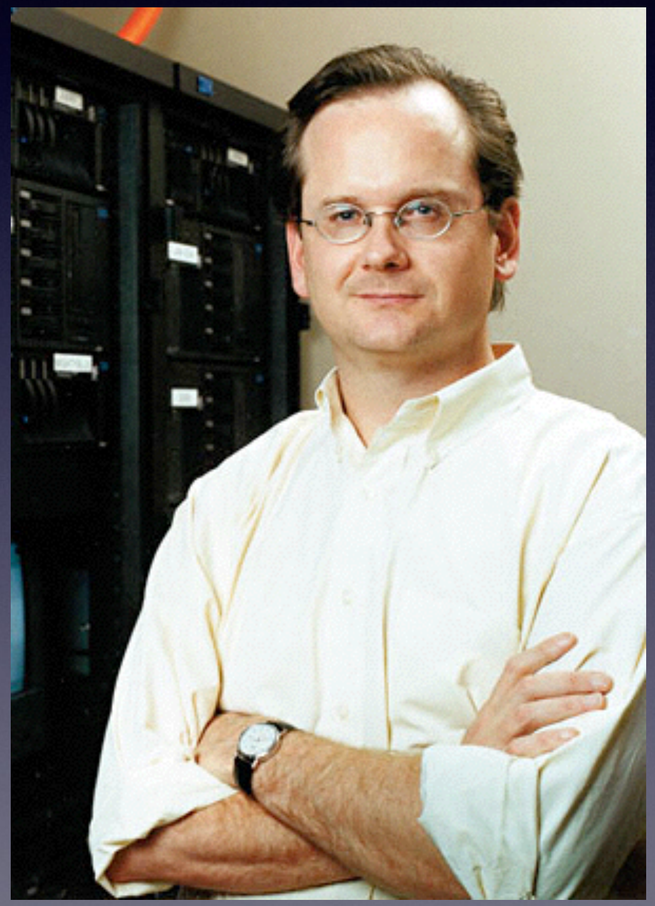
Exceptions and Limitations: Fair Use.

Responses Outside the Sciences 1: Open Source Software

- Software with licenses that communicate alternative terms of use to code developers, rather than the copyright default.
- Hundreds of open source software licenses:
  - GNU Public License (GPL)
  - (Modified) BSD License
  - MIT License
  - Apache 2.0 License
  - ... see http://www.opensource.org/licenses/alphabetical

Responses Outside the Sciences 2: Creative Commons

- Founded in 2001, by Stanford Law Professor Larry Lessig, MIT EECS Professor Hal Abelson, and advocate Eric Eldred.
- Adapts the Open Source Software approach to artistic and creative digital works.



Response from Within the Sciences

The *Reproducible Research Standard* (*RRS*) (Stodden, 2009)

- A suite of license recommendations for computational science:
    - Release media components (text, figures) under CC BY,
    - Release code components under Modified BSD or similar,
    - Release data to public domain or attach attribution license.

➡ Remove copyright's barrier to reproducible research and,

➡ Realign the IP framework with longstanding scientific norms.

Winner of the Access to Knowledge Kaltura Award 2008

Copyright and Data

- Copyright adheres to raw facts in Europe.
- In the US raw facts are not copyrightable, but the original "selection and arrangement" of these facts is copyrightable. (Feist Publns Inc. v. Rural Tel. Serv. Co., 499 U.S. 340 (1991)).
- the possibility of a residual copyright in data (attribution licensing or public domain certification).
- Law doesn't match reality on the ground: What constitutes a "raw" fact anyway?

Bayh-Dole Act (1980)

Promote the transfer of academic discoveries for commercial development, via licensing of patents (ie. Technology Transfer Offices),

Bayh-Dole Act gave federal agency grantees and contractors title to government-funded inventions and charged them with using the patent system to aid disclosure and commercialization of the inventions.

Greatest impact in biomedical research collaborations and drug discovery. Now, software patents also impact science.

Disclosure of Research Codes

Claim: Codes would (eventually) be fully open in the absence of Bayh-Dole:

- Grassroots "Reproducible Research" movement in computational science (policy development, best practices, tool development),
- Changes in funding agency requirements
- Changes in journal publication requirements

Sharing Code..

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Best Practices for Scientific Computing

Greg Wilson, D. A. Aruliah, C. Titus Brown, Neil P. Chue Hong, Matt Davis, Richard T. Guy, Steven H. D. Haddock, Kathryn D. Huff, Ian M. Mitchell, Mark D. Plumbley, Ben Waugh, Ethan P. White, Paul Wilson

Published: January 07, 2014 • DOI: 10.1371/journal.pbio.1001745

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"Setting the Default to Reproducible" in Computational Science Research

June 3, 2013

Following a late-2012 workshop at the Institute for Computational and Experimental Research in Mathematics, a group of computational scientists have proposed a set of standards for the dissemination of reproducible research.

Victoria Stodden, Jonathan Borwein, and David H. Bailey

Computation is now central to the scientific enterprise, and the emergence of powerful computational hardware, combined with a vast array of computational software, presents novel opportunities for researchers. Unfortunately, the scientific culture surrounding computational work has evolved in ways that make it difficult to verify findings, efficiently build on past research, or even apply the basic tenets of the scientific method to computational procedures.

As a result, computational science is facing a credibility crisis [1,2,4,5]. The enormous scale of state-of-the-art

Courtesy of S. Harris, ScienceCartoonsPlus.com.

Abstract

http://ssrn.com/abstract=2322276

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Best Practices for Computational Science: Software Infrastructure and Environments for Reproducible and Extensible Research

Victoria Stodden
Columbia University - Department of Statistics

Sheila Miguez
Columbia University

September 6, 2013

Abstract:
Scholarly dissemination and communication standards are changing to reflect the increasingly computational nature of scholarly research, primarily to include the sharing of the data and code associated with published results. This paper presents a formalized set of best practice recommendations for computational scientists wishing to disseminate reproducible research, facilitate innovation by enabling data and code re-use, and enable broader communication of the output of digital scientific research. We distinguish two forms of collaboration to motivate choices of software environment for computational scientific research. We also present these Best Practices as a living, evolving, and changing document on wiki.

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Top Ten Reasons To Not Share Your Code (and why you should anyway)

April 1, 2013

Randall J. LeVeque

There is no . . . mathematician so expert in his science, as to place entire confidence in any truth immediately upon his discovery of it. . . . Every time he runs over his proofs, his confidence encreases; but still more by the approbation of his friends; and is raised to its utmost perfection by the universal assent and applauses of the learned world.---David Hume, 1739*

Journal Policy?

- Journal Policy setting study design:
- Select all journals from ISI classifications "Statistics & Probability," "Mathematical & Computational Biology," and "Multidisciplinary Sciences" (this includes Science and Nature).
- N = 170, after deleting journals that have ceased publication.
- Create dataset with ISI information (impact factor, citations, publisher) and supplement with publication policies as listed on journal websites, in June 2011 and June 2012.

Journal Data Sharing Policy

	2011	2012
Required as condition of publication, barring exceptions	10.6%	11.2%
Required but may not affect editorial decisions	1.7%	5.9%
Encouraged/addressed, may be reviewed and/or hosted	20.6%	17.6%
Implied	0%	2.9%
No mention	67.1%	62.4%

Source: Stodden, Guo, Ma (2013) PLoS ONE, 8(6)

Journal Code Sharing Policy

	2011	2012
Required as condition of publication, barring exceptions	3.5%	3.5%
Required but may not affect editorial decisions	3.5%	3.5%
Encouraged/addressed, may be reviewed and/or hosted	10%	12.4%
Implied	0%	1.8%
No mention	82.9%	78.8%

Source: Stodden, Guo, Ma (2013) PLoS ONE, 8(6)

Findings

- Changemakers are journals with high impact factors.
- Progressive policies are not widespread, but being adopted rapidly.
- Close relationship between the existence of a supplemental materials policy and a data policy.
- No statistically significant relationship between data and code policies and open access policy.
- Data and supplemental material policies appear to lead software policy.

Editorial: ACM TOMS Replicated Computational Results Initiative

MICHAEL A. HEROUX, Sandia National Laboratories

The scientific community relies on the peer review process for assuring the quality of published material, the goal of which is to build a body of work we can trust. Computational journals such as the *ACM Transactions on Mathematical Software* (TOMS) use this process for rigorously promoting the clarity and completeness of content, and citation of prior work. At the same time, it is unusual to independently confirm computational results.

ACM TOMS has established a *Replicated Computational Results* (RCR) review process as part of the manuscript peer review process. The purpose is to provide independent confirmation that results contained in a manuscript are replicable. Successful completion of the RCR process awards a manuscript with the Replicated Computational Results Designation.

This issue of ACM TOMS contains the first [Van Zee and van de Geijn 2015] of what we anticipate to be a growing number of articles to receive the RCR designation, and the related RCR reviewer report [Willenbring 2015]. We hope that the TOMS RCR process will serve as a model for other publications and increase the confidence in and value of computational results in TOMS articles.

- provide independent confirmation that results contained in a manuscript are correct and replicated.

- Successful completion of the RCR process gives the manuscript a Replicated Computational Results designation on the first page of the published article.

3. Statistical Reproducibility

- False discovery, chasing significance, p-hacking (Simonsohn 2012), file drawer problem, overuse and mis-use of p-values, lack of multiple testing adjustments.
- Low power, poor experimental design,
- Data preparation, treatment of outliers, re-combination of datasets, insufficient reporting/tracking practices,
- Poor statistical methods (nonrandom sampling, inappropriate tests or models, model misspecification..)
- Model robustness to parameter changes and data perturbations,
- Investigator bias toward previous findings; conflicts of interest.

Journal Requirements

In January 2014 Science enacted new policies that will check for:

1. a “data-handling plan” i.e. how outliers will be dealt with,
2. sample size estimation for effect size,
3. whether samples are treated randomly,
4. whether experimenter blind to the conduct of the experiment.

Statisticians added to the Board of Reviewing Editors.

Updating Reproducibility

- **Failure of traditional reporting methods** vs adaptation of standards to accommodate changes in the research process.
- **Benchmarking and testing**: either nonexistent or over reliance on inappropriate benchmarks (see e.g. http://www.in-cites.com/scientists/DrDavidDonoho.html)
- **Collective action problem**: coordination of researcher incentives, universities, funding agencies, journals, scientific societies, legal and policy environment, libraries, the public.

Postdoc on Reproducibility in HPC

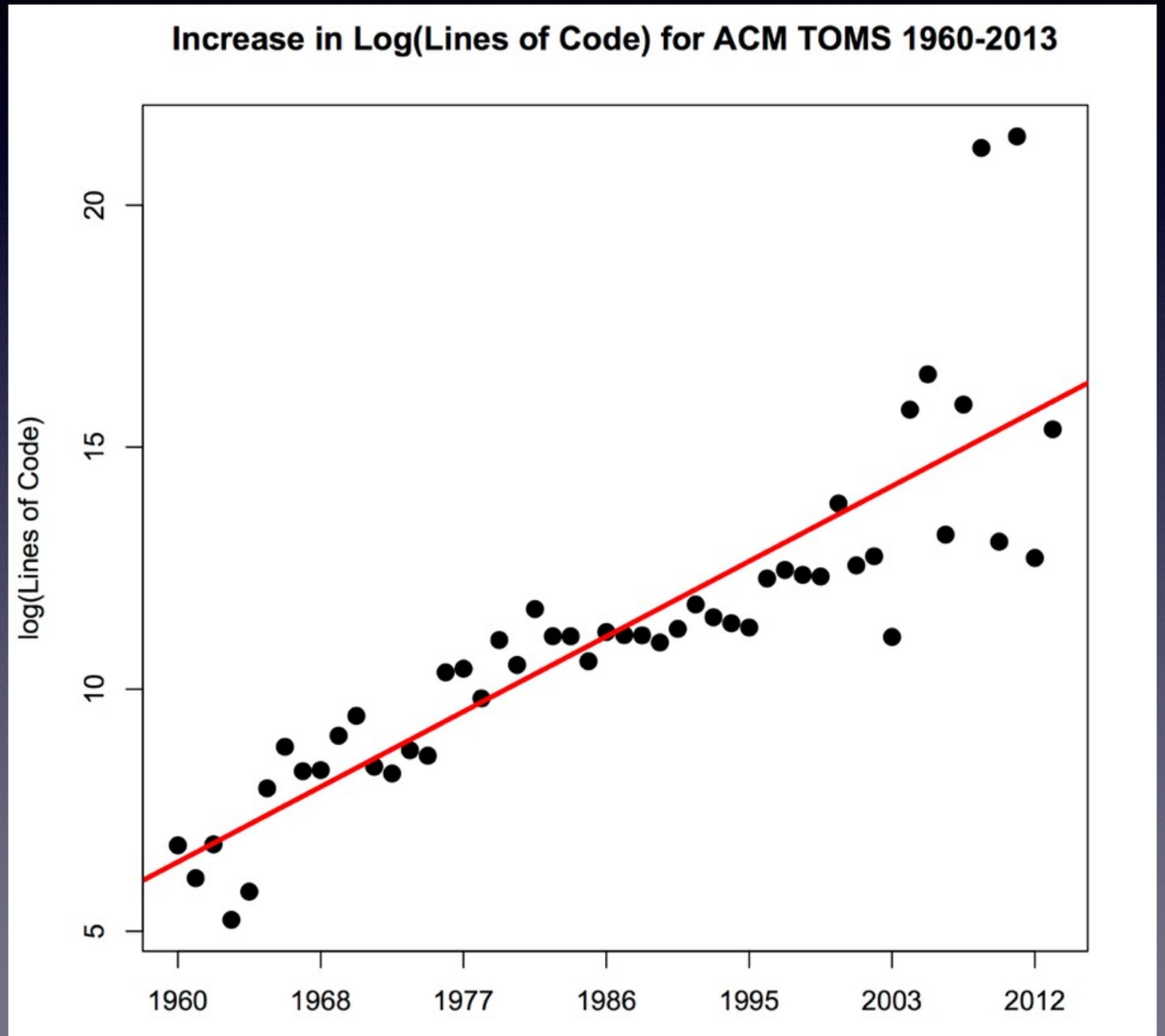
One-year postdoctoral fellowship at UIUC in reproducibility

One Postdoctoral Researcher Position within the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign, full-time, 100% (1-year duration, with possibility of extension, contingent upon performance and funding)

Summary: This postdoctoral appointment provides an opportunity to help develop a new area of transdisciplinary research in reproducibility in computational and data-intensive research. Researchers, journals, scientific societies and funding agencies are requiring the reproducibility of computational findings, which introduces new aspects to research including understanding factors that drive or prevent reproducibility, and enabling factors such as software and data access, interoperability, provenance, workflow capture, discoverability, and policy development. The postdoc will develop research on all these fronts including a focus on high end computing and cyberinfrastructure.

The position is funded by the Computing and Data Sciences Theme at NCSA, and the successful applicant will be working primarily with Dr. Victoria Stodden. The successful candidate will use one of the most advanced supercomputers for open scientific research, Blue Waters, and also work with a team of leading computational and data scientists at NCSA.

ACM TOMS Code Size Over Time



Reproducibility at SC16 with the Student Cluster Competition

Got transparency (or How naked are your results)?

Reproducibility and independent verification are essential to the scientific method, which lead to better scientific practices, data transparency, and research lifecycles.

- Authors of technical papers accepted at SC15 and previous years are invited to submit proposals to reproduce their paper results
  - Submissions accepted: December 1, 2015 - January 15, 2016
- Selected paper's software application will be featured as a competition application in the Student Cluster Competition at SC16
- Papers will be judged on their reproducibility as well as viability as a Student Cluster Competition application
- Further information, CfP, and contacts at: http://tinyurl.com/SCC16Apps

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available at http://www.stodden.net