### Reliability and Reproducibility in Cyber Security Research

Victoria Stodden Graduate School of Library and Information Science University of Illinois at Urbana-Champaign

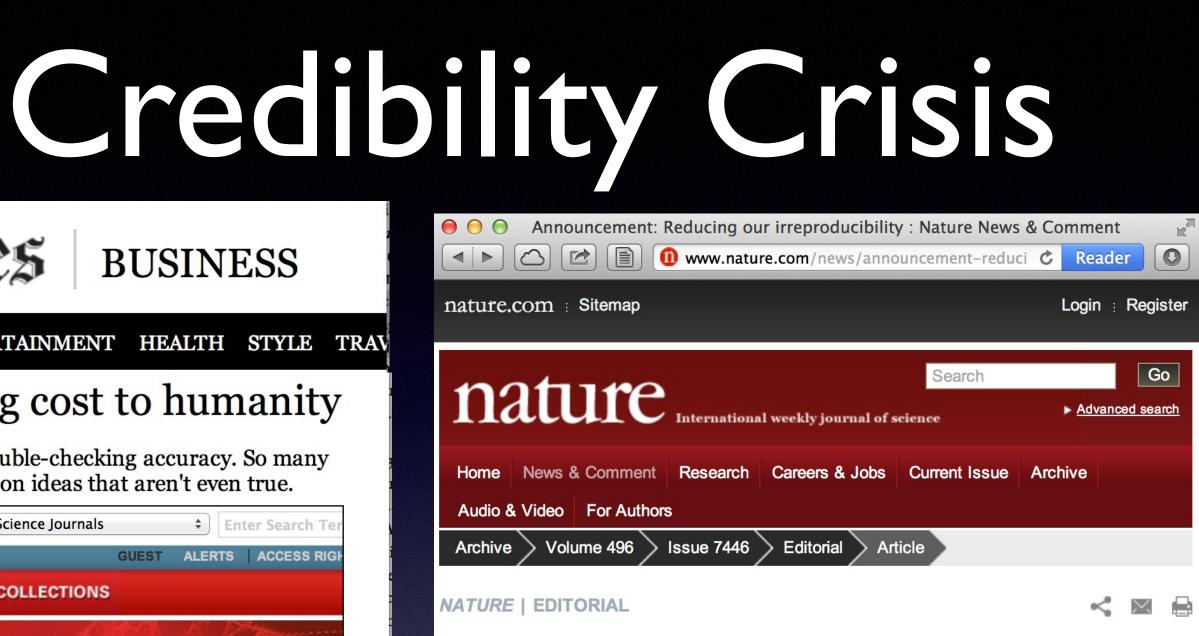
Workshop on the Science of Cyber-Security 67th Meeting of IFIP Working Group 10.4 on Dependable Computing and Fault Tolerance Tortworth, Bristol, UK January 23, 2015





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### Announcement: Reducing our irreproducibility

4 April 2013

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ver the past year, Nature has published a string of articles th liability and reproducibility of published research (collected a



ducibility prove the quality of scientific research.





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



# Unpacking "Reproducibility"

### "Empirical Reproducibility"

### Science AAAS.ORG AAAS Current Issue Science Home Home > *Science* Magazine > <u>17</u> January 2014 > McNutt, **343** (6168): 229 **Article Views** Summary **EDITORIAL** Full Text Full Text (PDF) Article Tools Save to My Folders

### "Computational Reproducibility"

### "Statistical Reproducibility"

### nature Home News & Comment Research Careers & Jobs Curre Volume 506 > Issue 7487 > Archive

### **NATURE | NEWS FEATURE**

### Scientific method: Statistical errors

P values, the 'gold standard' of statistical validity, are not as reliable as many scientists assume.

### **Regina Nuzzo**

12 February 2014



Society for Industrial and Applied Mathematics

### SIAM NEWS >

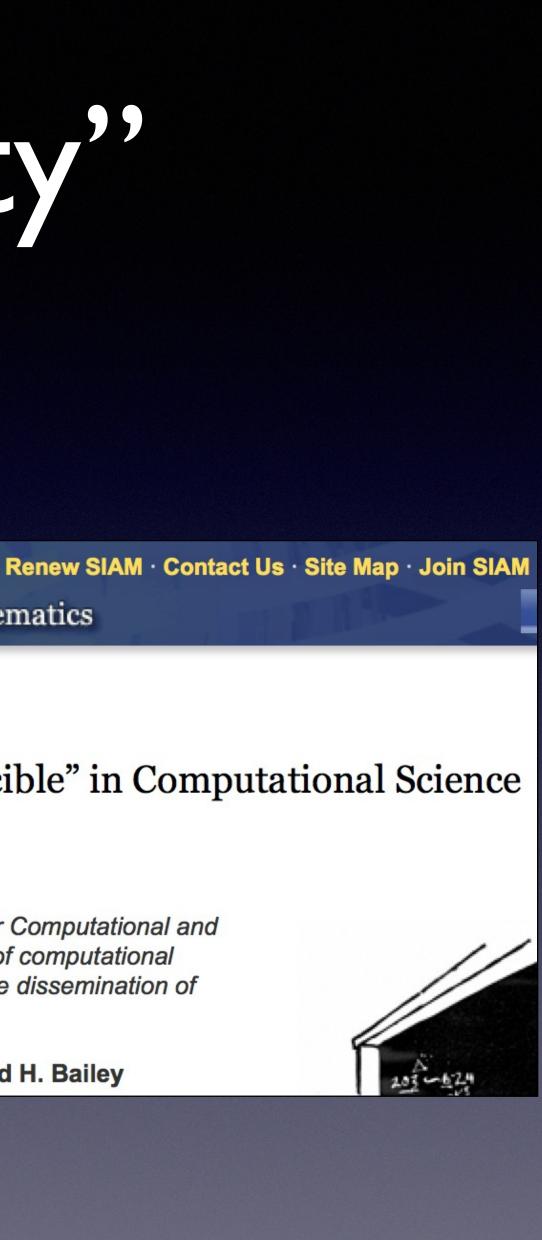
### "Setting the Default to Reproducible" in Computational Science Research

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

### V. Stodden, IMS Bulletin (2013)





Skepticism requires that the claim can be independently verified,

This in turn requires transparency in the communication of the research process.

Instantiated by Robert Boyle and the Transactions of the Royal Society in the 1660's.

Advances in the technology used for scientific discovery have changed how scientists effect reproducibility.

## I. Empirical Reproducibility





## Examples

### **Cell Reports** Commentary

### Sorting Out the FACS: A Devil in the Details

William C. Hines,<sup>1,5,\*</sup> Ying Su,<sup>2,3,4,5,\*</sup> Irene Kuhn,<sup>1</sup> Kornelia Polyak,<sup>2,3,4,5</sup> and Mina J. Bissell<sup>1,5</sup>

<sup>1</sup>Life Sciences Division, Lawrence Berkeley National Laboratory, Mailstop 977R225A, 1 Cyclotron Road, Berkeley, CA 94720, USA <sup>2</sup>Department of Medical Oncology, Dana-Farber Cancer Institute, Boston, MA 02215, USA

<sup>3</sup>Department of Medicine, Brigham and Women's Hospital, Boston, MA 02115, USA

<sup>4</sup>Department of Medicine, Harvard Medical School, Boston, MA 02115, USA

<sup>5</sup>These authors contributed equally to this work

\*Correspondence: chines@lbl.gov (W.C.H.), ying\_su@dfci.harvard.edu (Y.S.) 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 interestnamely, the heterogeneity of the human breast. Despite using seemingly identical methods, reagents, and specimens, our two laboratories guite 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



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About T



### **Reproducibility Issues in Research with Animals and Animal Models**

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

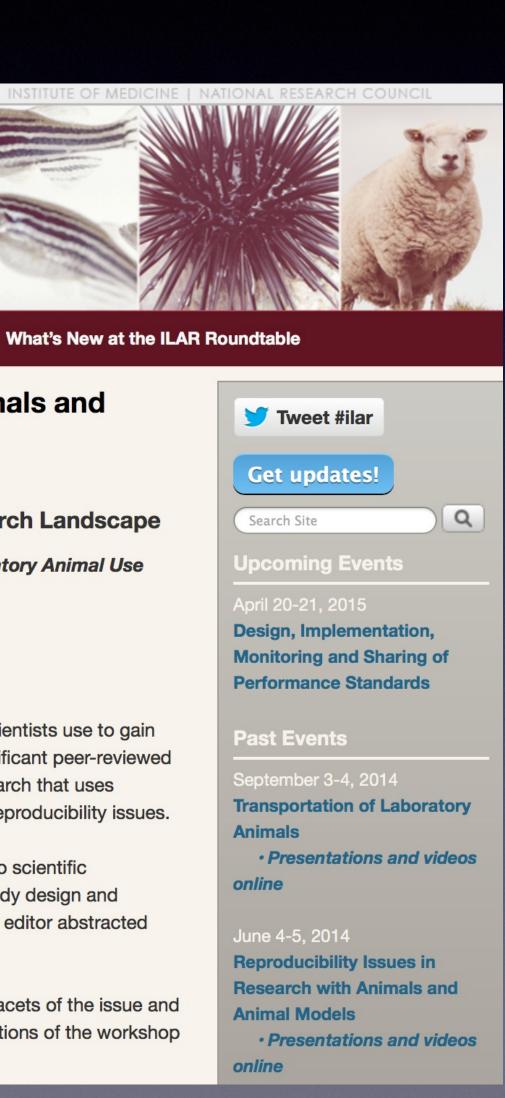
A workshop of the Roundtable on Science and Welfare in Laboratory Animal Use

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.



# 2. Computational Reproducibility

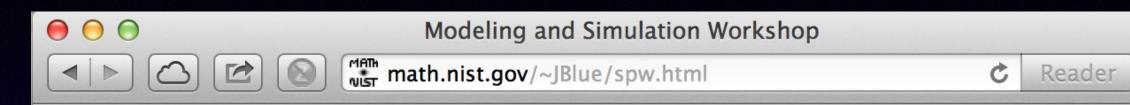
Traditionally two branches of the scientific method: Branch I (deductive): mathematics, formal logic,

Many claim the emergence of new branches: computational science.

- Branch 2 (empirical): statistical analysis of controlled experiments.
- Branch 3,4? (computational): large scale simulations / data driven

### Commonly believed...

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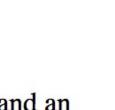
### Modeling and Simulation: A NIST Multi-Laboratory Strategic Planning Workshop

### Gaithersburg, MD September 21, 1995 Workshop Overview

The workshop consisted of an introduction; five talks, each followed by a discussion period; and an <u>open discussion session</u>. Capsule versions follow immediately; more substantial summaries follow later.

Jim Blue opened the workshop with brief <u>introductory remarks</u>. He emphasized that the purpose of doing modeling and simulation is to gain understanding and insight. The three benefits are that modeling and simulation can be cheaper, quicker, and better than experimentation alone. It is common now to consider computation as a third branch of science, besides theory and experiment.

"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 FOURTH PARADIGM

**DATA-INTENSIVE SCIENTIFIC DISCOVERY** 

EDITED BY TONY HEY, STEWART TANSLEY, AND KRISTIN TOLLE



# The Impact of Technology

- I. 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.



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.

comparable standards.

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

# Scoping the Issue

JASA June	Computational A
1996	9 of 20
2006	33 of 35
2009	32 of 32
2011	29 of 29

loannidis (2011): of 500 papers studied, 9% had full primary raw data deposited. Stodden (to come): estimates that the computations in 27% of scientific articles published in Science today are reproducible.

Examples: Voodoo Correlation in fMRI, Nevins/Potti Duke case, ...

### Articles Code Publicly Available 0% 9% 6% 21%



## CERM Workshop



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Programs & Events

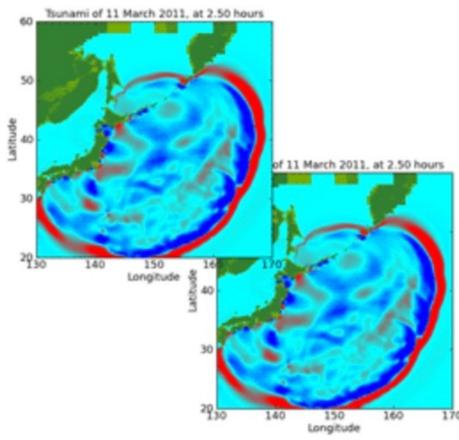
Participate

Proposals

Resou

### Description

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.



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

Click for code to create this image.

### **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<sup>1</sup>

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<sup>1</sup>—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."

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

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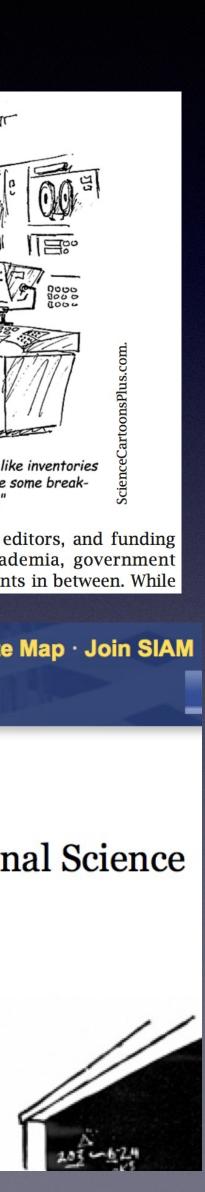
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### SIAM NEWS >

### "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 asse
Comp. Approach (#2)	A statement of the comput hypothesized assertions.
Software Cited (#3 & 4)	Complete statements of, or auxiliary software (both res
Hardware Discussed (#5)	Salient details of the test er of processors utilized.
Analysis (#6)	Salient details of data reduc
Parameter Discussed (#7)	Discussion of the adequacy
Parameters Given (#7)	Were necessary run param
Results (#8)	Full statement (or at least a
Available Code (#10)	Availability of computer co documentation.
Functions Calls	Which precise functions we
Comp. Instructions (#12)	Instructions for repeating c
Alternate Avenues (#14)	Avenues of exploration exa negative findings.
Citation (#15)	Proper citation of all code

ertions to be made in the paper.

tational approach, and why it constitutes a rigorous test of the

or references to, every algorithm employed, and salient details of esearch and commercial software) used in the computation.

environment, including hardware, system software and the number

ction and statistical analysis methods.

y of parameters such as precision level and grid resolution.

neters given?

a valid summary) of experimental results.

ode, input data and output data, with some reasonable level of

vere called, with what settings?

computational experiments described in the paper.

camined throughout development, including information about

and data used, including that generated by the authors.



# Supporting Computational Science

• Dissemination Platforms:

ResearchCompendia.org MLOSS.org Open Science Framework

- Workflow Tracking and Research Environments:

   <u>VisTrails</u>
   <u>Galaxy</u>
   <u>GenePattern</u>
   <u>Jupyter / IPython Notebook</u>
  - <u>Sumatra</u>

- <u>Taverna</u>
- Embedded Publishing:
   <u>Verifiable Computational Research</u> SOLE <u>knitR</u>
   Collage Authoring Environment <u>SHARE</u> <u>Sweave</u>

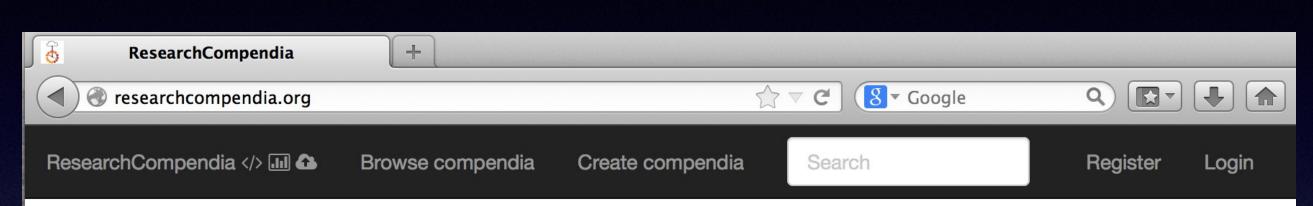
orgIPOLMadagascarthedatahub.orgnanoHUB.orgeworkRunMyCode.org

na <u>Pegasus</u>

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.

## Research Compendia



### **Research Compendia**

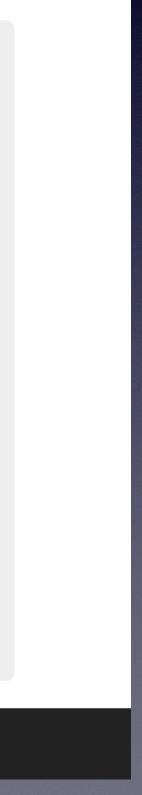
Help science stand on your shoulders

Science should be reproducible. Reproducible research is easy to build upon, is more citeable and more influential. As computational analysis, methods and digital data archival have become the standard in scientific research, it is important that this information is archived, curated, and documented in a way that most Scientific journals do not currently support.

With ResearchCompendia, we provide tools for researchers to connect their data, code and computational methods to their published or soon to be published research in an elegant, convenient, and easily citeable form.

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### 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

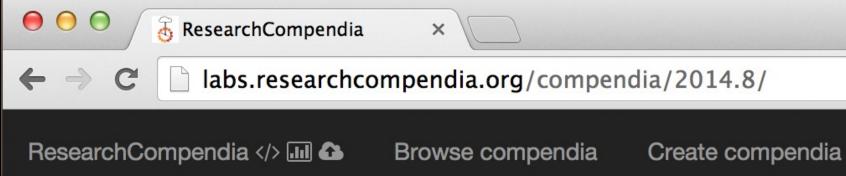
A word like Huh?-used as a repair initiator when, for example, one has not clearly heard what someone just saidis found in roughly the same form and function in spoken languages across the globe. We investigate it in naturally occurring conversations in ten languages and present evidence and arguments 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.

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Nord? Conversational				



### 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.

Article Verify Jul data

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 Code License: MIT License

### Verification

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verification code

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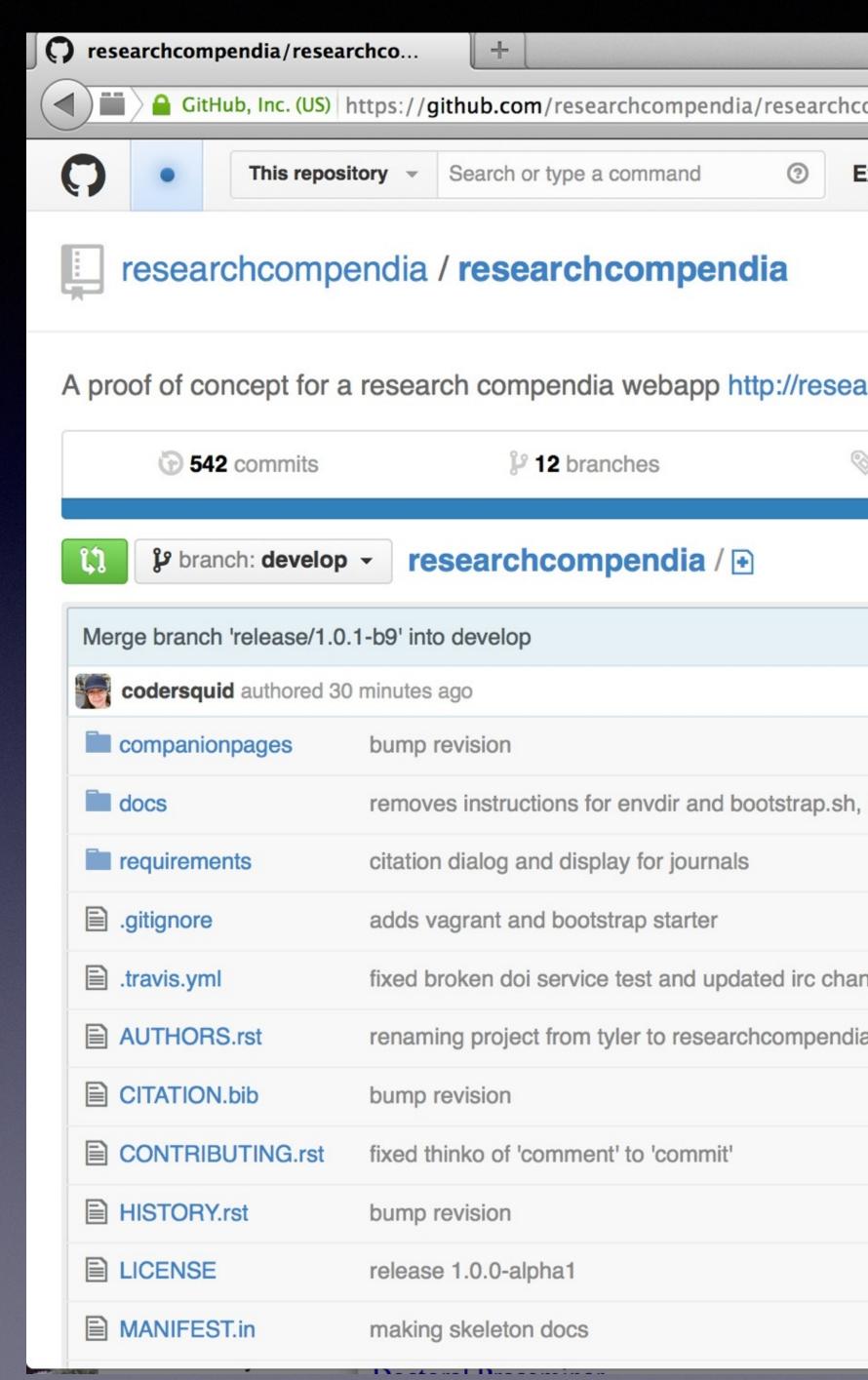
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# Journal Policy?

- 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

Required as condition of publication, barr

Required but may not affect editorial deci

Encouraged/addressed, may be reviewed a

Implied

No mention

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

Sharing Policy				
	2011	2012		
ring exceptions	10.6%	11.2%		
cisions	1.7%	5.9%		
and/or hosted	20.6%	17.6%		
	0%	2.9%		
	67.1%	62.4%		





# Journal Code

Required as condition of publication, barr

Required but may not affect editorial deci

Encouraged/addressed, may be reviewed

Implied

No mention

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

e Sharing Policy				
	2011	2012		
ring exceptions	3.5%	3.5%		
cisions	3.5%	3.5%		
and/or hosted	10%	12.4%		
	0%	1.8%		
	82.9%	78.8%		





- Changemakers are journals with high impact factors.
- policy and a data policy.
- and open access policy.

## Findings

Progressive policies are not widespread, but being adopted rapidly.

Close relationship between the existence of a supplemental materials

• No statistically significant relationship between data and code policies

Data and supplemental material policies appear to lead software policy.

### **The R Series**

### Implementing Reproducible Research



Edited by Victoria Stodden Friedrich Leisch Roger D. Peng



Three sections:

I. Tools

2. Practices and Guidelines

3. Platforms

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

- 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.

# 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



# Really Reproducible Research

• "Really Reproducible Research" (1992) inspired by Stanford Professor on Claerbout:

[and data] which generated the figures." David Donoho, 1998

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

# ournal Requirements

- In January 2014 Science enacted new policies. The will check for: I. 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

- Failings of traditional reporting methods vs adaptation of standards to accommodate changes in the research process.
- Interaction of computational systems in the process of scientific discovery viz. reliability of parameter estimates and models.
- Benchmarking and testing: either nonexistent or over reliance on inappropriate benchmarks (see e.g. <u>http://www.in-cites.com/scientists/</u> <u>DrDavidDonoho.html</u>)
- Collective action problem: coordination of researcher incentives, universities, funding agencies, journals, scientific societies, legal and policy environment,



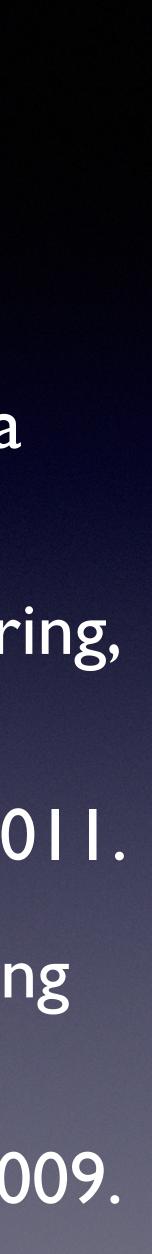
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- "Reproducible Research in Computational Harmonic Analysis", IEEE Computing in Science and Engineering, 11(1), January 2009
- "Enabling Reproducible Research: Open Licensing for Scientific Innovation," 2009.
  - available at http://www.stodden.net



## 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.

Code 91% 90% 86% 82% 85% 81% 85% 78% 71%

Encourage scientific advancement Encourage sharing in others Be a good community member Set a standard for the field Improve the calibre of research Get others to work on the problem Increase in publicity Opportunity for feedback Finding collaborators

### Sharing Incentives

Data 81% 79% 79% 76% 74% 79% 73% 71% 71%

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



Code 77% 52% 44% 40% 34% 30% 30% 20%

Time to document and clean up Dealing with questions from users Not receiving attribution Possibility of patents Legal Barriers (ie. copyright) Time to verify release with admin Potential loss of future publications Competitors may get an advantage Web/disk space limitations

# Barriers to Sharing

Data 54% 34% 42% 41% 38% 35% 33% 29%

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



## 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)

- (papers, code, figures, tables..)
- - reproduce the work

Exceptions and Limitations: Fair Use.

Original expression of ideas falls under copyright by default

Copyright secures exclusive rights vested in the author to:

- prepare derivative works based upon the original

# Responses Outside the Sciences I: Open Source Software

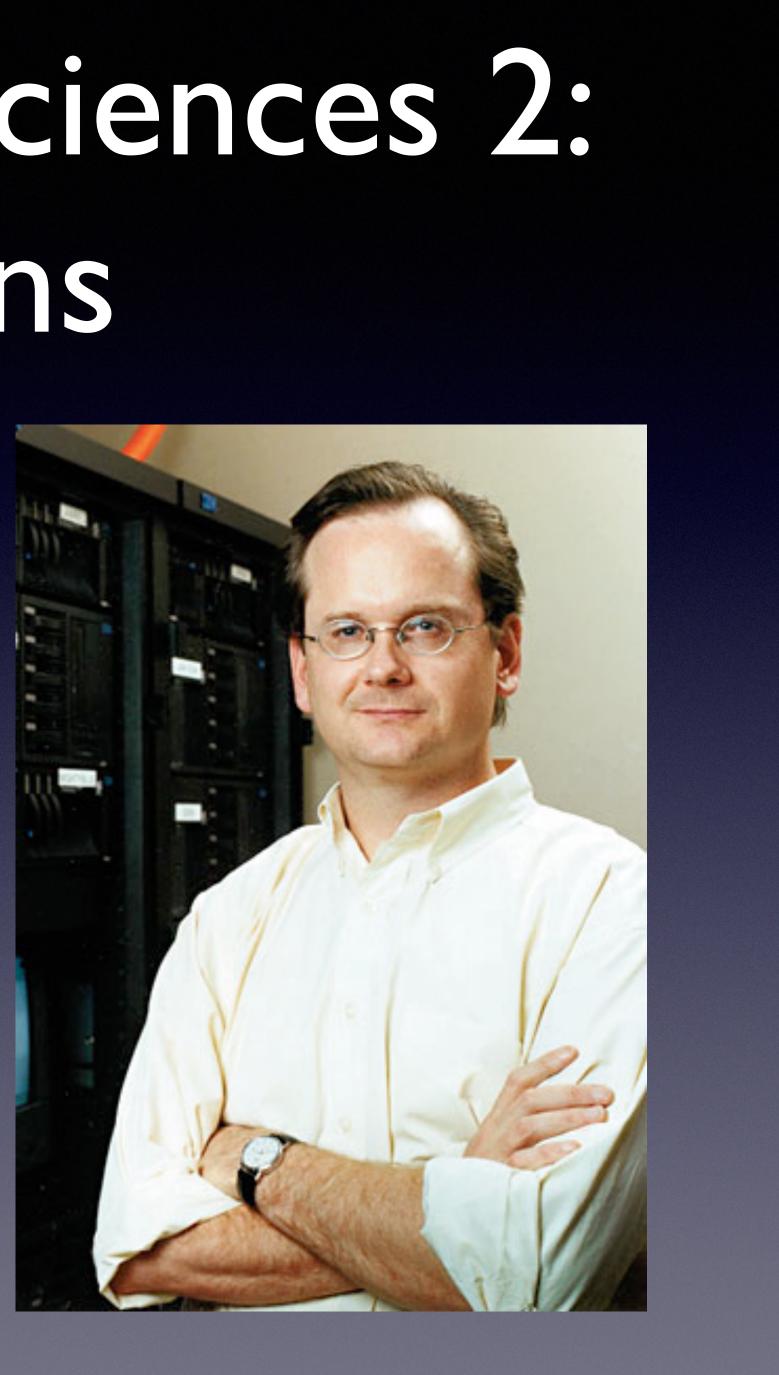
- Software with licenses that communicate alternative terms of use to code developers, rather than the copyright default.
- Hundreds of open source software licenses:
  - GNU Public License (GPL) -
  - (Modified) BSD License
  - MIT License
  - Apache 2.0 License
  - ... see <u>http://www.opensource.org/licenses/alphabetical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





## 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)

- 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,

Winner of the Access to Knowledge Kaltura Award 2008

• A suite of license recommendations for computational science:

 $\Rightarrow$  Realign the IP framework with longstanding scientific norms.

# Copyright and Data

- Copyright adheres to raw facts in Europe.
- Serv. Co., 499 U.S. 340 (1991)).
- public domain certification).
- anyway?

• 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.

• the possibility of a residual copyright in data (attribution licensing or

Law doesn't match reality on the ground: What constitutes a "raw" fact

