

Please download presentation slides at

https://sbonaretti.github.io/_attachments/2019_02_25_QMSKI_transparency.pdf

Hands-on transparent QMSKI: open-access data, reproducible workflows, and interactive publications

Serena Bonaretti

<https://sbonaretti.github.io/>

22nd International Workshop on Quantitative Musculoskeletal Imaging

February 25, 2019



Disclosures

- My first workshop on transparent research: Feel free to add and discuss information
- I will show some of the tools for transparent research, chosen among the most commonly used
- I do not have conflict of interest

What are openness and reproducibility?

- **Open science** refers to the free availability of data, software, and methods developed by researchers with the aim to share knowledge and tools to professionals and citizens ([Woelfle 2011](#))
- **Reproducibility** is the ability of researchers to duplicate the results of a previous study using the same data, software, and methods used by the original authors ([Bollen 2015](#))
 - **Replicability** is the recreation of same results using new data but the same experimental design ([Gorgolewski](#))

Note: In some fields the two definitions are inverted

Replication crisis

- Discovery of personalized cancer treatment at Duke



A Genomic Strategy to Refine Prognosis in Early-Stage Non-Small-Cell Lung Cancer

Anil Potti, M.D., Sayan Mukherjee, Ph.D., Rebecca Petersen, M.D., Holly K. Dressman, Ph.D., Andrea Bild, Ph.D., Jason Kootz, M.D., Robert Kratzke, M.D., Mark A. Watson, M.D., Ph.D., Michael Kelley, M.D., Geoffrey S. Ginsburg, M.D., Ph.D., Mike West, Ph.D., David H. Harpole, Jr., M.D., et al.

(Potti 2006)



Article | Published: 22 October 2006

Genomic signatures to guide the use of chemotherapeutics

Anil Potti, Holly K Dressman, Andrea Bild, Richard F Riedel, Gina Chan, Robyn Sayer, Janel Cragun, Hope Cottrill, Michael J Kelley, Rebecca Petersen, David Harpole, Jeffrey Marks, Andrew Berchuck, Geoffrey S Ginsburg, Phillip Febbo, Johnathan Lancaster & Joseph R Nevins

▲ This article was retracted on 07 January 2011

(Potti 2006)



2006-2010



FAST TRACK — ARTICLES | VOLUME 8, ISSUE 12, P 1071-1078, DECEMBER 01, 2007

RETRACTED: Validation of gene signatures that predict the response of breast cancer to neoadjuvant chemotherapy: a substudy of the EORTC 10994/BIG 00-01 clinical trial

Prof Hervé Bonnefoi, MD □ Anil Potti, MD □ Mauro Delorenzi, PhD □ Louis Mauriac, MD □ Mario Campone, MD
Michèle Tubiana-Hulin, MD □ et al. Show all authors

Published: November 14, 2007 • DOI: https://doi.org/10.1016/S1470-2045(07)70345-5

(Bonnefoi 2007)



An American Society of Clinical Oncology Journal

Pharmacogenomic Strategies Provide a Rational Approach to the Treatment of Cisplatin-Resistant Patients With Advanced Cancer

David S. Hsu, Bala S. Balakumaran, Chaitanya R. Acharya, Vanja Vlahovic, Kelli S. Walters, Katherine Garman, Carey Anders, Richard F. Riedel, Johnathan Lancaster, David Harpole, Holly K. Dressman, Joseph R. Nevins, Phillip G. Febbo, Anil Potti

From the Division of Medical Oncology, Department of Medicine; Institute for Genome Sciences and Policy; Department of Surgery, Duke University, Durham, NC; and the Division of Gynecologic Oncology, H. Lee Moffitt Cancer Center, Tampa, FL

Show Less

A retraction has been published.

(Hsu 2007)



Info Current issue All issues Search

Ann. Appl. Stat.
Volume 3, Number 4 (2009), 1309-1334.

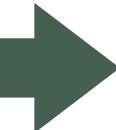
← Previous article TOC Next article →

Deriving chemosensitivity from cell lines: Forensic bioinformatics and reproducible research in high-throughput biology

Keith A. Baggerly and Kevin R. Coombes

(Baggerly 2009)

V. Stodden¹: “None of that was picked up in peer-review. Nobody looks under the covers that deeply in peer-review. They were able to read the paper. This kind of thing is in the code and in the data itself”



¹<https://www.youtube.com/watch?v=dF1-nkgwmjl> from min 13:30, and <https://www.youtube.com/watch?v=eV9dcAGaVU8>

Replication crisis

- Replication of studies in oncology



Comment | Published: 28 March 2012

Drug development

Raise standards for preclinical cancer research

C. Glenn Begley & Lee M. Ellis ✉

Nature 483, 531–533 (29 March 2012) | Download Citation ↓

(Begley 2012)



"Fifty-three papers were deemed 'landmark' studies...[S]cientific findings were confirmed in only 6 (11%) cases. Even knowing the limitations of preclinical research, this was a shocking result."

REPRODUCIBILITY OF RESEARCH FINDINGS

Preclinical research generates many secondary publications, even when results cannot be reproduced.

Journal impact factor	Number of articles	Mean number of citations of non-reproduced articles*	Mean number of citations of reproduced articles
>20	21	248 (range 3–800)	231 (range 82–519)
5–19	32	169 (range 6–1,909)	13 (range 3–24)

Results from ten-year retrospective analysis of experiments performed prospectively. The term 'non-reproduced' was assigned on the basis of findings not being sufficiently robust to drive a drug-development programme.

*Source of citations: Google Scholar, May 2011.

Replication crisis

- Other fields: psychology



SHARE RESEARCH ARTICLE



0

Estimating the reproducibility of psychological science

Open Science Collaboration^{*,†}

* See all authors and affiliations



Science 28 Aug 2015:
Vol. 349, Issue 6251, aac4716
DOI: 10.1126/science.aac4716



(Open Science Collaboration 2015)

"We conducted replications of 100 experimental and correlational studies [...]. Thirty-six percent of replications had statistically significant results; 47% of original effect sizes were in the 95% confidence interval"



Replication crisis

- Daily update on paper retraction



<https://retractionwatch.com/>



Article	Year of retraction	Citing Articles before retraction	Citing Articles after retraction	Total cites (journals indexed by Web of Science)
<u>Primary Prevention of Cardiovascular Disease with a Mediterranean Diet.</u> N Engl J Med April 4, 2013 Estruch R, Ros E, Salas-Salvado J, Covas MI, Corella, D, Aros F, Gomez-Gracia E, Ruiz-Gutiérrez V, Fiol M, Lapetra J, Lamuela-Raventos RM, Serra-Majem L, Pinto X, Basora J, Munoz MA, Sorli JV, Martinez JA, Martinez-Gonzalez MA, et al., for the PREDIMED Study Investigators	2018	1792	79	1917

<https://retractionwatch.com/the-retraction-watch-leaderboard/top-10-most-highly-cited-retracted-papers/>

Computational reproducibility crisis

HOW TO ENCOURAGE AND PUBLISH REPRODUCIBLE RESEARCH

Jelena Kovačević

Depts. of Biomedical Engineering & Electrical and Computer Engineering
Carnegie Mellon University
Email: jelenak@cmu.edu

([Kovacevic 2007](#))

15 papers from IEEE Transactions on image processing:

- 33% data available
- 0% code available
- 60% pseudo code available



Computational reproducibility crisis

Reproducible Research in Signal Processing

[What, why, and how]

[Patrick Vandewalle, Jelena Kovačević, and Martin Vetterli]

([Vandewalle 2009](#))

134 papers from IEEE Transactions
on image processing in 2004:

- 33% data available
- 9% code available
- 33% pseudo code available



Computational reproducibility crisis

MIT Sloan School of Management

MIT Sloan School Working Paper 4773-10

The Scientific Method in Practice: Reproducibility in the Computational Sciences

Victoria Stodden
[\(Stodden 2010\)](#)



Survey at NIPS 2008
134 researchers

Before conference

- 74% willing to share code
- 67% willing to share data

After conference

- 30% shared some code
- 20% shared some data

Some reasons not to share:

- The time it takes to clean up and document for release
- The possibility that your data / code may be used without citation
- Competitors may get an advantage
- Dealing with questions from users about the code

Computational reproducibility crisis

To encourage repeatable research, fund repeatability engineering and reward commitments to sharing research artifacts.

BY CHRISTIAN COLLBERG AND TODD A. PROEBSTING

Repeatability in Computer Systems Research

[\(Collberg 2015a\)](#) [\(Collberg 2015b\)](#)



- 508 papers from 8 conferences and 5 journals (2012)
- Team of undergraduate students, graduate students, and postdocs
- They could reproduce algorithms of 226 (44%)

Why is it so difficult to reproduce studies?

- Papers must be concise ([Vandewalle 2012](#))
 - Limited amount of words, figures, and tables
 - Authors have to select methods and parameters to present
- Data and software are in the supplementary material
 - Not in the paper body ([Vandewalle 2012](#))
- Until a few years ago there were no permanent, large, and free repositories for data and software with DOI
 - Personal repositories often get deleted ([Gil 2016](#))
- “Publish or perish” might favor quantity over quality and scientific bias (results have to be good) ([Fanelli 2010](#))



Current way of publishing

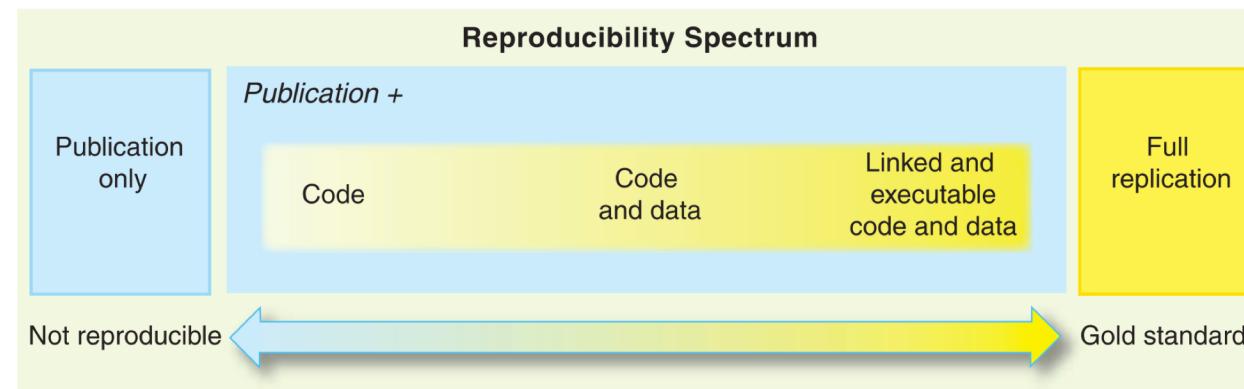
- Publications are the tip of the iceberg
- “It’s impossible to verify most of the results that computational scientists present at conferences and in papers” [Donoho 2009](#)
- “Scientific and mathematical journals are filled with pretty pictures of computational experiments that the reader has no hope of repeating” [LeVeque 2009](#)



Publications for transparent research

- “An author attaches to every figure caption a pushbutton or a name tag usable to recalculate the figure from all its data, parameters, and programs. This provides a concrete definition of reproducibility in computationally oriented research” [Claerbout 1992](#)
- “An article about computational science in a scientific publication is not the scholarship itself, it’s merely scholarship advertisement. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures” [Donoho 2009](#)

- [Peng 2011](#):



What are the benefits of transparent research?

- Openness and reproducibility are essential to researchers to:
 - Assess the value of scientific claims ([Sandve 2013](#))
 - Compare new methods to existing ones ([Freire 2018](#))
 - Build on the work of other scientists with confidence and efficiency, i.e. without "reinventing the wheel" ([Rule 2018](#))
 - Collaborate to improve and expand robust scientific workflows to accelerate scientific discoveries ([Donoho 2009](#), [Munafo 2017](#))



What are the benefits of transparent research?

- Increased citation rate

OPEN ACCESS Freely available online



Sharing Detailed Research Data Is Associated with Increased Citation Rate

Heather A. Piwowar*, Roger S. Day, Douglas B. Fridsma

Department of Biomedical Informatics, University of Pittsburgh School of Medicine, Pittsburgh, Pennsylvania, United States of America

Background. Sharing research data provides benefit to the general scientific community, but the benefit is less obvious for the investigator who makes his or her data available. **Principal Findings.** We examined the citation history of 85 cancer microarray clinical trial publications with respect to the availability of their data. The 48% of trials with publicly available microarray data received 85% of the aggregate citations. Publicly available data was significantly ($p = 0.006$) associated with a 69% increase in citations, independently of journal impact factor, date of publication, and author country of origin using linear regression. **Significance.** This correlation between publicly available data and increased literature impact may further motivate investigators to share their detailed research data.

[\(Piwowar 2007\)](#)

REPRODUCIBLE RESEARCH
FOR SCIENTIFIC COMPUTING

PATRICK VANDEWALLE

Code Sharing Is Associated with Research Impact in Image Processing

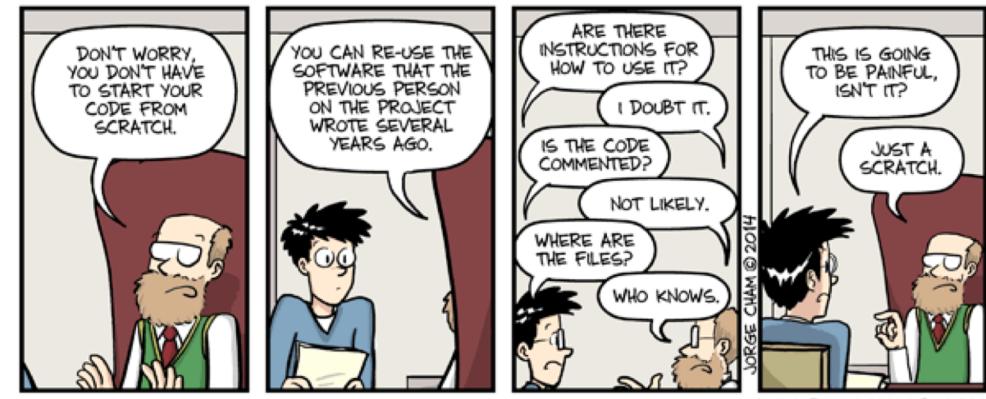
In computational sciences such as image processing, publishing usually isn't enough to allow other researchers to verify results. Often, supplementary materials such as source code and measurement data are required. Yet most researchers choose not to make their code available because of the extra time required to prepare it. Are such efforts actually worthwhile, though?

[\(Vandewalle 2012\)](#)

"The median number of citations [...] increases with a factor of 3 when code is available online"

- Personal and group self-discipline ([Donoho 2009](#))

- Reproducibility helps defeat self-deception ([Nuzzo 2015](#))



Funding agencies support transparent research

- Europe: [EOSC](#), [Horizon 2020](#), [OpenAire](#)
- US: [NIH](#), [Gates Foundation](#), [Chan-Zuckerberg Initiative](#)
- Canada: [Open data](#)
- Australia, New Zealand, Asia, ...

How can we conduct transparent research?

- Historically, research data, tools, and processes were rarely openly available because of limited storage and computational power ([Munafo 2017](#))
- Nowadays there are several tools to conduct transparent research
 - Open access data
 - Reproducible workflows
 - Interactive publications



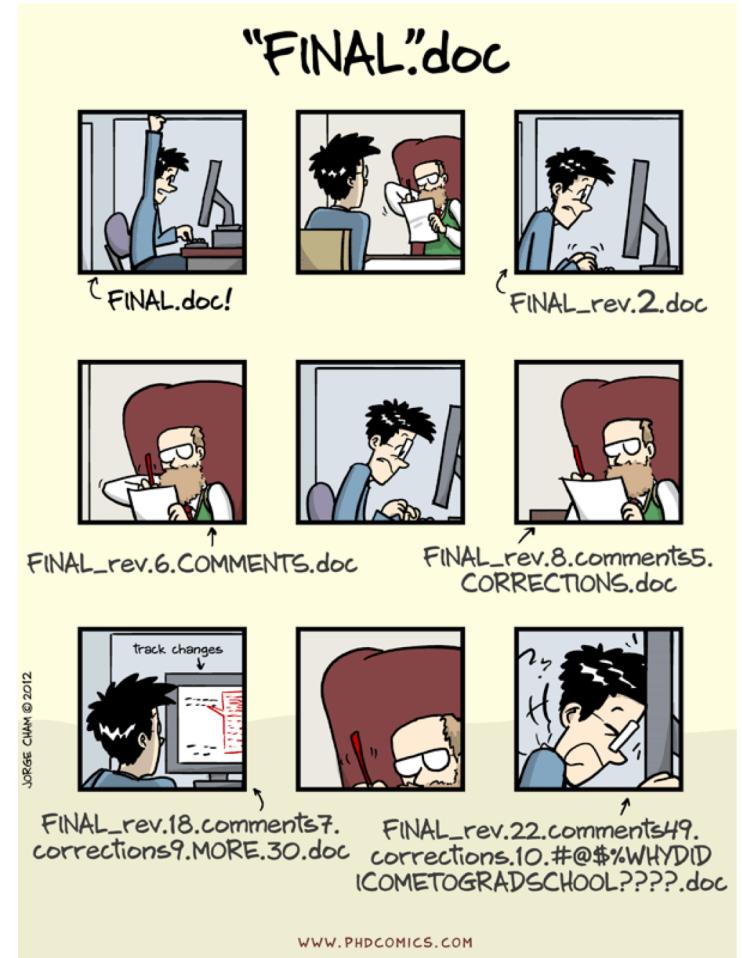
A few questions about our research practice

- How many of us have uploaded data and/or code to a public repository?
- How many of us use Jupyter notebook or R markdown for reproducible workflows?
- How many of us have written an interactive publication?

Hands-on transparent QMSKI:
open-access data,
reproducible workflows,
and interactive publications

About open data

- Data = data and software
- Why open repositories?
 - Personal repositories often get deleted ([Gil 2016](#))
 - Provide a DOI → Data and software are citable
 - Version control
- Metadata and documentation
 - Data provenance and usage



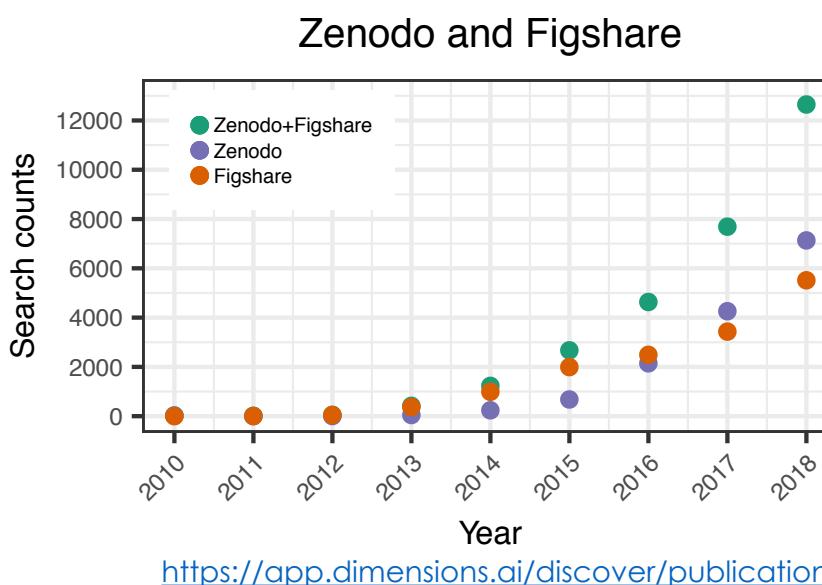
Data repositories

The screenshot shows the Zenodo homepage with a blue header. It displays two recent uploads: "Ambient air ozone concentrations using metal-oxide low-cost sensors: Spain and Italy, summer 2018" and "Research Software (RS) Careers: Generic Learnings from King's Digital Lab, King's College London". A sidebar on the right contains sections for "Zenodo now supports usage statistics!", "Using GitHub?", and "Zenodo in a nutshell".

<https://zenodo.org/>

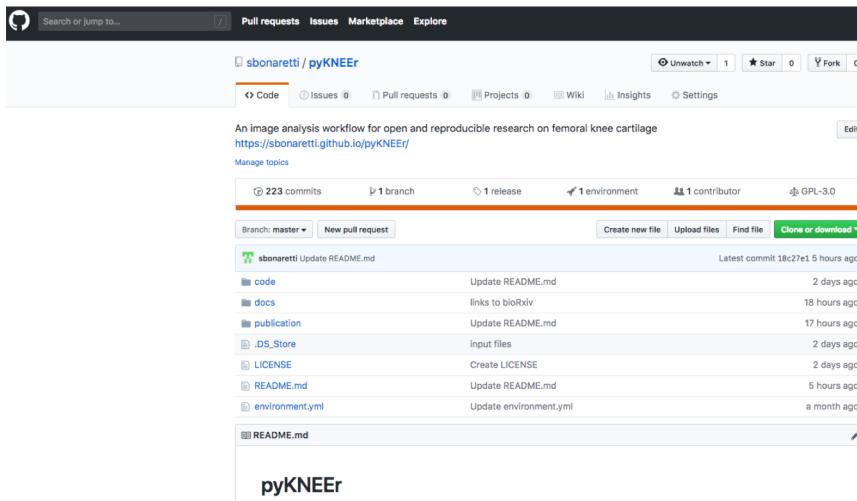
The screenshot shows the figshare homepage with a dark background featuring a mountain image. It highlights features like "store, share, discover research" and "get more citations for all of the outputs of your academic research over 5000 citations of figshare content to date".

<https://figshare.com/>



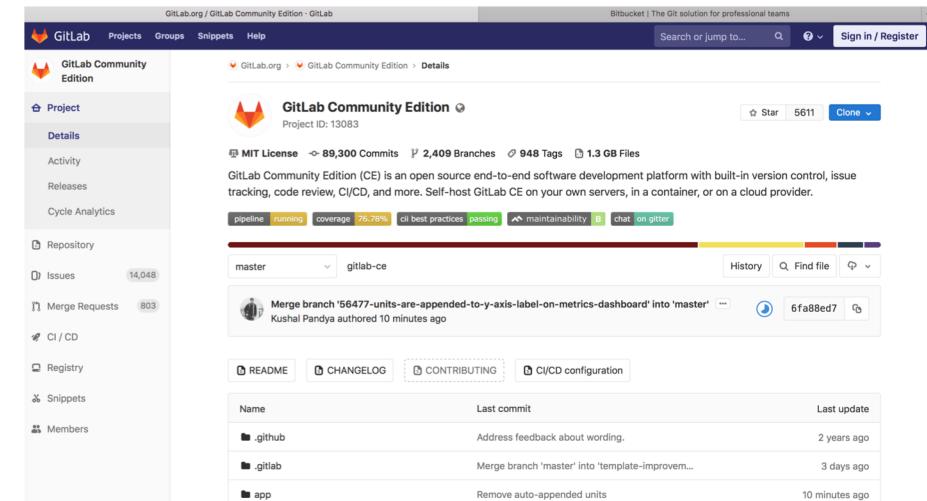
- More repositories: a list on [Nature](#)

Software repositories



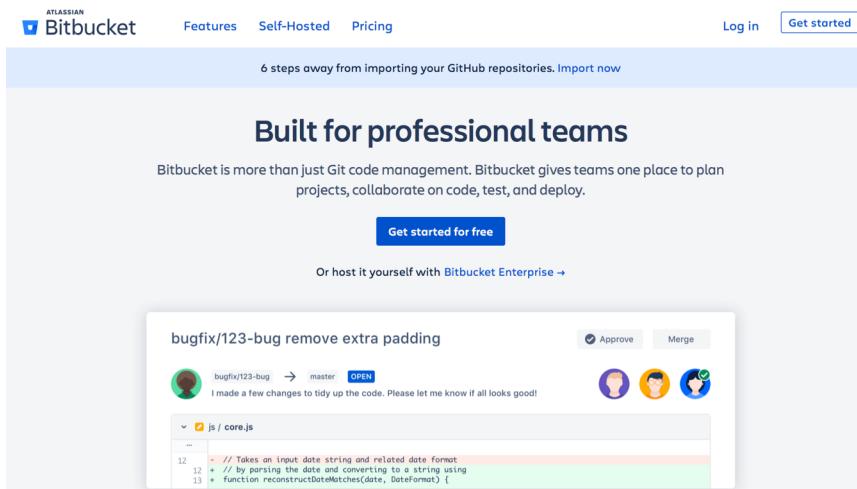
A screenshot of a GitHub repository page for 'sbonaretti/pyKNEEr'. The repository has 223 commits, 1 branch, 1 release, 1 environment, and 1 contributor. The code is licensed under GPL-3.0. The README.md file shows updates from 5 hours ago. The repository is described as 'An image analysis workflow for open and reproducible research on femoral knee cartilage'.

<https://github.com/>



A screenshot of a GitLab project page for 'GitLab Community Edition'. The project has 89,300 commits, 2,409 branches, 948 tags, and 1.3 GB files. It is licensed under MIT. The pipeline is running, coverage is 75.70%, and CI/CD is best practices passing. The repository has 14,048 issues and 803 merge requests. The README, CHANGELOG, CONTRIBUTING, and CI/CD configuration files are shown.

<https://about.gitlab.com>



The Bitbucket homepage features a 'Get started for free' button and a 'Built for professional teams' section. It highlights that Bitbucket is more than just Git code management, providing a platform for planning, collaborating, testing, and deploying projects. A screenshot of a pull request titled 'bugfix/123-bug remove extra padding' is shown, with the status 'OPEN' and three reviewers.

<https://bitbucket.org>

- Version control for reproducibility and collaborations

Metafiles and documentation

- Provenance of raw data
- Computational provenance of derived data
- Software documentation for code reuse
- Fields in repositories (e.g. Zenodo)
- Text files
- README.md in GitHub
- API
- Website
- ...

License

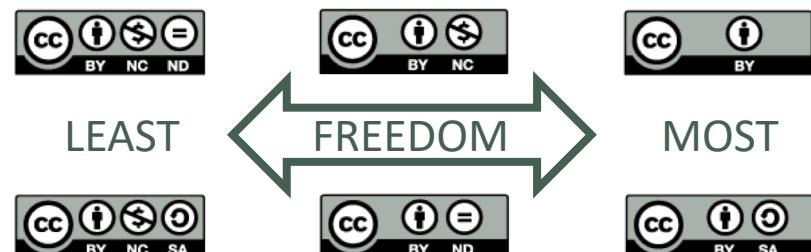
"Free software does not mean public-domain software. Free software is copyrighted, but it comes with a public license that allows you to use it, copy it, and redistribute it provided you follow certain guidelines" [Claerbout 1992](#)

- Online material is automatically protected by copyright
- If you want your material to be used:
Choose a license, “any” license

Data, publications, and code licenses

Data and publications

- Creative commons
(<https://creativecommons.org/choose>)



Reproduced from: <https://www.youtube.com/watch?v=8YkbeycRa2A>

Code

(<https://choosealicense.com/licenses/>)

	GNU AGPLv3	GNU GPLv3	GNU LGPLv3	Mozilla Public License 2.0	Apache License 2.0	MIT License	The Unlicense
Commercial use	●	●	●	●	●	●	●
Distribution	●	●	●	●	●	●	●
Modification	●	●	●	●	●	●	●
Patent use	●	●	●	●	●	●	●
Private use	●	●	●	●	●	●	●
Disclose source	●	●	●	●	●	●	●
License and copyright notice	●	●	●	●	●	●	●
Network use is distribution	●						
Same license	●	●	●	●	●	●	●
State changes	●	●	●				
Liability	●	●	●	●	●	●	●
Warranty	●	●	●	●	●	●	●
Trademark use				●	●	●	●

Hands-on transparent QMSKI:
open-access data,
reproducible workflows,
and interactive publications

How do we create reproducible workflows?

OPEN  ACCESS Freely available online



Editorial

Ten Simple Rules for Reproducible Computational Research

Geir Kjetil Sandve^{1,2*}, Anton Nekrutenko³, James Taylor⁴, Eivind Hovig^{1,5,6}

1 Department of Informatics, University of Oslo, Blindern, Oslo, Norway, **2** Centre for Cancer Biomedicine, University of Oslo, Blindern, Oslo, Norway, **3** Department of Biochemistry and Molecular Biology and The Huck Institutes for the Life Sciences, Penn State University, University Park, Pennsylvania, United States of America, **4** Department of Biology and Department of Mathematics and Computer Science, Emory University, Atlanta, Georgia, United States of America, **5** Department of Tumor Biology, Institute for Cancer Research, The Norwegian Radium Hospital, Oslo University Hospital, Montebello, Oslo, Norway, **6** Institute for Medical Informatics, The Norwegian Radium Hospital, Oslo University Hospital, Montebello, Oslo, Norway

(Sandve 2013)



EDITORIAL

Ten Simple Rules for Taking Advantage of Git and GitHub

Yasset Perez-Riverol^{1*}, Laurent Gatto², Rui Wang¹, Timo Sachsenberg³, Julian Uszkoreit⁴, Felipe da Veiga Leprevost⁵, Christian Fufezan⁶, Tobias Ternet¹, Stephen J. Eglen⁷, Daniel S. Katz⁸, Tom J. Pollard⁹, Alexander Konovalov¹⁰, Robert M. Flight¹¹, Kai Blin¹², Juan Antonio Vizcaíno^{1*}

1 European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Trust Genome Campus, Hinxton, Cambridge, United Kingdom, **2** Computational Proteomics Unit, Cambridge Systems Biology Centre, University of Cambridge, Cambridge, United Kingdom, **3** Applied Bioinformatics and Department of Computer Science, University of Tübingen, Tübingen, Germany, **4** Medizinisches Proteom-Center, Ruhr-Universität Bochum, Bochum, Germany, **5** Department of Pathology, University of Michigan, Ann Arbor, Michigan, United States of America, **6** Institute of Plant Biology and Biotechnology, University of Münster, Münster, Germany, **7** Centre for Mathematical Sciences, University of Cambridge, Cambridge, United Kingdom, **8** National Center for Supercomputing Applications and Graduate School of Library and Information Science, University of Illinois, Urbana, Illinois, United States of America, **9** MIT Laboratory for Computational Physiology, Institute for Medical Engineering and Science, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States of America, **10** Centre for Interdisciplinary Research in Computational Algebra, University of St Andrews, St Andrews, United Kingdom, **11** Department of Molecular Biology and Biochemistry, Markey Cancer Center, Resource Center for Stable Isotope-Resolved Metabolomics, University of Kentucky, Lexington, Kentucky, United States of America, **12** The Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark, Hørsholm, Denmark

(Perez-Riverol 2016)



PERSPECTIVE

Good enough practices in scientific computing

Greg Wilson^{1*}, Jennifer Bryan², Karen Cranston³, Justin Kitzes⁴, Lex Nederbragt⁵, Tracy K. Teal⁶

1 Software Carpentry Foundation, Austin, Texas, United States of America, **2** RStudio and Department of Statistics, University of British Columbia, Vancouver, British Columbia, Canada, **3** Department of Biology, Duke University, Durham, North Carolina, United States of America, **4** Energy and Resources Group, University of California, Berkeley, Berkeley, California, United States of America, **5** Centre for Ecological and Evolutionary Synthesis, University of Oslo, Oslo, Norway, **6** Data Carpentry, Davis, California, United States of America

(Wilson 2016)

arXiv.org > cs > arXiv:1810.08055

Computer Science > Other Computer Science

Ten Simple Rules for Reproducible Research in Jupyter Notebooks

Adam Rule, Amanda Birmingham, Cristal Zuniga, Ilkay Altintas, Shih-Cheng Huang, Rob Knight, Niema Moshiri, Mai H. Nguyen, Sara Brin Rosenthal, Fernando Pérez, Peter W. Rose

(Submitted on 13 Oct 2018)

Reproducibility of computational studies is a hallmark of scientific methodology. It enables researchers to build with confidence on the methods and findings of others, reuse and extend computational pipelines, and thereby drive scientific progress. Since many experimental studies rely on computational analyses, biologists need guidance on how to set up and document reproducible data analyses or simulations.

In this paper, we address several questions about reproducibility. For example, what are the technical and non-technical barriers to reproducible computational studies? What opportunities and challenges do computational notebooks offer to overcome some of these barriers? What tools are available and how can they be used effectively?

We have developed a set of rules to serve as a guide to scientists with a specific focus on computational notebook systems, such as Jupyter Notebooks, which have become a tool of choice for many applications. Notebooks combine detailed workflows with narrative text and visualization of results. Combined with software repositories and open source licensing, notebooks are powerful tools for transparent, collaborative, reproducible, and reusable data analyses.

(Rule 2018)

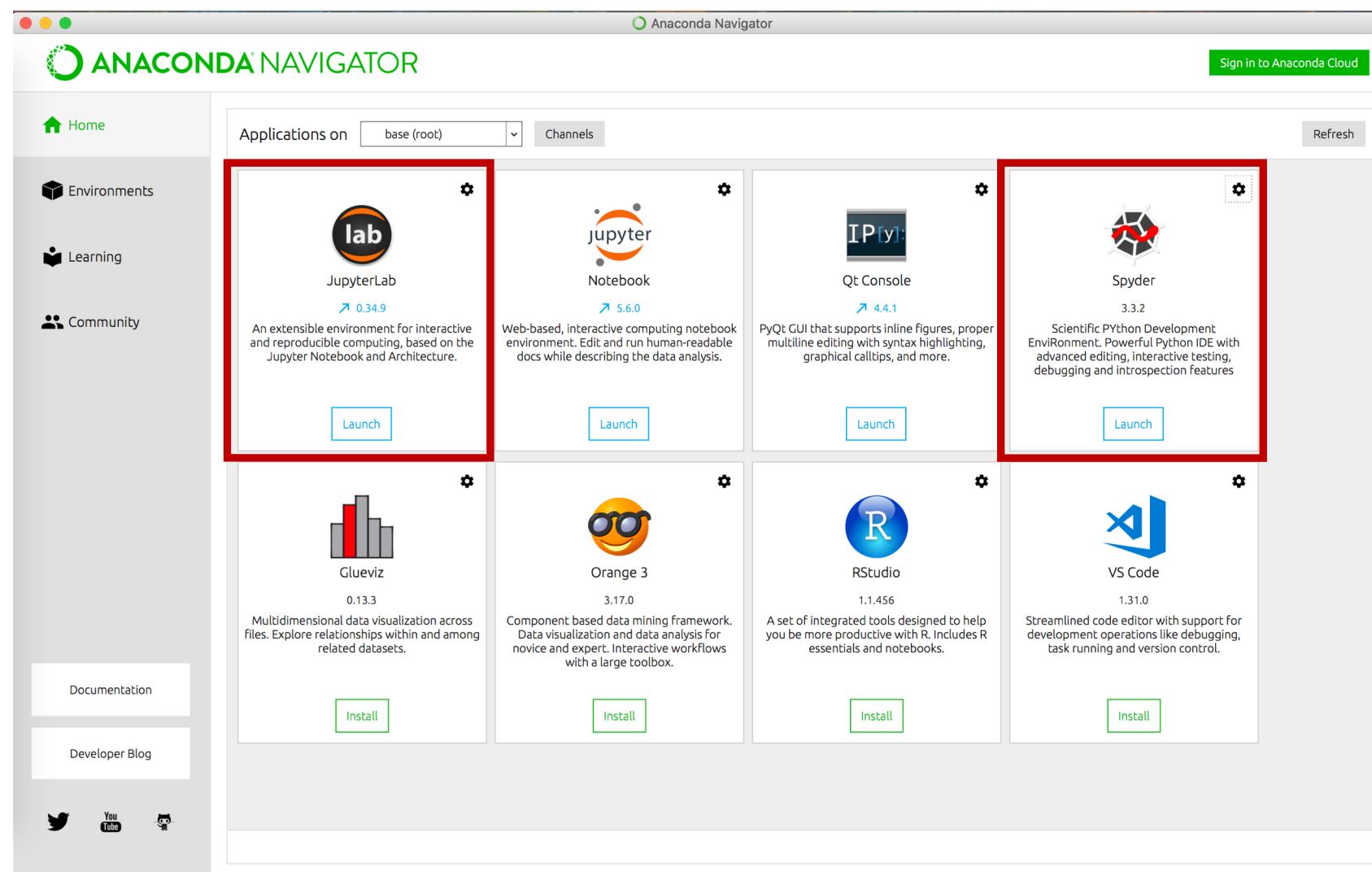
Summary of rules

- Use open source programming language and file formats
 - e.g. python, R, .txt, .csv, ...
- Automate data analysis
 - Avoid manual data manipulation
 - Tidy data tables with scripts
 - Always store raw data behind plots
- For every result keep track of how it was produced
 - Share and explain your data and code
 - Document the process, not just the results
 - Use version control, record dependencies
- Be your own user
 - Code well, be transparent, be simple
- Contribute to reproducible and open research
 - Don't be a perfectionist: "release early, release often"



TheVirtualPresenter.com

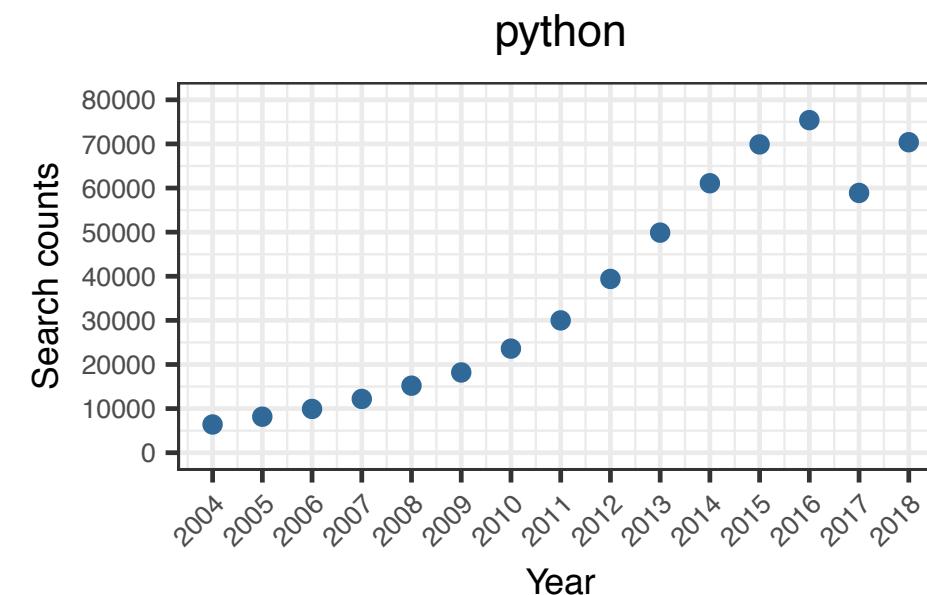
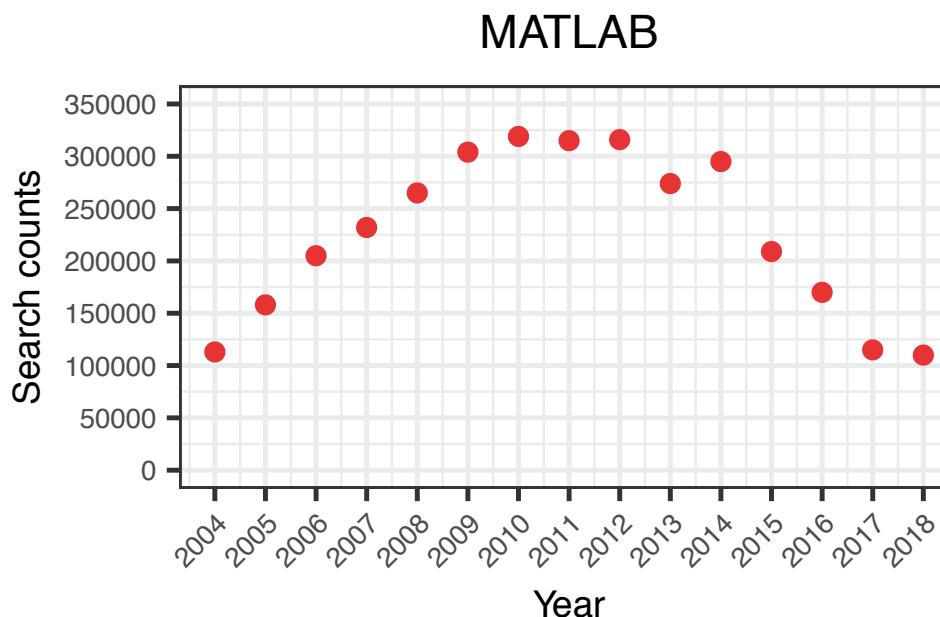
Open access language: python environment



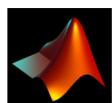
[Download Anaconda](#)

Open access language

- Compatible with open and reproducible research
- A large amount of packages and shared code
- No license purchase



From MATLAB to python: Differences



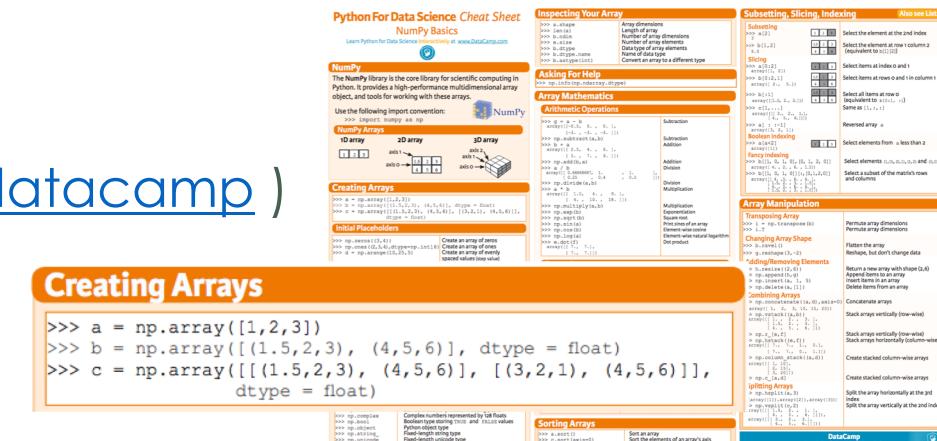
```
% initialize and print an array  
% array name = [start:step:stop];  
  
C = [2:2:8];  
_____  
% if structure  
  
if a == 1 && b ~= 3  
    fprintf('a=1 and b not 3 \n');  
    fprintf('OK? \n');  
end  
_____  
% plotting  
  
x = linspace(0,2*pi,100);  
y = sin(x);  
plot(x,y)  
ylabel('sin(x)')  
xlabel('x')
```

```
# initialize and print an array  
# array name = arange(start,stop,step)  
  
import numpy as np  
C = np.arange(2,10,2)  
_____  
# if structure  
  
if a == 1 and b != 3:  
    print('a=1 and b not 3');  
    print('OK?')  
_____  
# plotting  
  
import numpy as np  
import matplotlib.pyplot as plt  
x = np.linspace(0,2*np.pi,100)  
y = np.sin(x)  
plt.plot(x,y)  
plt.ylabel('sin(x)')  
plt.xlabel('x')  
plt.show()
```

http://reactorlab.net/resources-folder/matlab/P_to_M.html

From MATLAB to python: Practical tips

- To start, translate part of your current code to python
 - Open MATLAB and Spyder, and translate lines one-to-one
 - Focus on syntax, not algorithm
- Every time you are stuck, search for solutions online
 - There are plenty of question-and-answer sites (e.g. Stack Overflow) and blogs
- Take advantage of online material
 - Structured knowledge: Free online courses (e.g. [datacamp](#))
 - Free style: Blogs, cheat sheet, and YouTube
- Take advantage of shared code
 - Look for already developed code, don't reinvent the wheel



Jupyter notebooks

```
pyKNEEr
Relaxometry of Femoral Knee Cartilage
Exponential and linear fitting
• Exponential fitting is computationally expensive but more accurate
• Linear fitting is faster as data are transformed to their log and then linearly interpolated. However, linear fitting is less accurate because the nonlinear logarithmic transform provides larger weight to outliers
The fitting is computed:
• directly on the acquired images or after rigid registration of the following echo to the first echo
• voxel-wise, i.e. for each voxel the Echo-Times (dicom tag [0018,0081]) are the x-variable and the voxel intensities in each acquisition are the y-variable
• only in the mask volume to have short computation time
Image information
Inputs:
• input_file_name contains the list of the images used to calculate the relaxation maps
• method_flag is 0 if fitting is linear, 1 if fitting is exponential
• registration_flag is 0 for no registration, 1 for rigid registration
• output_file_name contains average and standard deviation of the fitting maps
In [1]: input_file_name = "image_list_relaxometry_fitting_0A11_T2.txt"
method_flag = 1 # 0 = linear, 1 = exponential
registration_flag = 1 # 0 = no rigid registration, 1 = execute rigid registration
n_of_cores = 4
output_file_name = "exp_fit_aligned_0A11_T2.csv"

Read image data
• image_data is a dictionary (or struct), where each cell corresponds to an image. For each image, information such as paths and file names are stored
In [2]: image_data = io.load_image_data_fitting(input_file_name, method_flag, registration_flag)

Calculate fitting maps
Align acquisitions
Images are aligned rigidly to remove occasional subject motion among acquisitions
Note: This step is optional and can be skipped, given that:
• When images are aligned, the fitting is calculated on interpolated values obtained with rigid registration
• When images are not aligned, the fitting is calculated on original intensities, but images might not be aligned
In [3]: if registration_flag == 1:
    rel.align_acquisitions(image_data, n_of_cores)

Compute the fitting
In [4]: rel.calculate_fitting_maps(image_data, n_of_cores)

Visualize fitting maps
2D MAP: For each image, fitting maps at medial and lateral compartments and flattened map
The flattened map is an average of neighboring voxels projected on the bone surface side of the femoral cartilage
In [5]: rel.show_fitting_maps(image_data)

3D MAP: Interactive rendering of fitting maps
(The error message "Error creating widget: could not find model" can appear when the notebook is moved to a different folder)
In [6]: # ID of the map to visualize (The ID is the one in the 2D visualization above)
image_ID = 1 - 1 # -1 because counting starts from 0

# read image
file_name = image_data[image_ID]["relaxometryFolder"] + image_data[image_ID]["mapFileName"]
image = tk.imread(file_name)

# view
viewer = view(image, gradient_opacity=0.0, ui_collapsed=False, shadow=False)
viewer

GRAPH: Dots represent the average value of fitting maps per image; bars represents the standard deviation
In [7]: rel.show_fitting_graph(image_data)

TABLE: Average and standard deviation of fitting maps per image
The table is saved as a .csv file for subsequent analysis
In [8]: rel.show_fitting_table(image_data, output_file_name)

References
[1] Borhani A., Wheaton AJ., Gougaud A.J., Akella S.V., Regatte RR., Charagundla S.R., Reddy R. In vivo measurement of T1rho dispersion in the human brain at 1.5 Tesla. J Magn Reson Imaging. Apr;19(4):403-9. 2004.
[2] Li X., Benjamin Ma C., Link TM., Castillo D.D., Blumenkrantz G., Lozano J., Carbajal-Garcia J., Ries M., Majumdar S. In vivo T1 and T2 mapping of articular cartilage in osteoarthritis of the knee using 3 T MRI. Osteoarthritis Cartilage. Jul;15(7):789-97. 2007.

Dependencies
In [9]: %load_ext watermark
%watermark -v -m SimpleITK,matplotlib,numpy,pandas,scipy,itkwidgets,multiprocessing
```

- Open-source web application integrating
 - Live code
 - Narrative text with equations
 - Visualizations
- Versatile
- Easy to share among researchers



Example of notebooks in medical imaging

- Bone microCT

- SimpleITK notebooks

- SPIE 2019 workshop

- Deep Learning Toolkit

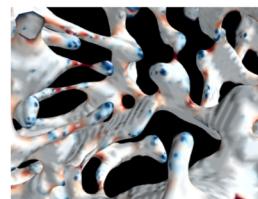
- VTK

- pyKNEEr

Processing X-ray tomography images with Python

X-ray tomography is an imaging technique that produces 3-D images of a scanned object. For most applications of tomography such as medical imaging or materials science, one often wishes to extract and label objects of interest from the 3-D tomography image.

This tutorial is an example of segmentation of 3-D tomography images, using the [scikit-image](#) Python package. Most image processing functions of [scikit-image](#) are compatible with 2-D as well as 3-D images, which makes it a tool of choice for processing tomography images. Furthermore, [scikit-image](#) is part of a larger ecosystem of Scientific Python packages, so that it is possible to use other packages, such as Mayavi for 3-D visualization.



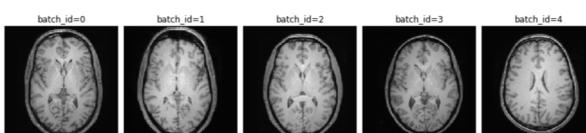
```
#matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
from time import time
```

```
# Visualise the 'dict_batch_feat' using matplotlib.
input_tensor_shape = dict_batch_feat.shape
center_slices = [s//2 for s in input_tensor_shape]

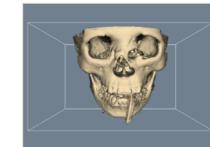
# Visualise the 'gen_batch_feat' using matplotlib.
f, axarr = plt.subplots(1, input_tensor_shape[0], figsize=(15,5));
f.suptitle('Visualisation of the "dict_batch_feat" input tensor with shape={}'.format(input_tensor_shape))

for batch_id in range(input_tensor_shape[0]): # Extract a center slice image
    img_slice_ = np.squeeze(dict_batch_feat[batch_id, center_slices[1], :, :, :])
    img_slice_ = np.flip(img_slice_, axis=0)

    # Plot
    axarr[batch_id].imshow(img_slice_, cmap='gray');
    axarr[batch_id].axis('off')
    axarr[batch_id].set_title('batch_id={}'.format(batch_id))
f.subplots_adjust(wspace=0.05, hspace=0, top=0.8)
plt.show();
```



[VTKExamples/Python/VisualizationAlgorithms/HeadBone](#)



Other Languages
See (Cxx)

Code

[HeadBone.py](#)

```
#!/usr/bin/env python

import vtk

def main():
    fileName = get_program_parameters()

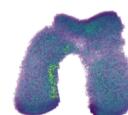
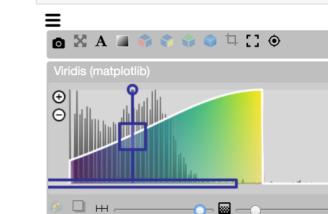
    colors = vtk.vtkNamedColors()
```

3D MAP: Interactive rendering of T_2 maps

```
# ID of the map to visualise (the ID is the one in the 2D visualization above)
image_ID = 1 - 1 # -1 because counting starts from 0

# read image
file_name = image_data[image_ID]["relaxometryFolder"] + image_data[image_ID]["t2mapMaskFileName"]

# view
viewer = view(image, gradient_opacity=0.0, ui_collapsed=False, shadow=False)
```



binder

- Online interactive computational environment



Turn a Git repo into a collection of interactive notebooks

Have a repository full of Jupyter notebooks? With Binder, open those notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere.

Build and launch a repository

GitHub repository name or URL

GitHub ▾

Git branch, tag, or commit

Path to a notebook file (optional)

File ▾

launch

Copy the URL below and share your Binder with others:

Fill in the fields to see a URL for sharing your Binder.

Copy the text below, then paste into your README to show a binder badge: launch [binder](#)

Computational environment

- Dependencies for reproducibility of computational environment
 - Package changes and future versions can be not compatible

Dependencies

```
%load_ext watermark  
%watermark -v -m -p matplotlib, numpy, pandas, scipy
```

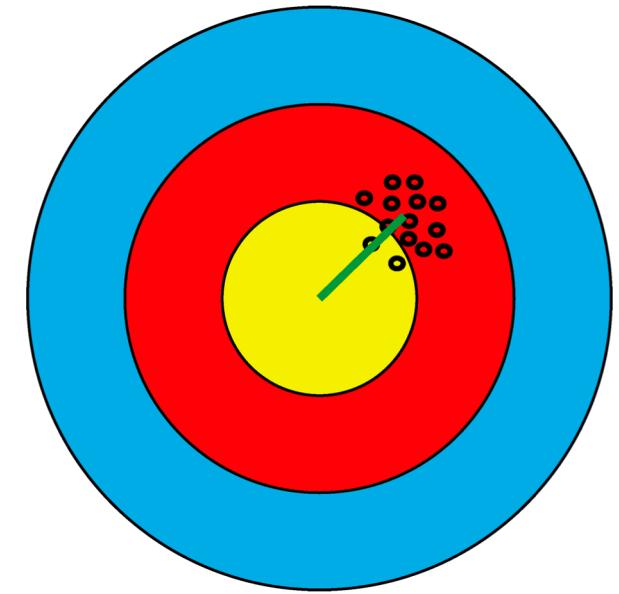
```
Cython 3.7.1  
IPython 7.2.0
```

```
matplotlib 2.2.3  
numpy 1.16.1  
pandas 0.24.1  
scipy 1.2.1
```

```
compiler    : Clang 4.0.1 (tags/RELEASE_401/final)  
system      : Darwin  
release     : 17.7.0  
machine     : x86_64  
processor   : i386  
CPU cores   : 4  
interpreter: 64bit
```

Last note on reproducibility

- Reproducibility does not imply correctness
- Lack of reproducibility does not imply incorrectness
- Incorrectness can be found with reproducibility



[Holmes 2018](#)

Hands-on transparent QMSKI:
open-access data,
reproducible workflows,
and interactive publications

Preprints and open access

- Paper repositories: [arXiv](#) and [bioRxiv](#)



arXiv.org @arxiv · Feb 14

Roses are red, violets are blue, we've reached another milestone all thanks to you! Last night we surpassed 1.5M articles--all open and free. This comes 4 years, 1 month and 16 days after reaching 1M, which took more than 23 years to reach. 2M seems just around the corner!

- Major publishers accept preprints ([list](#))
- Scientific journals:
 - Only open access: PLOS, Frontiers, F1000, ...
 - Allow open access publications: Wiley, Elsevier,...
 - Allocation for open access publication in grants



How do we make interactive publications?



Earth and Space Science

REVIEW

10.1002/2015EA000136

Special Section:
Geoscience Papers of the Future

Key Points:

- Describes best practices for documenting research to support open science
- Publishing computational provenance with software and data improves science transparency
- Promotes approaches to achieve equitable credit for all digital research products

Correspondence to:
Y. Gil,
gil@isi.edu

Toward the Geoscience Paper of the Future: Best practices for documenting and sharing research from data to software to provenance

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([Gil 2016](#))

On Reproducible AI

Towards reproducible research, open science, and digital scholarship in AI publications

Odd Erik Gundersen, Yolanda Gil and David W. Aha

Abstract

Background: Artificial intelligence, like any science, must rely on reproducible experiments to validate results.

Objective: To give practical and pragmatic recommendations for how to document AI research so that results are reproducible. **Method:** Our analysis of the literature shows that AI publications currently fall short of providing enough documentation to facilitate reproducibility. Our suggested best practices are based on a framework for reproducibility and recommendations for best practices given by scientific organizations, scholars, and publishers. **Results:** We have made a reproducibility checklist based on our investigation and described how every item in the checklist can be documented by authors and examined by reviewers.

Conclusion: We encourage authors and reviewers to use the suggested best practices and author checklist when considering submissions for AAAI publications and conferences.

([Gundersen 2018](#))

- Buttons and links to data and code
- Documentation of the computational provenance of results

Examples of interactive papers

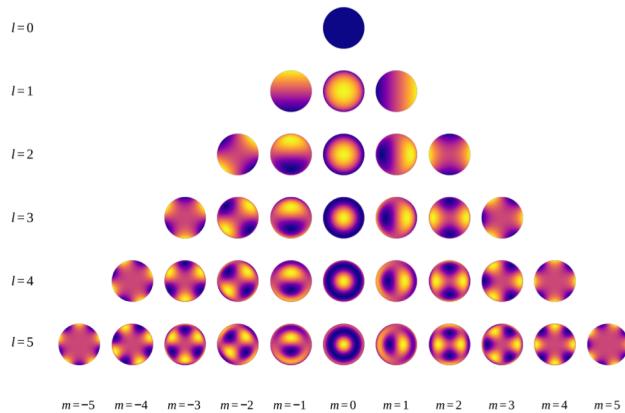


Figure 1. The real spherical harmonics up to degree $l = 5$ computed from Equation (1). In these plots, the x -axis points to the right, the y -axis points up, and the z -axis points out of the page.

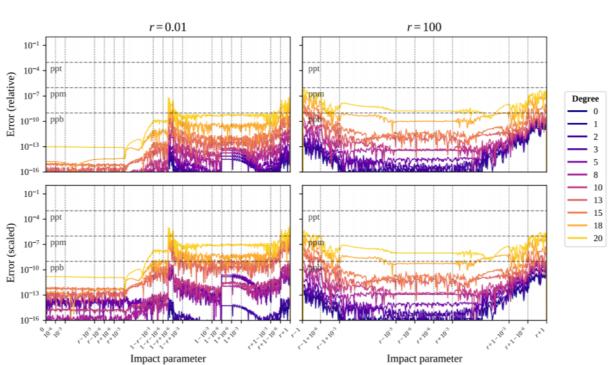


Figure 12. Similar to Figure 11, but showing instead the error on the derivative of the flux with respect to the impact parameter computed analytically with autodifferentiation. The error is computed relative to a numerical derivative computed at 128 bit precision.

(Luger 2018)

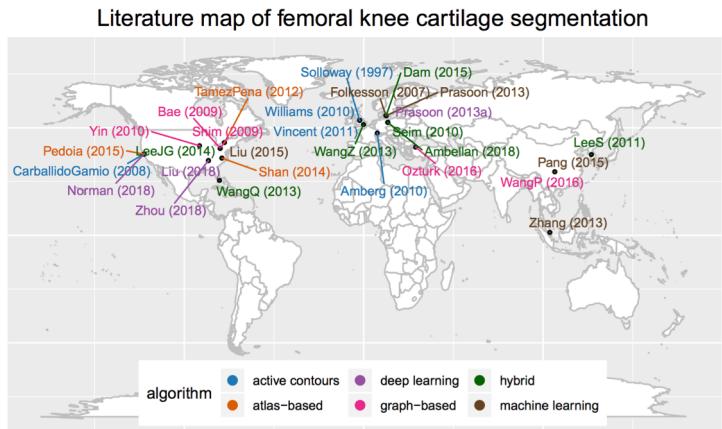


Figure 1: The visualization shows name of first author, year of publication, affiliation of last author, and segmentation method for 29 relevant publications on femoral knee cartilage segmentation from 1997 to 2018. Publications by segmentation method and in alphabetical order are: Active contours: Amberg(2010)[2], Carballido-Gamio(2008)[6], Solloway(1997)[62], Vincent(2011)[67], Williams(2010)[74]; Atlas-based: Pedoia(2015)[47], Shan(2014)[59], Tamez-Pena(2012)[64]; Deep-learning: Liu(2018)[33], Norman(2018)[43], Prasoon(2013a)[52], Zhou(2018)[81]; Graph-based: Bae(2009)[4], Ozturk(2016)[44], Shim(2009)[60], WangP(2016)[68], Yin(2010)[78]; Hybrid: Ambellan(2018)[1], Dam(2015)[11], LeeG(2014)[30], Lees(2011)[31], Seim(2010)[57], WangQ(2013)[69], WangZ(2013)[70]; Machine learning: Folkeson(2007)[18], Liu(2015)[34], Pang(2015)[46], Prasoon(2013)[51], Zhang(2013)[80]. This graph and graphs in Fig. 4 and Fig. 5 were made in Jupyter notebook using ggplot2 [71], an R package based on the grammar of graphics [72].

Software Used Preprocessing	Repository	Metadata / Documentation	Software / Language	License	DOI	Citation
elastix 4.8	Bitbucket GitHub	Wiki GitHub Wiki	C++, ITK C++, ITK	Apache Apache	https://doi.org/10.1016/j.media.2014.05.008 https://doi.org/10.1109/TMI.2009.2035616	[59]*
Developed pyKNEER	GitHub	Website	python, Jupyter notebook	GNU GPLv3	https://doi.org/10.5281/zenodo.2574172	Bonaretti S. et al. "pyKNEER" (v0.1). Zenodo. 2019. 10.5281/zenodo.2574172
Data Original	OAI	Website	-	Data user agreement	https://doi.org/10.1016/j.joca.2018.01.018	[49]*
Derived (results)	Zenodo	Jupyter notebook	-	CC-BY-NC-SA	https://doi.org/10.5281/zenodo.2630609	Bonaretti S. et al. Dataset used in (Bonaretti et al. 2019). Zenodo. 2019. 10.5281/zenodo.2530609

Dataset	OAII-DESS	OAII-T ₂	OAII-BL	OAII-FU	inHouse-DESS	inHouse-CQ
Number of subjects	19	19	88	88	4	4
I. Acquisition parameters						
Acquisition protocol	DESS sagittal	T ₂ -w sagittal	DESS sagittal	DESS sagittal	DESS sagittal	CubeQuant sagittal
Acquisition plane	2 (1 available) ^a	7	2 (1 available) ^a	2 (1 available) ^a	2 (1 available) ^a	4
Number of images in series	0.3646 x 0.3646	0.3125 x 0.3125	0.3646 x 0.3646	0.3646 x 0.3646	0.3125 x 0.3125	0.3125 x 0.3125
In-plane spacing [mm]	(0.420 x 0.420)*	(0.420 x 0.426)*	(0.420 x 0.426)*	(0.420 x 0.426)*	(0.420 x 0.426)*	-
Slice thickness [mm]	0.7 (0.75)*	3 (3.5)*	0.7	1.5	42.52	-
Echo time (TE) [ms]	4.7	10, 20, 30, 40,	4.7	4.7	4.7	-
Spin-lock time (TSL) [ms]	-	50, 60, 70	-	-	-	1, 10, 30, 60
Repetition time (TR) [ms]	16.32	2700 (2900)*	16.32	25	25	1302
Flip angle [°]	25	180	25	30	30	90
II. Ground truth segmentation						
Method	atlas-based	active models	femoral cartilage mask	femoral cartilage contour	-	-
Anatomy	femur, femoral cartilage	-	-	-	-	-
Type	-	-	-	-	-	-
III. Experimental results						
Image number in series	1	1	2-7	1	1	2
Preprocessing	-	-	-	-	-	1
Spatial standardization	•	•	•	•	•	•
Intensify standardization	-	-	-	-	-	-
Segmentation	4, 8, 10, 13, 16	-	-	-	-	-
Find reference	•	-	-	-	-	-
Intersubject	-	-	-	-	-	-
Longitudinal	-	-	-	-	-	-
Multimodal	-	•	-	-	-	-
Segmentation quality	-	-	-	-	-	-
Dice coefficient	•	-	-	-	-	-
Analysis	•	-	-	-	-	-
Morphology	•	•	•	•	•	•
Relaxation	-	•	-	-	•	•

(Bonaretti 2019)

Journal requirements



Acceptable Data-Sharing Methods

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PLOS journals will not consider manuscripts for which the following factors influence ability to share data:

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[See acceptable data access restrictions here.](#)

<https://blog.frontiersin.org/2018/02/21/open-data-figshare-partnership/>



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Frontiers partners with Figshare to promote open data

Posted on February 21, 2018 in [Frontiers Announcements](#), [Top News](#)

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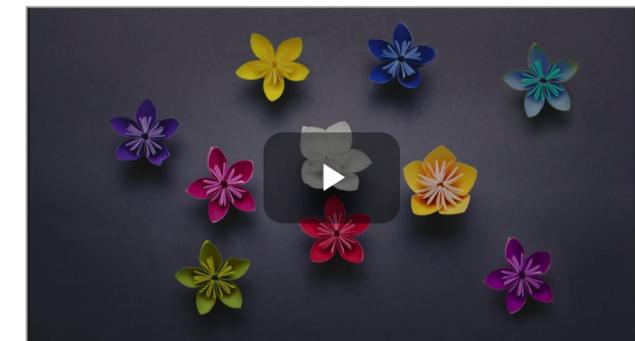
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Take home message



Hands-on transparent QMSKI: open-access data, reproducible workflows, and interactive publications

Serena Bonaretti

<https://sbonaretti.github.io/>

22nd International Workshop on Quantitative Musculoskeletal Imaging

February 25, 2019

