Reproducing and Preserving Research with ReproZip

Remi Rampin, Vicky Steeves, Fernando Chirigati

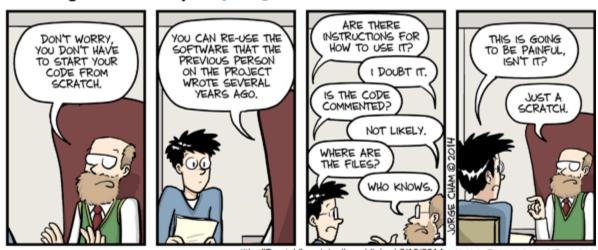
<u>@remram44, @VickySteeves, @fchirigati</u>

IASSIST 2017 | May 25, 2017



Obligatory PhD Comics strip...

Piled Higher and Deeper by Jorge Cham



title: "Scratch" - originally published 3/12/2014 WWW. PHDCOMICS. COM

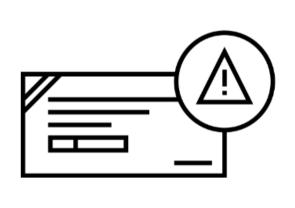
Reproducibility exists on a spectrum

- Reviewable Research: Sufficient detail for peer review & assessment.
- Replicable Research: Tools are available to duplicate the author's results using their data.
- Confirmable Research: Main conclusions can be attained independently without author's software.
- Auditable Research: Process & tools archived such that it can be defended later if necessary.
- Open/Reproducible Research: Auditable research made openly available.

Stodden et al ICERM report (2013)

Challenge 1: Everyone Messes Up

Human Errors



People make mistakes--and it impacts their research.

It's good to have other people check out your research and analyses--it's like having a copy editor for your data!



<u>Gap</u>: a tool to seamlessly review whole research projects without the reviewer having to manually install and debug all dependencies, code, and data.

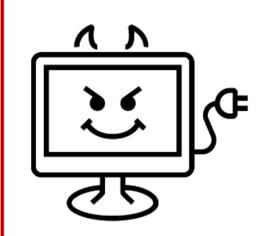
Excel is Terrible

American Economic Review: Papers & Proceedings 100 (May 2010): 573–578 http://www.aeaweb.org/articles.php?doi=10.1257/aer.100.2.573

<>	В	С		J	K	L	M
	2 Real GDP growth						
3			Debt/GDP				
4	Country	Coverage	30 or less	30 to 60	60 to 90	90 or above	30 or less
26			3.7	3.0	3.5	1.7	5.5
27	Minimum		1.6	0.3	1.3	-1.8	0.8
28	Maximum		5.4	4.9	10.2	3.6	13.3
29							
1 30	US	1946-2009	n.a.	3.4	3.3	-2.0	n.a.
31	UK	1946-2009	n.a.	2.4		2.4	n.a.
32	Sweden	1946-2009	3.6		2.7	n.a.	6.3
ic 33	Spain	1946-2009	1.5			n.a.	9.9
34	Portugal	1952-2009	4.8	2.5	0.3	n.a.	7.9
, 33	New Zealand	1948-2009	2.5	2.9	3.9	-7.9	2.6
36	Netherlands	1956-2009	4.1	2.7	1.1	n.a.	6.4
37	Norway	1947-2009	3.4		n.a.	n.a.	5.4
. 38	Japan	1946-2009	7.0		1.0	0.7	7.0
e 39	Italy	1951-2009	5.4	2.1	1.8	1.0	5.6
40	Ireland	1948-2009	4.4	4.5	4.0	2.4	2.9
41	Greece	1970-2009	4.0		2.7	2.9	13.3
42	Germany	1946-2009	3.9	0.9	n.a.	n.a.	3.2
43	France	1949-2009	4.9	2.7	3.0	n.a.	5.2
44	Finland	1946-2009	3.8			n.a.	7.0
45	Denmark	1950-2009	3.5	1.7	2.4	n.a.	5.6
p 46	Canada	1951-2009	1.9			n.a.	2.2
, 47	Belgium	1947-2009	n.a.	4.2	3.1	2.6	n.a.
48	Austria	1948-2009	5.2		-3.8	n.a.	5.7
49	Australia	1951-2009	3.2	4.9	4.0	n.a.	5.9
50							
51	ner countries. 1		4.1	2.8 Severe	2.8		E(L30:L44)

Challenge 2: Environments are Hard to Capture

Dependency Hell



You cannot expect people to find all the chains of dependencies!

You cannot expect people to install all the dependencies and run your code smoothly!



<u>Gap</u>: tools that can automatically capture all the dependencies in the original environment and automatically set them up in another environment.

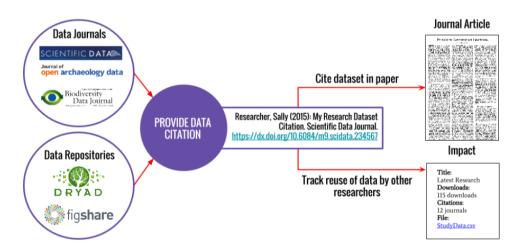
Even if runnable, results may differ

The Effects of FreeSurfer Version, Workstation Type, and Macintosh
Operating System Version on Anatomical Volume and Cortical
Thickness Measurements | June 1, 2012

We investigated the effects of data processing variables such as FreeSurfer version (v4.3.1, v4.5.0, and v5.0.0), workstation (Macintosh and Hewlett-Packard), and Macintosh operating system version (OSX 10.5 and OSX 10.6). Significant differences were revealed between FreeSurfer version v5.0.0 and the two earlier versions. [...] About a factor two smaller differences were detected between Macintosh and Hewlett-Packard workstations and between OSX 10.5 and OSX 10.6

The New Traditional Model

- Publish a paper.
- Publish the underlying code and data.
- Link the paper + code/data.
- Bump up your H-Index.



And I have slides on that model <u>here</u> and <u>here</u>.

ReproZip tries to solve...

Workload & Time Challenges

It is a time commitment to get data and code ready to share, and to share it

Otherwise known as...

the Incentive Problem

Reproducibility takes time, and is not always valued by the academic reward structure

"Insufficient time is the main reason why scientists do not make their data and experiment available and reproducible."

"77% claim that they do not have time to document and clean up the code."

Victoria Stodden, Survey of the

Carol Tenopir, Beyond the PDF2 | Machine Learning Community -

ReproZip tries to softe...

Technical Obsolescence

Technology changes affect the reproducibility

Normative Dissonance¹

Espoused values don't always match practice

Otherwise known as...

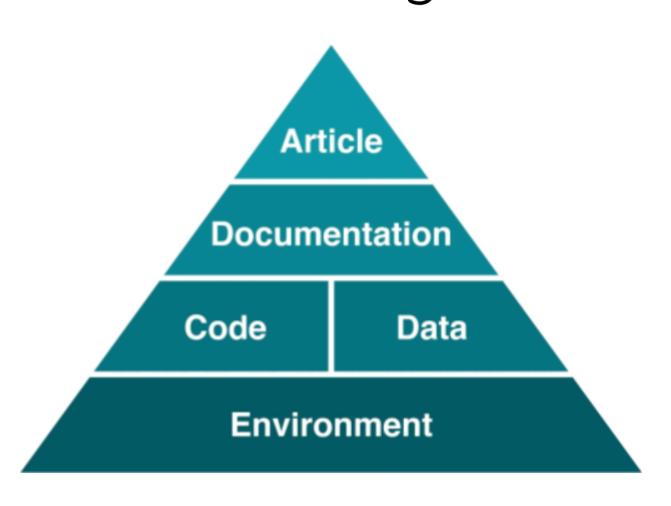
the Pipeline Problem

Reproducibility requires skills that are not included in most curriculums!

"It would require huge amount of effort to make our code work with the latest versions of these tools."

Collberg et al., Repeatability and Benefaction in Computer Systems Research, University of Arizona TR 14-04

But the article, code, and data are really just the tip of the iceberg



What does this mean for...

Librarians

We now have to help researchers license code + data + computer environments, select or build repositories to reliably store those objects, and preserve them forever.

Researchers

They have to clean up code and code, learn how to capture computer environments and make it shareable, without spending all their time + research budget on it.

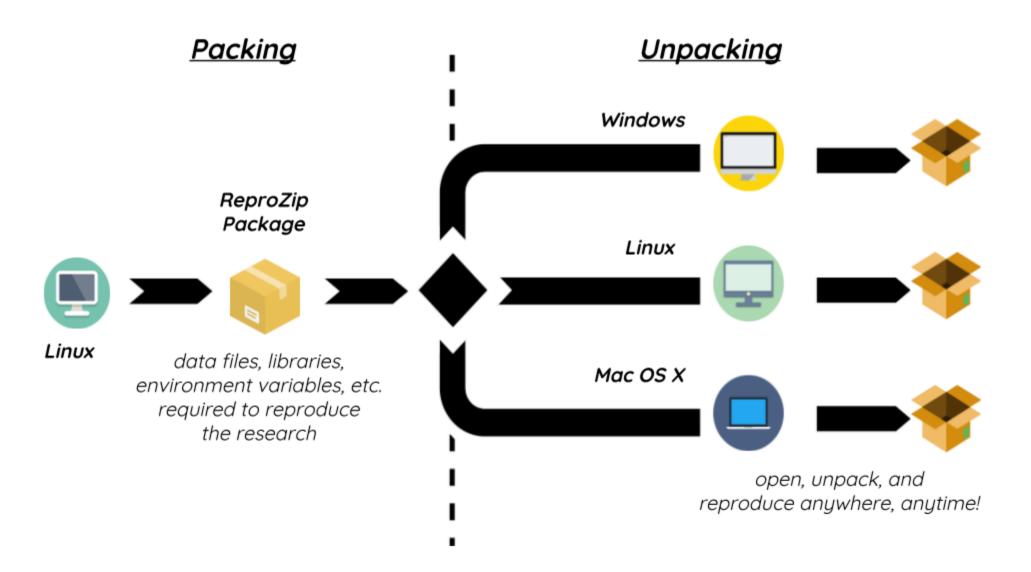
But what if I told you that you could put code + data + applications + environment in **one small file that has a ton of automatically captured metadata and provenance**?

Tool to Help: ReproZip!

ReproZip is a tool aimed at simplifying the process of creating reproducible...whatever. It can be research, it can be applications, it can be databases, it can be websites...if you can do it on a computer, chances are we can pack it!



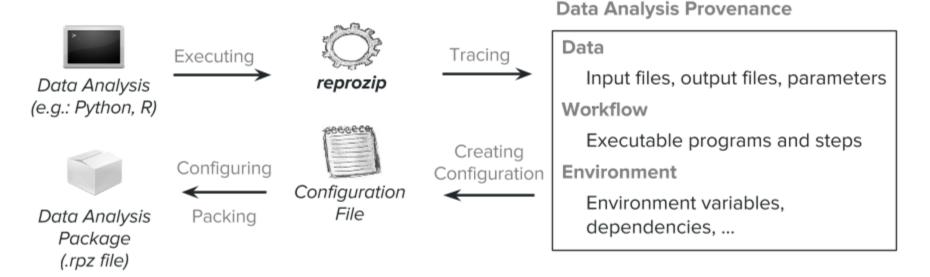
2 Steps to Reproducibility



Step 1: Trace & Pack

reprozip trace [command]

Computational Environment *E* (Linux)



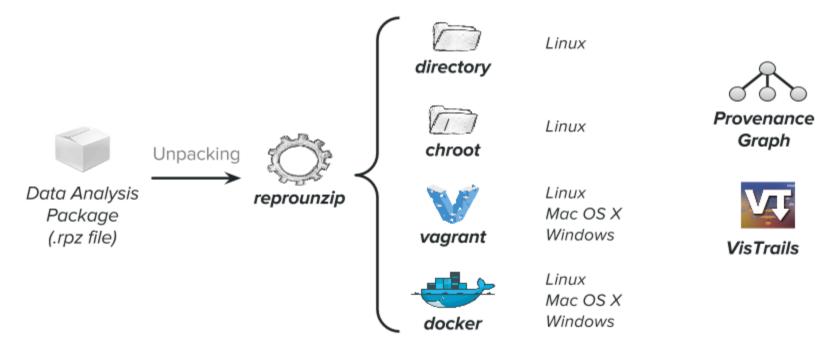
reprozip pack package-name.rpz

Before you pack, you can edit the config.yml (but it's not recommended). This is what a config looks like.

Step 2: Set up & Run

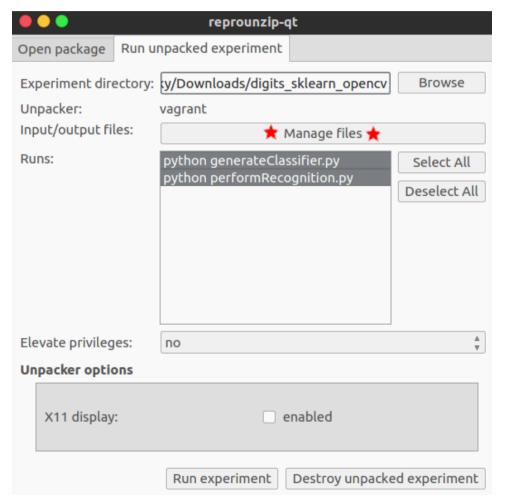
Double click on the RPZ file, and choose your unpacker!

Computational Environment *E'* (potentially different than *E*)



Not just simple reproduction...

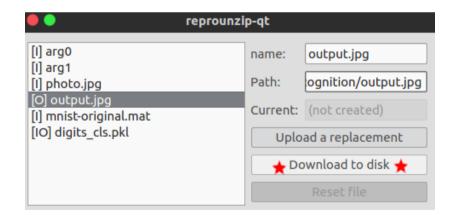
When you unpack your .rpz package with the GUI, you'll come to



this screen.

Download the results or add your own input!

Download Ouput



Upload New Inputs



ReproZip can pack

Data analysis scripts / software (any language, you name it!)

Graphical tools

Interactive tools

Client-server applications (including databases)

Jupyter notebooks

MPI experiments (setting up the experiment is involved though...)

... and much more!

Current Use Cases

Rec. by the <u>Information Systems</u>
<u>Journal</u>, Reproducibility Section

Rec. by the <u>ACM SIGMOD</u>
Reproducibility Review

Listed on the ACM <u>Artifact</u> <u>Evaluation Process Guidelines</u>

Integrated as a component of <u>Corr</u>

Archiving data journalism apps like <u>StackedUp</u>

... and many more!

Potential for

Reprozin in (Academic)

Libraries

<u>Liaison Librarians</u>

- Liaison libs have an excellent opportunity as the first line of contact with patrons to encourage and disseminate information on reproducible practices (e.g. using ReproZip).
- The library gains an excellent way to build collections of diverse, preservation-ready research outputs, and patrons easily adopt reproducible practices.

<u>Data Services</u>

Adding ReproZip to the curriculum of data services classes and workshops, and to the list of supported software, data services teams can become a center on campus for assisting the reproducibility of their patrons' scholarship.

Potential for ReproZip in (Digital) Libraries

<u>Digital Libraries</u>

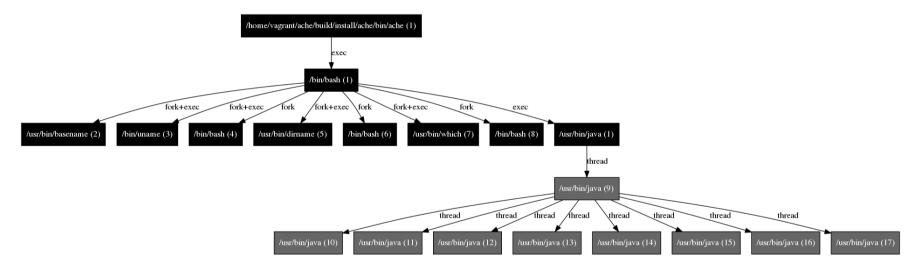
- ReproZip isn't relient on Docker or Vagrant; it uses a plugin model for unpackers, so new ones can be added for forward compatibility.
- If no containers or VMs exist in the future, then the archivist can still read and use the robust technical and administrative metadata in ReproZip's config.yml.

Repository Management

ReproZip contains extensive technical and administrative metadata, which can be an be exported a json file, which allows for extensible models of metadata – such as crosswalking to Resource Description Framework (RDF) or Dublin Core, automating ingest workflows.

Future Development Work

- Packing on <u>macOS</u> (beginning summer 2017)
- Improvements to <u>provenance graph visualization</u> (beginning summer 2017), because right now we've got...



- ReproZip <u>plugin</u> for Jupyter Notebooks (beginning summer 2017)
- Better MPI/HPC support

Conclusion

ReproZip is extensible enough to be used for reproducibility across research domains as well as across library services.

Because ReproZip is open-source software, the community drives its development – others can contribute, modify, and reuse it for a variety of purposes.

The library community can leverage ReproZip in instruction, consultation, repository services, digital archiving, and in their own research.

Other Resources for ReproZip

ReproZip Website:

https://reprozip.org

ReproZip Examples:

https://examples.reprozip.org

ReproZip GitHub:

https://github.com/ViDA-NYU/reprozip

ReproZip Mailing list: <u>reprozip-users@vgc.polu.edu</u>

ReproZip YouTube Demos:

General Demo:
 https://goo.gl/o1Hgrx

 Website packing: https://goo.gl/yMEOZJ

 Jupyter notebook: https://goo.gl/NvMHnw

ReproZip on Twitter:

https://goo.gl/d6NXoH

Thank You:

Prof. Juliana Freire, ReproZip Pl and reproducibility master.

Dr. Nicholas Wolf for his help in editing our paper.

The Gordon and Betty Moore
Foundation & the Alfred P. Sloan
Foundation, who support The
Moore-Sloan Data Science
Environment at NYU, which was
vital to the development of
ReproZin

Questions?

Get this Presentation:

https://vickysteeves.gitlab.io/2017-IASSIST-ReproZip

Email us:

reprozip-users@vgc.poly.edu

or

vicky.steeves@nyu.edu

or

remi.rampin@nyu.edu

or

fchirigati@nyu.edu