Preparing code and data for computationally reproducible collaboration and publication

FORCE11 Scholarly Communications Institute 2019, UCLA
Thursday, August 8, 2019

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- Participants should have:
  - A laptop or other computer.
  - A supported browser (not IE or Edge).
  - 1 x pink post-it note.
  - 1 x green post-it note.
  - 1 x workshop survey.
  - A handful of mixed candy.
- Participants should follow along with the slide deck at the bitly link.

Workshop POP

- **Purpose:** To introduce **skills and tools** in organization, documentation, automation, containerization, and dissemination of research.
- **Outcome:** You feel more confident applying relevant skills and tools to guide the sharing of your research code and data.
- **Process:** You adapt & apply some skills or tools we discuss today next time your share or publish your research.

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- Why are we here?
- What do we hope to accomplish together?

Agenda

Reproducibility guidance

Organization
Exercise 1: Data collection
Exercise 2: One repository
Exercise 3: Separate code & data

Documentation
Exercise 4: Specify environment
Exercise 5: Specify dependencies
Exercise 6: Containerization
Demo: Literate programming
Demo: Create a README file + data dictionary

Automation
Exercise 7: Create a master script
Exercise 8: Create relative paths

Dissemination
Exercise 9: Specify a license
Exercise 10: Share your code!

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- How will we try to accomplish our Workshop POP?
- This is an adaptable agenda:
  - We will take two breaks together.
  - Participants should feel free to take breaks whenever they wish.

Icebreaker

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Participants are asked to stand in a line ordered from **most recently coded** to **never coded**:

- How long has it been since you last touched research code?
- Participants must discuss with each other when they last touched research code.

Once the line is created:

- Facilitator makes these points:
  - There is a diversity of coding experience in the room - take a look who is near you who has less coding experience than you.
  - There are too many people in the room for one facilitator to troubleshoot alone, and there are lots of skilled people in the room.
  - We will use the post-it notes to signal when we have completed an exercise.
  - When you finish an exercise and switch your post-it note to green, look to your neighbors with a pink sticky - see if they could use some help!

With a show of hands, ask the participants whether they think there is a reproducibility crisis in their discipline:

1. Yes, a significant crisis.
2. Yes, a slight crisis.
3. Don't know.
4. No, there is no crisis.

Source information:

1,500 scientists lift the lid on reproducibility

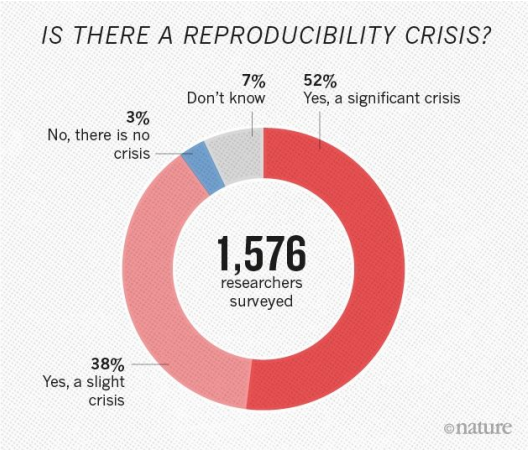
https://www.nature.com/news/1-500-scientists-lift-the-lid-on-reproducibility-1.19970 (2016)

"A minority of respondents reported ever having tried to publish a replication study. When work does not reproduce, researchers often assume there is a perfectly valid (and probably boring) reason. What's more, incentives to publish positive replications are low and journals can be reluctant to publish negative findings. In fact, several respondents who had published a failed replication said that editors and reviewers demanded that they play down comparisons with the original study."

"The survey — which was e-mailed to Nature readers and advertised on affiliated

websites and social-media outlets as being 'about reproducibility' — probably selected for respondents who are more receptive to and aware of concerns about reproducibility.”

A crisis? *(Nature 2016)*



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- Most researchers think that reproducibility is an issue in their discipline, but may disagree about the urgency.

Communication during exercises:

1. Post a **pink sticky note** on your laptop at the start of the exercise.
2. Switch to a **green sticky note** when you finish and have no questions.
3. If you finish early, find someone with a **pink sticky note** and see if you can help!
4. If you are colorblind, the **pink sticky note** has a "**p**" written on it.

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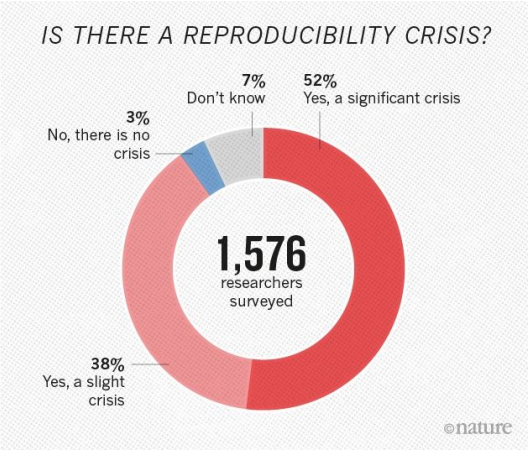
- At the beginning of each exercise, I will remind you to put a pink sticky note on your laptop.
- When you finish the exercise and have no questions, switch to a green sticky note.
- Since we are a large group and we can learn from each other, see if a neighbor who is still working is interested in some help.

Your experience? *(Nature 2016)*



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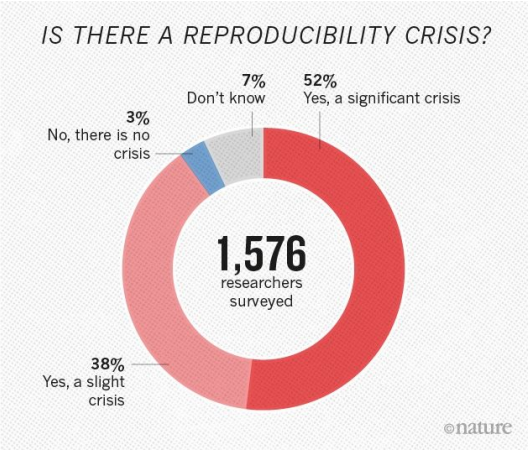
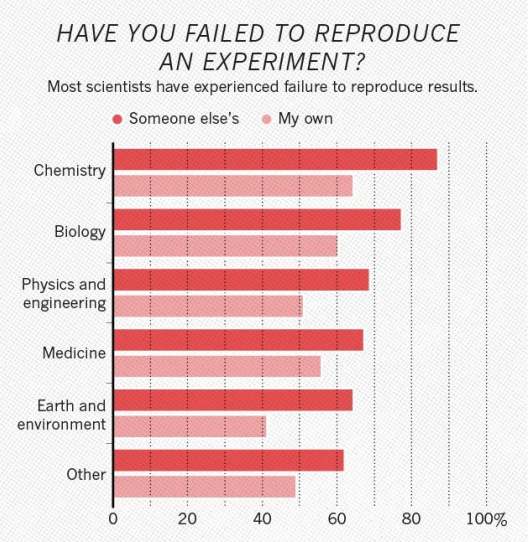
- However, we are going to frame this question in a different way.
  - With a show of hands, how many participants have had difficulty reproducing someone else's work?
  - And how many participants have had difficulty reproducing your own work a few weeks, months, or years later?

A common experience *(Nature 2016)*





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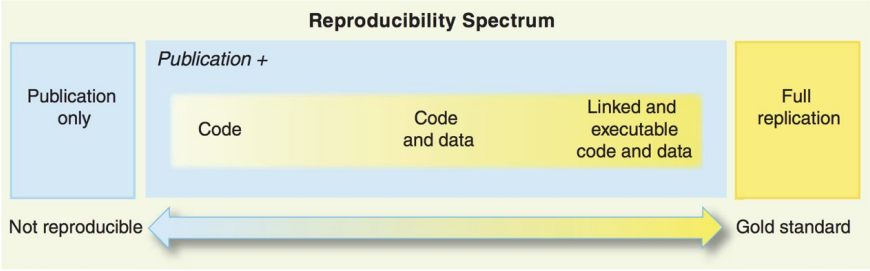
- This is how I prefer to frame issues about reproducibility.
- Difficulty reproducing our own work or the work of peers is very, very common in research.
- Many of the steps that a researcher can take to address irreproducibility of published research also improves the reusability of their research for themselves, labmates, and close collaborators.

An opportunity to help your future self

"It takes some effort to organize your research to be reproducible… the **principal beneficiary is generally the author herself**."- Schwab & Claerbout



Peng, R.D. (2011) Science

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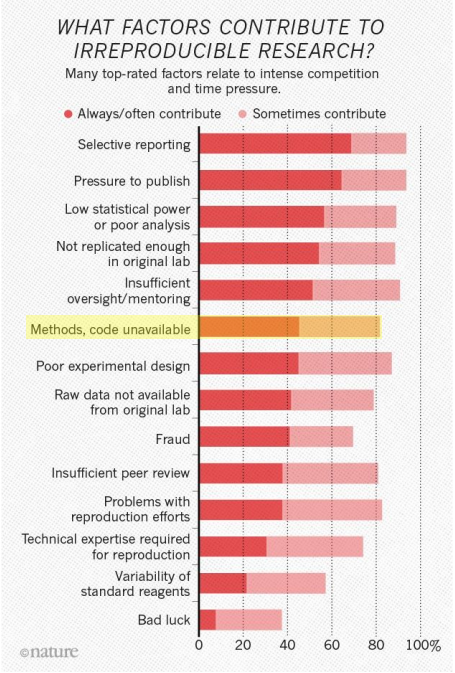
- Therefore, when thinking about adopting best practices to tackle reproducibility, adopt first those practices that will benefit yourself first - as your future self is the most frequent reuser of your research.
- Remember that, like reproducibility generally, computational reproducibility is a spectrum. Integrating one or two new practices into your research will make your research more reproducible - it is not all or nothing. And each of these steps will benefit yourself first!

Computational reproducibility

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

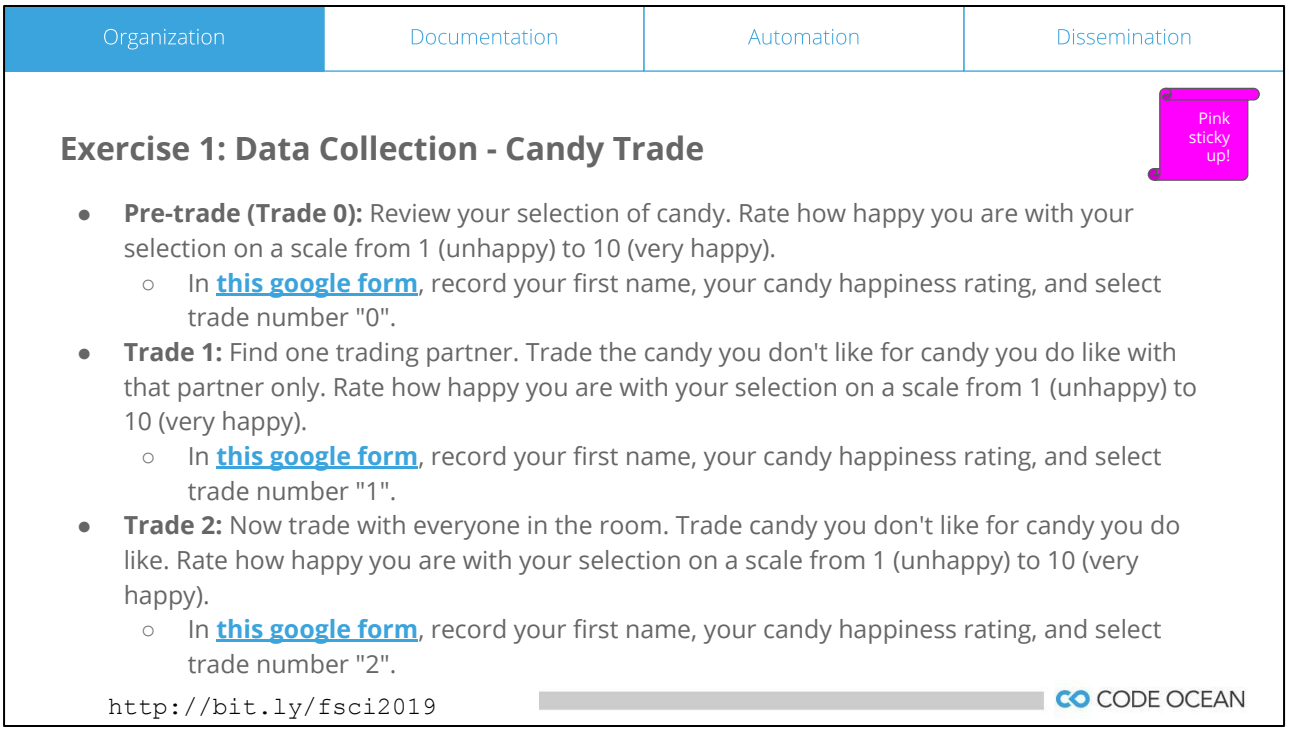
- Buckheit and Donoho (1995)'s distillation of Claerbout and Karrenbach (1992)

`http://bit.ly/fsci2019`



Nature 2016

- Professor Stodden et al. talked a lot about reproducibility yesterday and I just assume you were there
- For our purposes, computational reproducibility is the ability for a new researcher to rerun the data and code of the original research to create the same figures, tables, and values shared by the original researcher.
    - Almost all research relies on software and code for some aspect of its methods. Computational reproducibility relies on the sharing of that software and code in addition to a published narrative of the methods. This is why the founders of our idea of reproducibility describe a published article as just an advertising of the research. The actual research includes our research software and code.
- Unavailable code and methods is a barrier to computational reproducibility. So to improve computational reproducibility, we want to know how best to share our methods and code.
-



- Because some participants did not bring their own data and code, we will run a short data collection exercise.
- This exercise is followed by a 10 minute break.
- Instructor: During the break:
  - Download the responses: https://docs.google.com/forms/d/13_i1jKlyTwhl0UaUkmqhfZuG-M9i4l5_6Q81vz54Ypw/edit#responses.
  - Remove the “Timestamp” column.
  - Save as a CSV file.
  - Upload to CSV file, named “data.csv”, to this github repo: https://github.com/aprilcs/candy_trade. Be sure to delete the existing “data.csv” file if there already is one in the repo.

10 MINUTE BREAK

Tools we will use:

- Github https://github.com/
- Code Ocean https://codeocean.com/
- Binder (does not need account)

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CODE OCEAN

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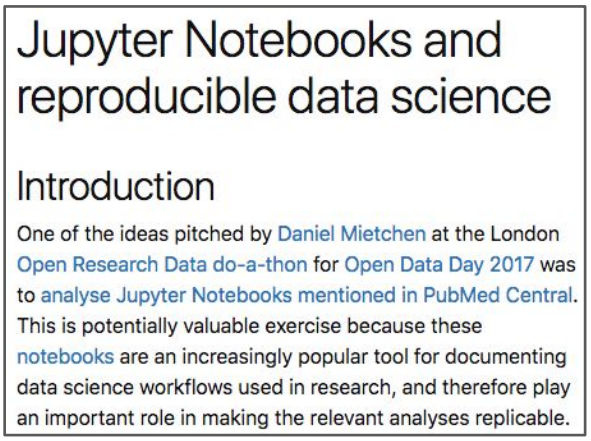
Lessons learned: testing computational reproducibility

- PMC “jupyter OR ipynb” -> 107 papers
- “My initial thought was that analysing the validity of the notebooks would simply involve searching the text of each article for a notebook reference, then downloading and executing it … **It turned out that this was hopelessly naive**…”



Jupyter Notebooks and reproducible data science

Introduction

One of the ideas pitched by Daniel Mietchen at the London Open Research Data do-a-thon for Open Data Day 2017 was to analyse Jupyter Notebooks mentioned in PubMed Central. This is potentially valuable exercise because these notebooks are an increasingly popular tool for documenting data science workflows used in research, and therefore play an important role in making the relevant analyses replicable.

Mark Woodbridge, Daniel Sanz, Daniel Mietchen, & Ross Mounce (2017). Jupyter Notebooks and reproducible data science, https://markwoodbridge.com/2017/03/05/jupyter-reproducible-science.html.

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- We mentioned before the break that sharing code, data, and methods is necessary for computational reproducibility.
- However, sharing just the code and methods does not ensure reproducibility. This was demonstrated by an informal study by Woodbridge et al. to reproduce code from published papers in the form of Jupyter Notebooks.
- They were able to successfully execute only one of the ~25 notebooks that we downloaded.
- We don’t have to be naive like them - we can learn from their attempt.

If people do not know what a jupyter notebook is, you can talk about the uses of notebooks:

- Documentation of analyses
  - A Modularized Efficient Framework for Non-Markov Time Series Estimation: https://codeocean.com/2018/01/16/a-modularized-efficient-framework-for-non-markov-time-series-estimation/code
- Programming or statistical education
  - Fractal Generation with L-Systems: https://codeocean.com/2017/12/08/fractal-generation-with-l-systems/code

- Executable article
    - On Writing Reproducible and Interactive Papers: https://codeocean.com/2018/06/28/on-writing-reproducible-and-interactive-papers/code

What *Woodbridge et al.* found:

- Files, data, dependencies needed to execute analyses **were often missing**.

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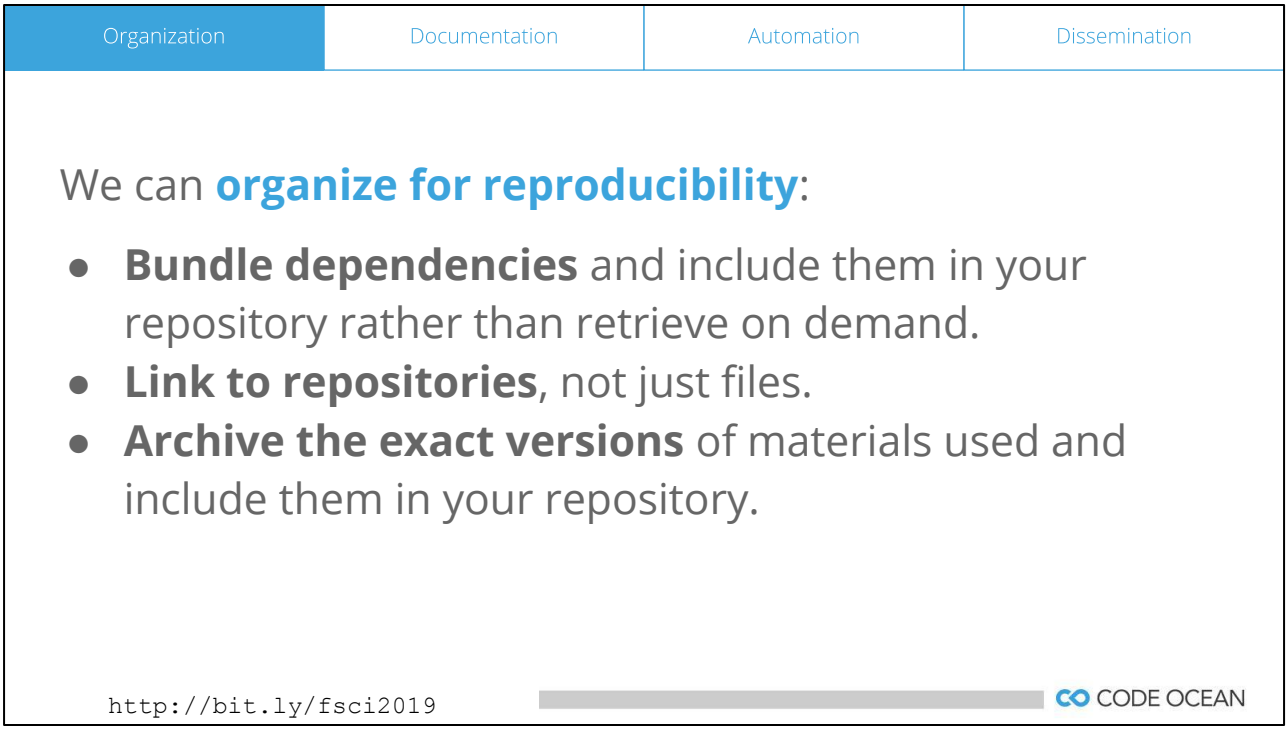
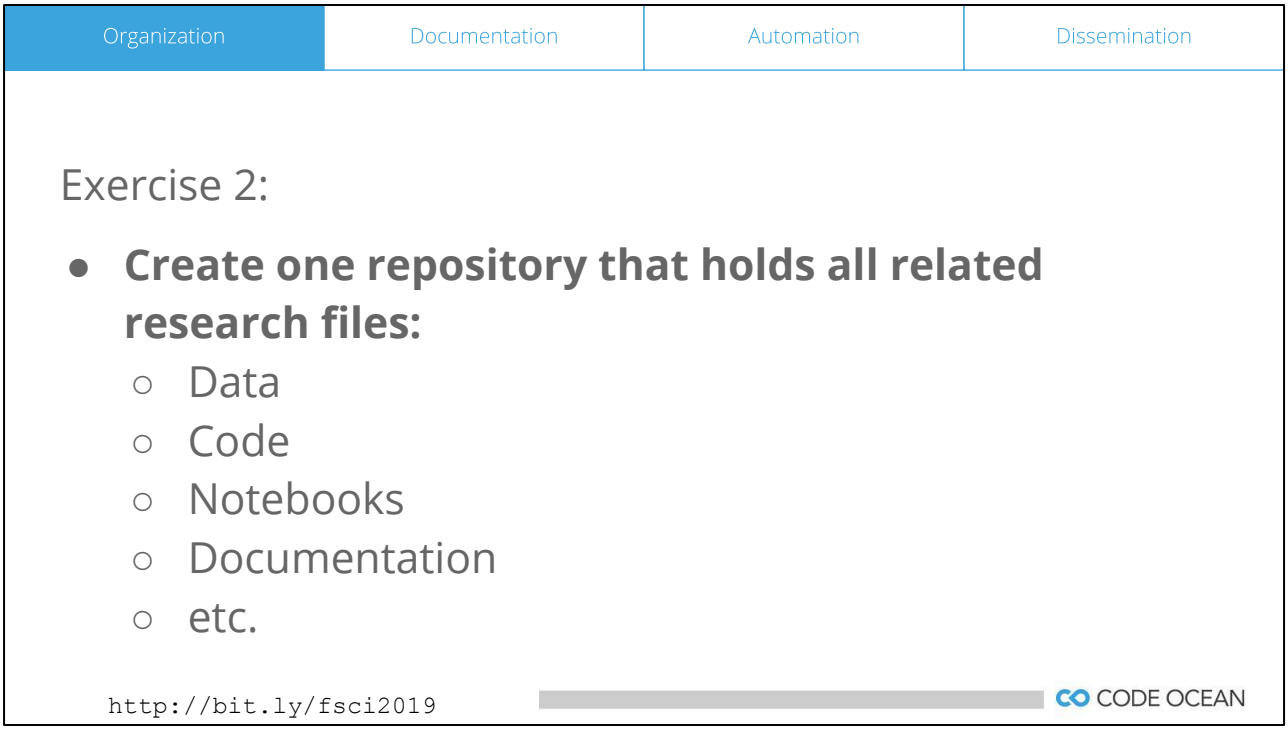
- The first thing that Mark Woodbridge and his colleagues learned was that the files, data, and dependencies needed to execute analyses were often missing from the publication or accompanying repository.



Learning from Woodbridge's finding, we can organize for reproducibility:

- Archive the exact versions of data used and include them in your repository.
- Bundle dependencies and include them in your repository rather than retrieve on demand.
- Link to repositories rather than individual code files or data files.



So, the first way to overcome the risk of missing files, data, or dependencies that Woodbridge found is to put everything in one repository.

Therefore, exercise 2 will be to create one repository for all our research materials. We will use Code Ocean in this workshop, but you could do this locally with a file folder or using a git repository.

Exercise 3:

- **Organize your research to separate code from data.**


```
.
|-- CITATION
|-- README
|-- LICENSE
|-- requirements.txt
|-- data
|   -- birds_count_table.csv
|-- doc
|   -- notebook.md
|   -- manuscript.md
|   -- changelog.txt
|-- results
|   -- summarized_results.csv
|-- src
|   -- sightings_analysis.py
|   -- runall.py
```

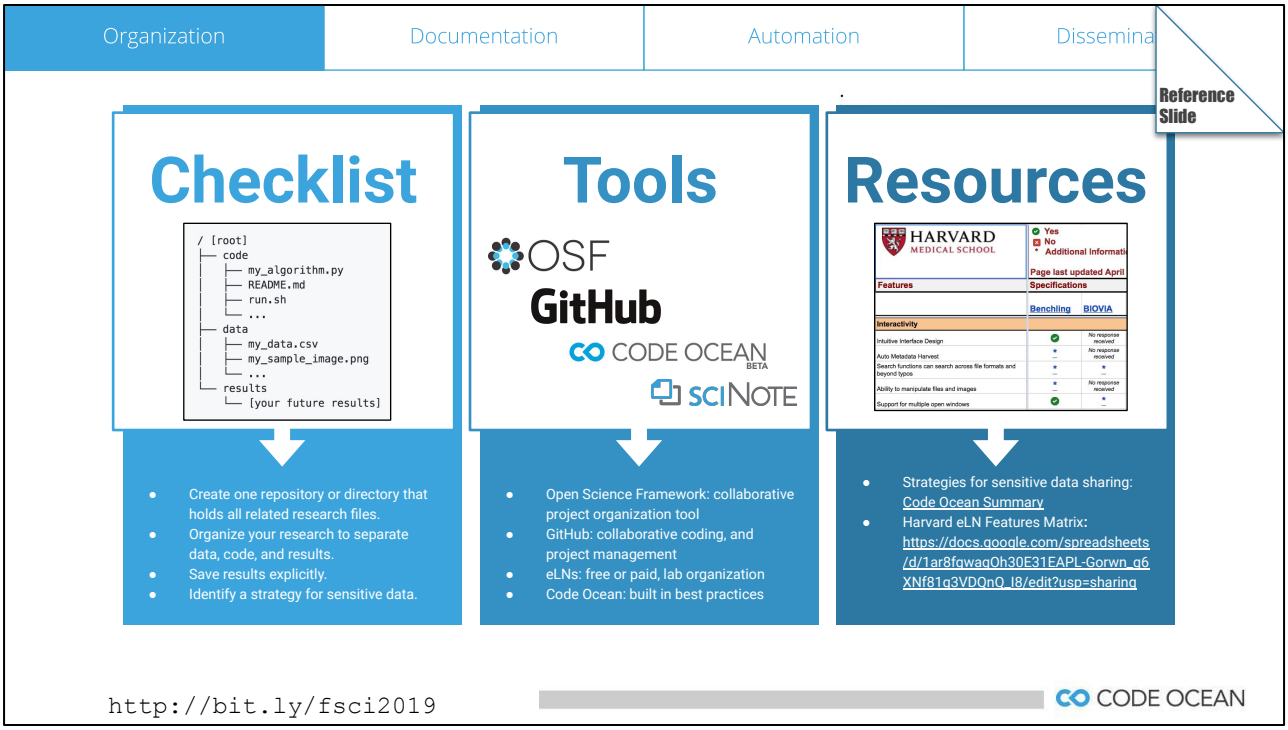
Resource on reproducible organization:

- Karl Broman: http://kbroman.org/steps2rr/pages/organize.html

Join our Candy Swap project

R: https://github.com/aprilcs/sips-workshop

Python: https://github.com/aprilcs/sips-workshop-py



How do we organize for reproducibility?

- For your reference, we have created these reference slides within the slide deck with key points, tools, and resources.
- We won't spend time on these reference slides as they are intended for your future reference, and will just go over the main points.

Reproducible organization includes:

- Creating one repository for all your research materials.
- Separating data and code.
- And saving your results explicitly as a function of your data and code.

Free tools are available to help organize your research materials:

- The OSF is a free, open source, collaboration tool.
- Github provides free public repositories for collaborative coding and project management.
- Electronic lab notebooks help to organize a lab, and Harvard's Features Matrix is a great place to start comparing them.
- Code Ocean structures their repository to separate data and code and save results explicitly.

What *Woodbridge et al.* found:

- There is no way to **directly express dependencies** of published code.

We can **publish using containers**:

- Use container technology to **directly express dependencies.**
- **Configure an image** for your analyses with Docker, binder, WholeTale, or Code Ocean.

The terms:

- **Dockerfile**: Readable instructions for how to build an image.
- **Image**: Everything your application needs to run, all bundled together (includes Dockerfile, libraries, and code).
- **Layer**: A Dockerfile directs Docker to build the initial image layer from a base image, and then other layers are built on top.
- **Container**: Started and created from an image.
- **Registry**: Images are stored and retrieved from registries.

Hale, Jeff. *Learn Enough Docker to be Useful*. https://towardsdatascience.com/learn-enough-docker-to-be-useful-b7ba70caeb4b

The metaphor: PIZZA!

- **Dockerfile**: The recipe.
- **Image**: The recipe and the ingredients combined as an all-in-one pizza-making-kit.
- **Layer**: The ingredients are the layers. You've got crust, sauce, and cheese for this pizza.
- **Container**: Cooked pizza. Cooked by Docker (the oven).
- **Registry**: All-in-one pizza-making-kit factories?

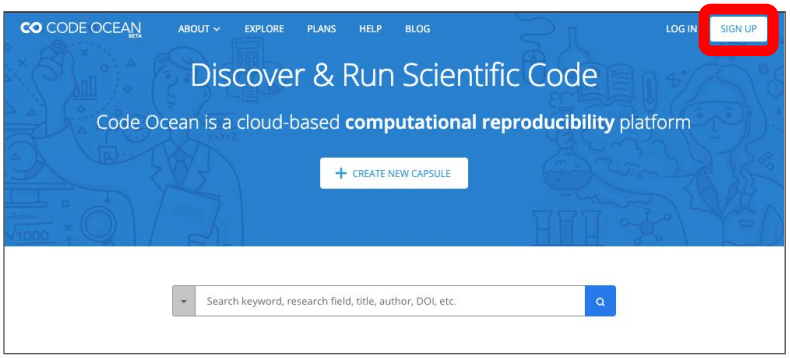
Hale, Jeff. *Learn Enough Docker to be Useful*. https://towardsdatascience.com/learn-enough-docker-to-be-useful-b7ba70caeb4b

Containers solve:

- Dependency Hell - install, error, google, install, error...
  - Provides other researchers with a binary image in which all the software has already been installed, configured, and tested.
- Imprecise documentation - missing installation info.
  - Dockerfile provides a human readable summary of the necessary software dependencies needed to execute the code. Dependencies are automatically documented as they are installed.
- Code rot - dependencies change, the code breaks
  - Reduced risk with archiving images

Boettiger, Carl. *An introduction to Docker for reproducible research.* 10.1145/2723872.2723882

Create a Code Ocean account



Pink sticky up!

- https://codeocean.com/
- You can **delete it and opt out of any communications** if you wish! For completing the exercises only. :)
- You will need to verify your email address

http://bit.ly/fsci2019

CODE OCEAN

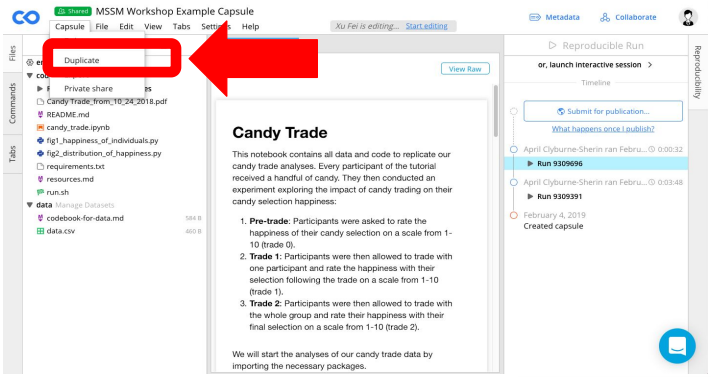
- Everyone put your pink sticky up!
- We are going to create a Code Ocean account to create a repository, called a “capsule”, on Code Ocean for all research materials.
- Participants should:
  - Go to https://codeocean.com/
  - Sign up
  - They will need to verify their email address (sometimes they will need to resend this several times).
- Participants can delete their account and opt out of any communications if you wish! There is a check box on the survey where they should select “No” to receiving news if they wish.
- Code Ocean is for completing the exercises only, but the exercises can make code more reproducible no matter which platform participants which to use for themselves in the future.
- Once they have successfully created an account, they should switch to a green sticky.

Duplicate this capsule:

R: http://bit.ly/r-example

Python: http://bit.ly/py-example

Pink sticky up!



- Click “Capsule”
- Select “Duplicate”

http://bit.ly/fsci2019

CODE OCEAN

- Everyone put your pink sticky up!
- Participants should
  - Ensure they are in “Classic” Code Ocean mode for the workshop.
  - Select the ellipses [...].
  - Click Duplicate
- Duplicating this capsule creates a copy owned by you, and you know you are successful when you have a capsule named “____ Workshop (copy)”
- Once they have successfully duplicated the capsule, they should switch to a green sticky.

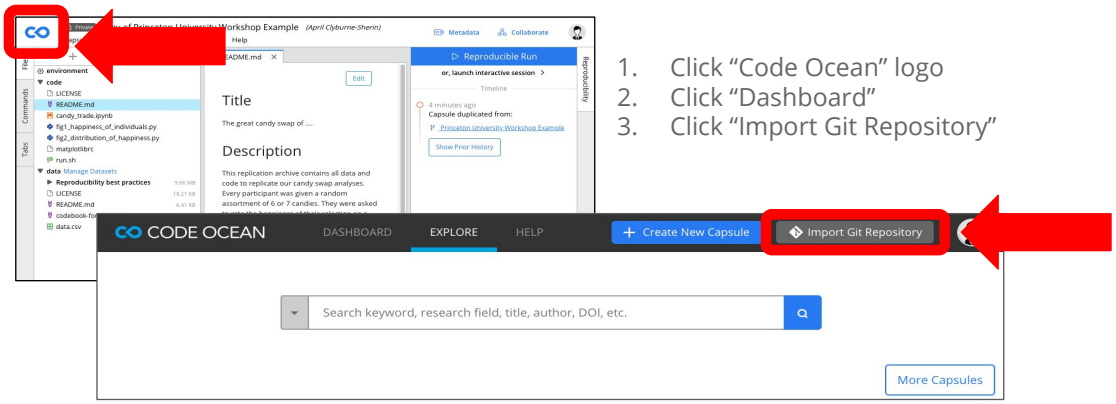
About this capsule:

- This is an example and reference capsule for the workshop.
- It is a skeleton example of where are headed with our exercises.
- It also includes 3 papers that can be great resources for computational reproducibility if you wish to read further.

Create a new compute capsule

Pink sticky up!

Import Git Repository:
R: https://github.com/aprilcs/sips-workshop
Python: https://github.com/aprilcs/sips-workshop-py



1. Click “Code Ocean” logo
2. Click “Dashboard”
3. Click “Import Git Repository”

Organization | Documentation | Automation | Dissemination

Pink sticky up!

Exercise 4:

- **Specify the run environment for your analyses.**

```
> sessionInfo()
R version 3.6.0 (2019-04-26)
Platform: x86_64-apple-darwin15.6.0 (64-bit)
Running under: macOS Mojave 10.14.5
```

Example: **Base Environment: R (3.5.3) or Python (3.7.0)**

http://bit.ly/fsci2019

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This comes with miniconda and is called conda.

Python --version, when you open a terminal and type python

Pink sticky up!

Exercise 5:

- **Specify your packages and dependencies with versions.**
  - Python: pip freeze > /requirements.txt
  - R: install.r and runtime.txt

runtime.txt

```
1 r-2019-07-01
```

install.r

```
1 install.packages("bitops")
2 install.packages("rmarkdown")
3 install.packages("caTools")
4 install.packages("ggplot2")
5 install.packages("knitr")
6 install.packages("rprojroot")
7
```

R packages: **apt-get** pandoc; **CRAN** bitops, markdown, caTools, ggplot2, knitr, rprojroot

Python packages: **conda** matplotlib, pandas, numpy, jupyter

Resource on documenting dependencies:

- Binder: https://mybinder.readthedocs.io/en/latest/config_files.html

Exercise 6:

- **Use container technology to create an image of your complete computational environment.**
  - Code Ocean
  - Binder

Export your capsule to see how an image and Dockerfile were created through your specifications.

Inspect the Dockerfile.

We will demonstrate building a container with repo2docker using mybinder and github.

Demo:

- **Consider using literate programming to document the analysis narrative with the code.**
  - Jupyter Notebooks
  - RMarkdown

Explore Jupyter notebooks in this example capsule: http://bit.ly/uiuc-example

Explore RMarkdown in this example capsule: http://bit.ly/rmarkdown-example

- **Create a README file and data dictionary.**

Documenting your file overview and dependencies in your README:

- AJPS Replication Package: https://dataverse.harvard.edu/dataset.xhtml?persistentId=doi:10.7910/DVN/EZSJ1S

Documenting your data in a codebook or data dictionary:

- DataONE: https://www.dataone.org/best-practices/create-data-dictionary

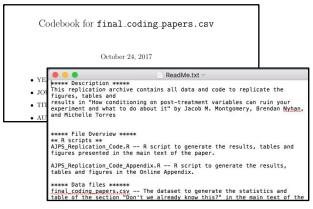
Resource on using markdown:

- GitHub: https://github.com/adam-p/markdown-here/wiki/Markdown-Cheatsheet

Organization | Documentation | Automation | Dissemina

Reference Slide

Checklist



- Consider literate programming.
- Document each element or variable in your dataset with a data dictionary / codebook.
- Create a README file.

Tools

GitHub

jupyter

CODE OCEAN BETA

- Version control: git and GitHub tracks changes to documents and metadata
- Literate programming: knits documentation with code (Jupyter)
- Document & share metadata: Code Ocean renders documentation, notebooks, and records metadata

Resources

DCC because good research needs good data

Popular Licenses

The following OSI-approved licenses are popular, widely used,

- Apache License 2.0
- BSD 3-Clause "New" or "Revised" license
- BSD 2-Clause "Simplified" or "FreeBSD" license
- GNU General Public License (GPL)
- GNU Library or "Lesser" General Public License (LGPL)
- MIT license

- DataONE: https://www.dataone.org/best-practices/create-data-dictionary
- Cornell: https://data.research.cornell.edu/content/readme
- Digital Curation Center: http://www.dcc.ac.uk/resources/how-guides/license-research-data
- OSI: https://opensource.org/licenses

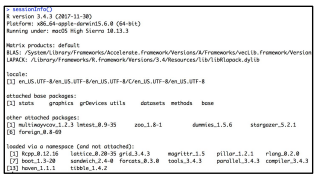
http://bit.ly/fsci2019

CODE OCEAN

Organization | Documentation | Automation | Dissemina

Reference Slide

Checklist



- Specify your computational environment and package versions.
- Configure a container to make your analysis portable and reusable.

Tools

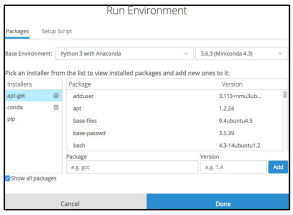
CODE OCEAN

docker

binder (beta)

- Container technology: packages data, code, metadata, & computational environment for portable analyses
- Docker: container technology for devs
- Code Ocean: easy configuring, preservation, & reuse of containers for researchers
- Binder: configure & share containers

Resources



- Documenting dependencies: http://mybinder.readthedocs.io/en/latest/using.html#preparing-a-repository-for-binder
- Specifying environments: https://help.codeocean.com/getting-started/the-computational-environment/selecting-a-base-environment

http://bit.ly/fsci2019

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What *Woodbridge et al.* found:

- **Manual manipulation or setup** was needed to reproduce results, often without documentation of how the results were produced.

We can **automate the execution of our analyses**:

- Create a master script to execute all analyses.
- Reproduce results automatically as a function of the data & the code; Save results explicitly.
- Use relative paths.

Exercise 7:

- **Create a master script to execute your code.**

- In R, use a run.r or main.r master script
  - Use source() to run your scripts
  - Run your install.r script
- In Python, use a main.py or run.sh master script
  - In your run.sh script, use nbconvert to execute your notebook into the results directory.
- Case study: https://www.practicereproducibleresearch.org/core-chapters/3-basic.ht

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Exercise 8:

- **Change absolute paths to relative paths.**

Resource explaining paths:

- Karl Broman: http://kbroman.org/steps2rr/pages/organize.html

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Show an example of changing a path:

- In the python code “fig1_happiness_of_individuals”
  - Change “data = pd.read_csv('../data/data.csv')” to “data = pd.read_csv('C:/Users/SomeOne/Projects/data/data.csv')”

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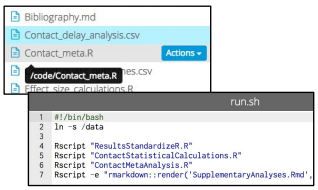
Reference Slide

Checklist



- Use relative rather than absolute paths.
- Create a master script that runs your scripts in sequence.

Tools

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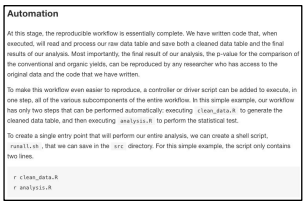
docker

binder (beta)

- Docker: share automated code for devs
- Code Ocean: easy configuring, preservation, & reuse of automated code
- Binder: share automated code for using containers

Resources



- Karl Broman on paths: http://kbroman.org/steps2rr/pages/organize.html
- Resource on automation using a master script: https://www.practicereproducibleresearch.org/core-chapters/3-basic.html

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What *Woodbridge et al.* found:

- There is no standardized way of **attaching code to published articles**.
- Therefore it is difficult to **discover and retrieve** code.

We can **embed or link code persistently**:

- **Obtain a DOI for your repository and use this link throughout your article.**
  - Example: Github -> Binder -> Zenodo -> DOI linked in article
  - Example: CodeOcean -> DOI in article
- **Cross link repository with published article in metadata of each.**
- **Embed executable capsule within the article.**
  - Example: https://doi.org/10.1017/bpp.2018.25

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Exercise 9:

- **Specify a license for your data and your code.**

Resource on choosing a data licence:

Digital Curation Center: http://www.dcc.ac.uk/resources/how-guides/license-research-data

Resources on choosing a code licence:

- Karl Broman: http://kbroman.org/steps2rr/pages/licenses.html
- License picker: https://choosealicense.com/
- Open Source Initiative: https://opensource.org/licenses

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Add a licence.txt file to your project or select one in the metadata section (CO or GitHub)

- Consider Creative Commons licenses for data and text, either CC-0 or CC-BY.
- For software, we recommend a permissive open source license such as the MIT, BSD, or Apache license

Exercise 10:

- **Share your code!**

- Check whether your container is ready to publish by hitting "Run".

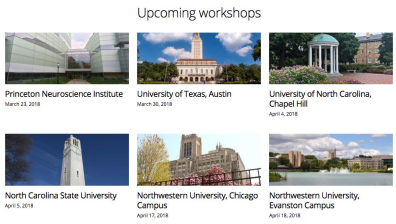
Reproducibility support

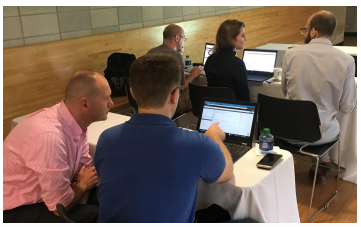
Workshops & Webinars

- Theory or hands-on
- Customized to researcher needs
- Request a workshop or webinar at https://codeocean.com/events

1:1 Computational Reproducibility Consult

- In person
  - Lab meeting
  - Office visit
- Virtual
- Request at april@codeocean.com or https://doodle.com/codeocean





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Reproducibility community

Reproducibility Ambassador Program

- **Scholarships** to present your research at conferences
- **Support** for lab events, journal clubs, meetups
- **Training**, mentorship, and community forum
- **Opportunities** to share your perspective on reproducibility
- **Co-development** role to help us meet your needs and try out new features

Preprint journal club

- Build peer review **skills** including code review
- **Contribute** feedback to new research

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Thank you for your time :)

Please fill out an evaluation so we can keep improving!
http://bit.ly/workshop-survey-2019

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