A conversation on reproducibility and interactive notebooks with RMarkdown



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Learning objectives

- What about "reproducibility"?
- What is Markdown?
- Hands on:
 - Create an Rmarkdown document and "knit" it
 - Working with Rmarkdown files and git + GitHub
- (As time allows) examples of other document types
 - Journal article templates (eg with "rticles" package)
 - Bookdown
 - Blogdown



Why reproducible research? Robustness

PHYSICS TODAY

22 Aug 2018 in Research & Technology

The war over supercooled water

How a hidden coding error fueled a seven-year dispute between two of condensed matter's top theorists.

"Limmer maintains that he and his mentor weren't trying to hide anything. "I had and was very willing to share the code," he says. What he didn't have, he says, was the time or personnel to prepare the code in a form that could be useful to an outsider"

"Suddenly it made sense that the Berkeley researchers hadn't seen a second liquid phase; they were effectively running their simulations at temperatures well above the critical point."

https://physicstoday.scitation.org/do/10.1063/PT.6.1. 20180822a/full/

Why reproducible research? Records

Email from grad student to Berkeley professor in 2017:

"...The citation on the slide is [your report on a state government website].

I downloaded that PDF and do not see [important statistic] anywhere in it. Table 3 seems to have [different value], Table 15 has [related value] in California...

...The closest match that I've found is [other statistic] from Table 15... Is it possible there was an error in transcription? If not, can you help me figure out what's going on here? What does [important statistic] on [slide] represent?"

Response from Berkeley professor:

"I don't remember the details. [Former student], do you? Thanks in advance."

[Former student] never responded

Why reproducible research? Reusability









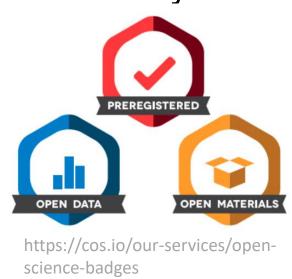
WWW.PHDCOMICS.COM

Why is this important?

- Show evidence of the correctness of our results
- Enable others to make use of our methods and results (including future you)
- Increasingly encouraged or required by funders and journals

http://ropensci.github.io/reproducibility-guide/sections/introduction/

https://www.stat.berkeley.edu/~stark/Seminars/reproNE16.htm



"reproducibility"

What does reproducibility mean? Three ideas to distinguish

- 1. Reproducibility (sometimes called repeatability or even 'preproducibility') [6]
 - Data, and/or statistical methods, code, software environment are available so data analysis can be repeated and get a similar result [1, 2, 3]
- 2. Replicability (sometimes called reproducibility)
 - Another researcher is able to conduct the same experiment and get similar results

3. Correctness

- Is your analysis appropriate? Is your hypothesis correct?
 - → Reproducible research can still be wrong! [4]

4 - Reproducible research can still be wrong, Leek, Peng PNAS 2015, DOI: 10.1073/pnas.1421412111

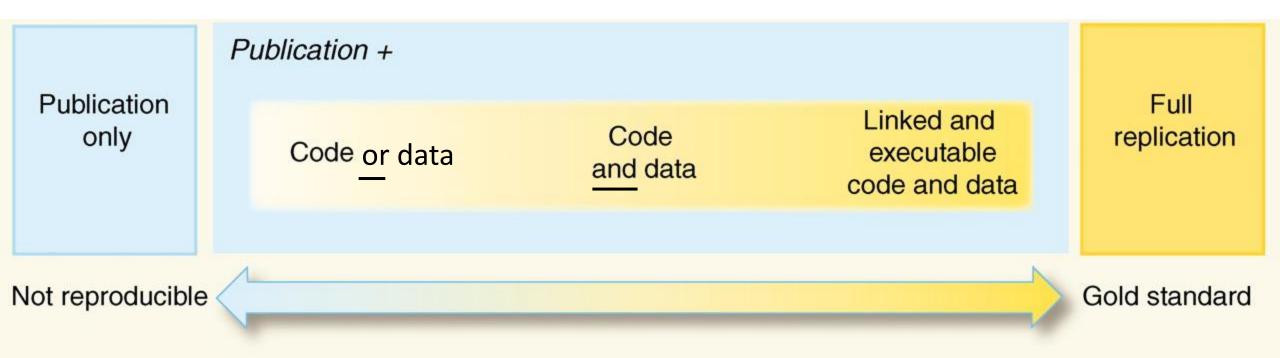
^{1 -} Peng Science 2011, DOI: 10.1126/science.1213847

^{2 -} http://ropensci.github.io/reproducibility-guide/sections/introduction/

^{3 -} https://simplystatistics.org/2014/06/06/the-real-reason-reproducible-research-is-important/, Peng 2014

⁵⁻ https://www.nature.com/news/muddled-meanings-hamper-efforts-to-fix-reproducibility-crisis-1.20076#/b1, citing https://www.ascb.org/wp-content/uploads/2015/11/How-can-scientist-enhance-rigor.pdf citing Schmidt, Stefan. (2009). Shall We Really Do It Again? The Powerful Concept of Replication Is Neglected in the Social Sciences. Review of General Psychology. 13. 90-100. 10.1037/a0015108.

A spectrum of practice (depends on project)



Adopted from:

Reproducible Research in Computational Science

By Roger D. Peng

Science 02 Dec 2011: 1226-1227

http://science.sciencemag.org/content/334/6060/1226.full

What are some examples of good practices we can start using now?

Data analysis

1. File organization

Suggest one folder per project, eg:

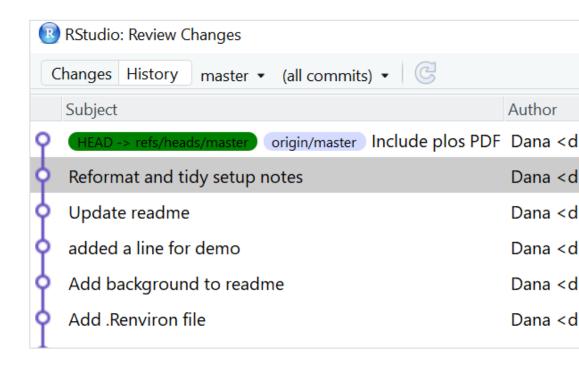
```
My_project
        Data
             raw data.csv
        Docs
            Manuscript.doc
        Results
            Processed_results.csv
        Scripts
            clean_data.R
            fit _model_and_graph.R
```

Resources:

- A Quick Guide to Organizing Computational Biology Projects
- Good enough practices in scientific computing

2. Version control (for code)

Like MS Word's Previous Versions → Restore, or unlimited undo for your R scripts



Resources:

- http://happygitwithr.com/
 - A quick introduction to version control with Git and GitHub

Sharing + publication of results

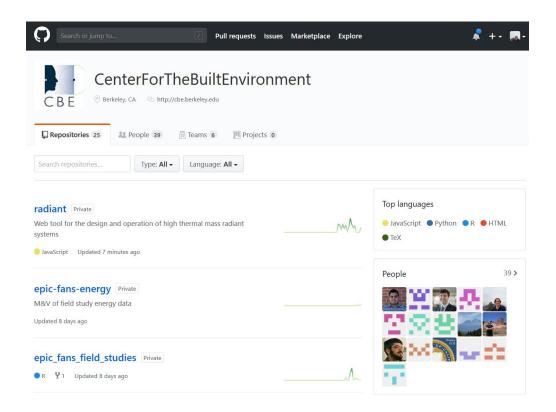
1. Data repositories

- UC system dash
- Example: <u>ASHRAE Global</u>
 Thermal Comfort Database II

Resources:

- Berkeley Research Data Management librarians!
- Other repositories include Zenodo, Open Science Framework, DataDryad, Figshare

2. Code repositories



Resources:

- Software Carpentry's Intro to Version Control for Novices
- A guick introduction to version control with Git and GitHub

Two very common (and free) interactive notebooks:

Other interactive notebooks: Beaker (Two Sigma) Zeppelin (Apache) **Databricks** (Databricks)

Jupyter

Sampling from the generative model

In this notebook, we will use the generative model of the HDHP (Hierarchical Dirichlet-Hawkes Process) in order to sample e We will start with a predifined number of users, say 10, and we will attempt to model their behavior as they are posting ques an online platform. For simplicity, our "vocabulary" will be dummy.

We start by importing all the libraries that will be required.

```
*matplotlib inline
import datetime
import string
import hdhp
import notebook_helpers
import seaborn as sns
```

Now, let us set some parameters for our model. These fall under two categories; the ones relevant to the content and then of

```
vocabulary = ['word' + str(i) for i in range(100)] # the 'words' of our documents
doc min length = 5
doc length = 10
words per pattern = 50
alpha_0 = (2.5, 0.75)
mu_0 = (2, 0.5)
```

overlap = notebook helpers.compute pattern overlap(process) sns.distplot(overlap, kde=True, norm_hist=True, axlabel='Content overlap')

Average overlap: 0.338826769742

https://github.

<matplotlib.axes._subplots.AxesSubplot at 0x10de8ca50>



R Markdown

Unit 3: Fisheries Collapse Module

This module will focus on understanding and replicating fisheries stock assessment data and fisheries collapse.

The Database

We will use data from the RAM Legacy Stock Assessment Database

First, load in the necessary libraries. Note that this time we need a package we haven't used before readx1. This package is useful for reading in .xls or .xlsx files. As always if you want more info on a package run ?readx1 after loading it

```
library("tidyverse")
library("readxl")
library ("scales") # For y-axis labels not in scientific notation - is there a better way to do this since
```

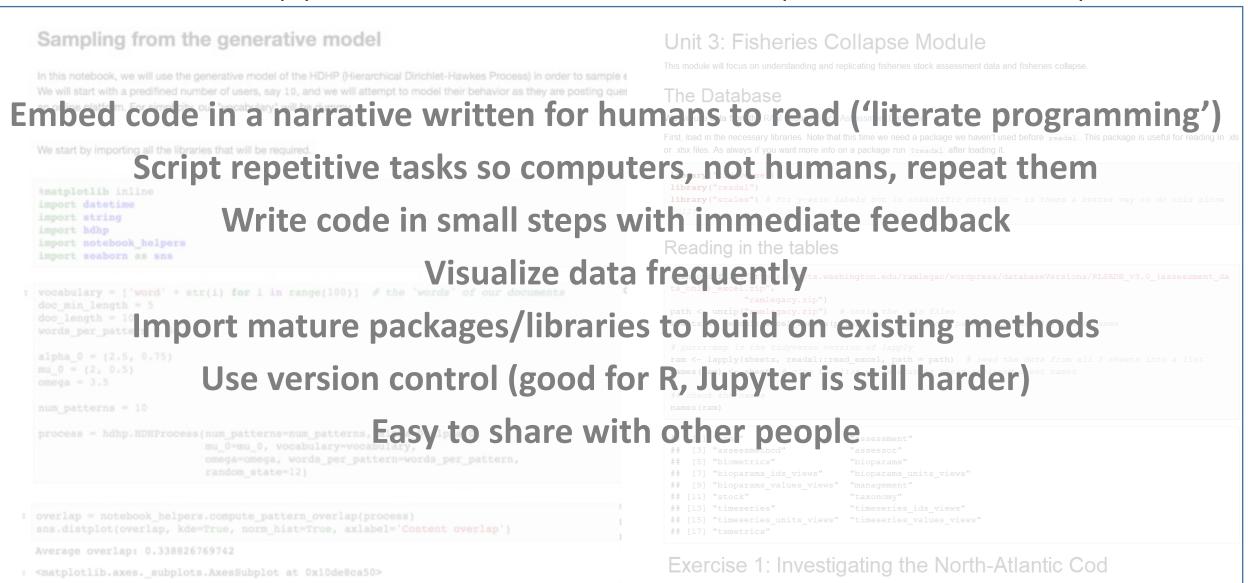
Reading in the tables

```
download.file("https://depts.washington.edu/ramlegac/wordpress/databaseVersions/RLSADB v3.0 (assessment da
ta only) excel.zip",
                                                                                                                      https://github.com/ds421/fish-template/blob/m
               "ramlegacy.zip")
path <- unzip("ramlegacy.zip") # unzip the .xls files
sheets <- readxl::excel sheets(path) # use the readxl package to identify sheet names
# purrr:map is the tidyverse version of lapply
ram <- lapply(sheets, readxl::read_excel, path = path) # read the data from all 3 sheets into a list
names (ram) <- sheets # give the list of datatables their assigned sheet names
## check the names
names (ram)
```

```
"assessment"
## [1] "area"
## [3] "assessmethod"
                                  "assessor"
## [5] "biometrics"
                                  "bioparams"
## [7] "bioparams ids views"
                                  "bioparams units views"
## [9] "bioparams values views"
                                  "management"
## [11] "stock"
                                  "taxonomy"
## [13] "timeseries"
                                  "timeseries ids views"
## [15] "timeseries_units_views"
                                  "timeseries_values_views"
## [17] "tsmetrics"
```

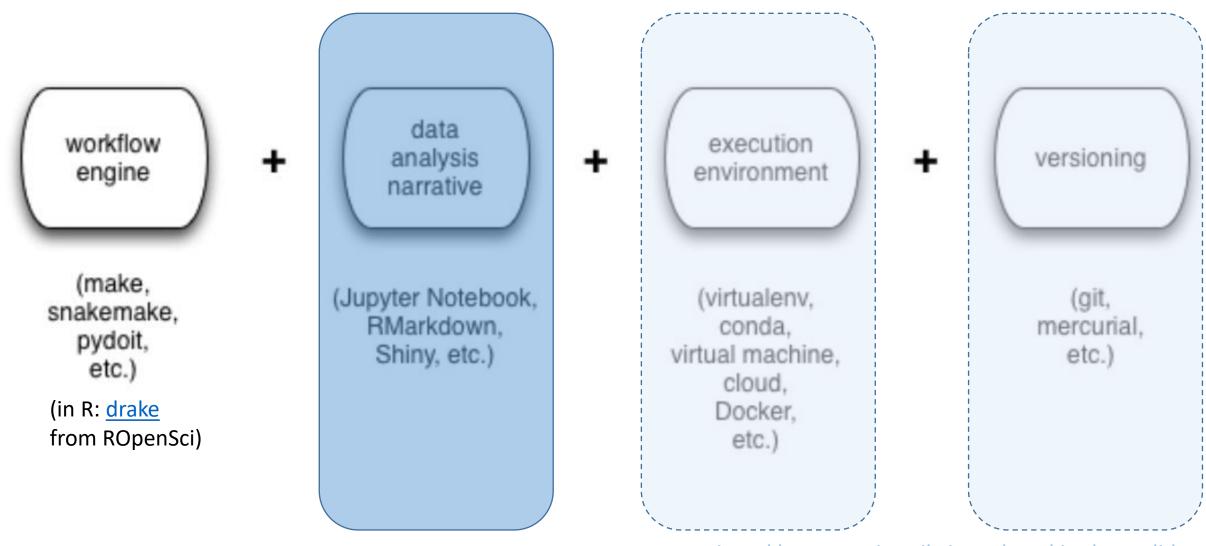
check our data

Similarities of Jupyter and R notebooks – compatible with best practices



All but data visualization based on Wilson G, Aruliah DA, Brown CT, Chue Hong NP, Davis M, Guy RT, et al. (2014) Best Practices for Scientific Computing. PLoS Biol 12(1): e1001745. https://doi.org/10.1371/journal.pbio.1001745

Interactive notebooks are one part of a toolset for reproducibility



introduced in these slides

mentioned but not primarily introduced in these slides

Background—what is literate programming?



https://en.wikipedia.org/wiki/ Donald_Knuth#/media/File:Kn uthAtOpenContentAlliance.jpg

D. E. Knuth; Literate
Programming, The
Computer Journal,
Volume 27, Issue 2, 1
January 1984, Pages
97–111,
https://doi.org/10.1
093/comjnl/27.2.97

"Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do."

- Donald Knuth (1984)

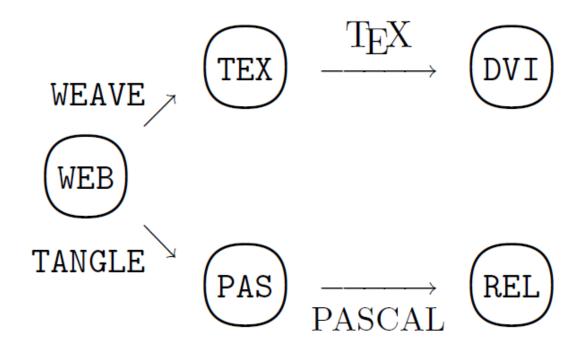
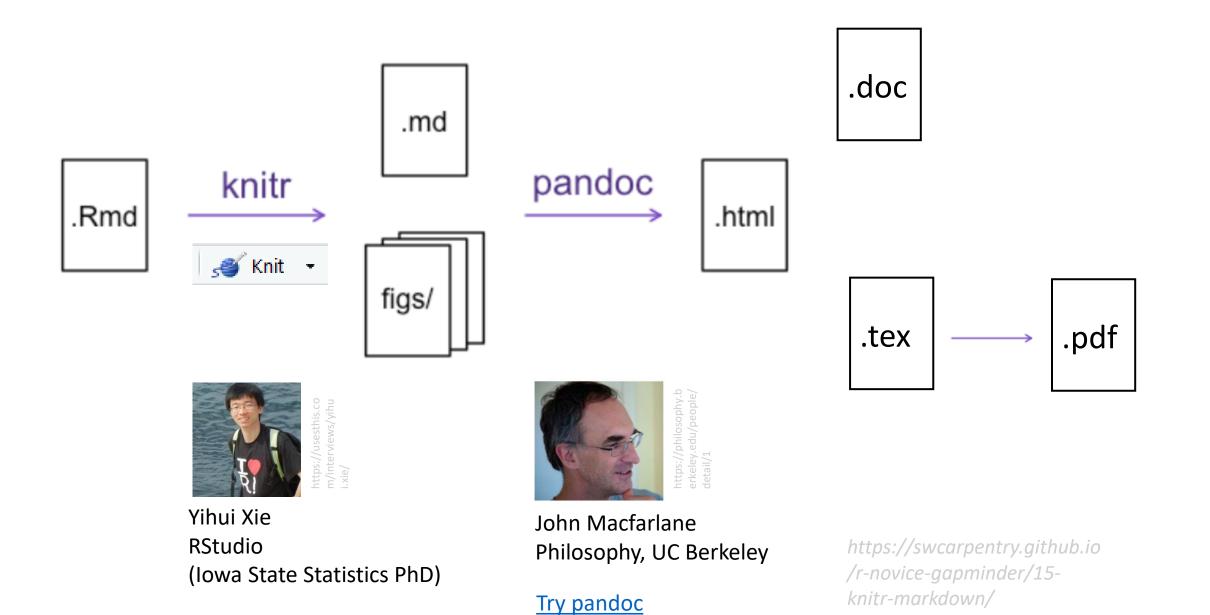


Figure 1. Dual usage of a WEB file.

What is markdown?

Text using Markdown syntax	Corresponding HTML produced by a Markdown processor	Text viewed in a browser
Heading	<h1>Heading</h1>	Heading [edit]
## Sub-heading	<h2>Sub-heading</h2>	Sub-heading [edit]
Paragraphs are separated	Paragraphs are separated by a blank line.	Paragraphs are separated by a blank line. Two spaces at the end of a line
by a blank line. Two spaces at the end of a line	Two spaces at the end of a line produces a line break.	produces a line break.
produces a line break.	Text attributes italic ,	Text attributes italic, bold, monospace. Horizontal rule:
<pre>Text attributes _italic_, **bold**, `monospace`.</pre>	bold , <code>monospace</code> .	Bullet list:
Horizontal rule:	Horizontal rule:	applesoranges
	<hr/>	• pears
Bullet list:	Sullet list:	Numbered list: 1. wash
<pre>* apples * oranges * pears</pre>	apples oranges	2. rinse3. repeat

.Rmd files combine code and text and convert to many formats



Literate programming example with R Markdown

Starting with one .Rmd file with both R code and text

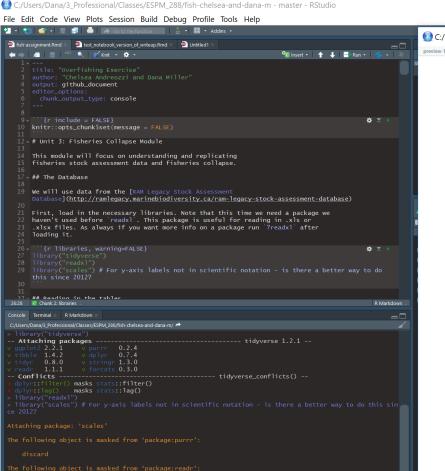
This button or command:

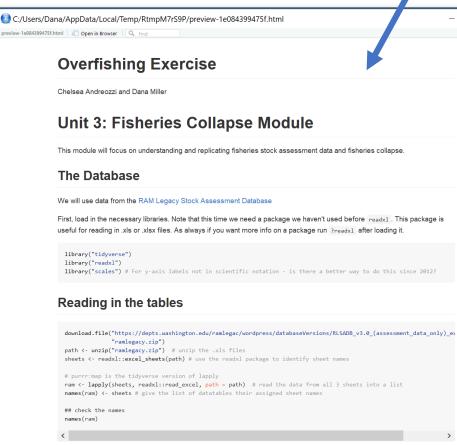


executes all R code (output shown in console) This button or command:



renders formatted document with executed code and text (.md, .pdf, .doc etc)





R Markdown documents – key features

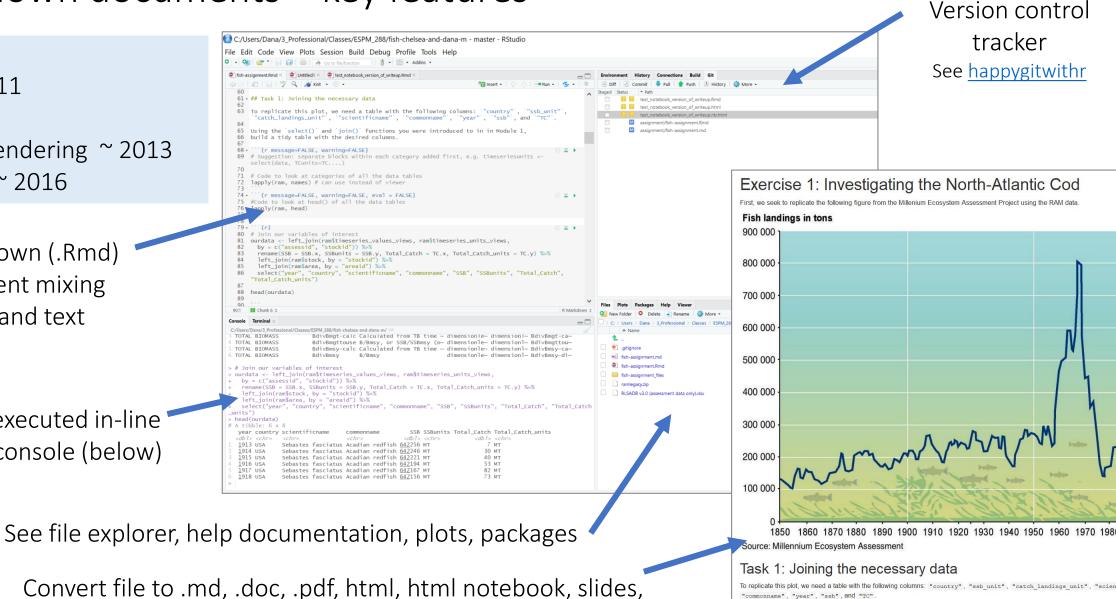
book, blog, dashboards, Shiny app, etc

See R Markdown output formats

History Rstudio ~ 2011 knitr ~ 2012 Markdown rendering ~ 2013 R Notebook ~ 2016

> R Markdown (.Rmd) document mixing code and text

Code can be executed in-line (above) or in console (below)



To replicate this plot, we need a table with the following columns: "country", "ssb_unit", "catch_landings_unit", "sciential to replicate this plot, we need a table with the following columns: "country", "ssb_unit", "catch_landings_unit", "sciential to replicate this plot, we need a table with the following columns: "country", "ssb_unit", "catch_landings_unit", "sciential to replicate this plot, we need a table with the following columns: "country", "ssb_unit", "catch_landings_unit", "sciential to replicate this plot, we need a table with the following columns: "country", "ssb_unit", "catch_landings_unit", "sciential to replicate this plot, we need a table with the following columns: "country", "ssb_unit", "catch_landings_unit", "sciential to replicate the plot of the plot of

Suggestion: separate blocks within each category added first, e.g. timeseriesunits <- selections

Using the select() and join() functions you were introduced to in in Module 1, build a tidy table with the desired column:

Demo: R Markdown

Learning objectives:

- 1.
- How to create a new R Markdown document in Rstudio
- Make edits
- Knit it
- Share it somewhere
- Have someone else download and run it
- 2.
- Example of paper written in R Markdown

Limitations of R + RMarkdown

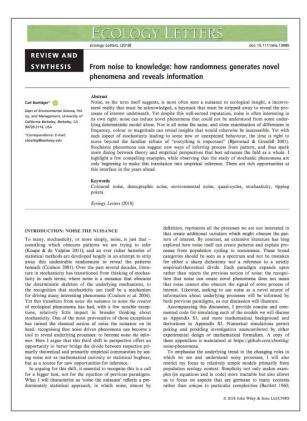
- Not a "general purpose programming language"
- By default, loads entire data into memory
- Less widely used in industry than python
- Possible to run chunks out of order (but can "run all")

Reference to set up git w/R: http://happygitwithr.com

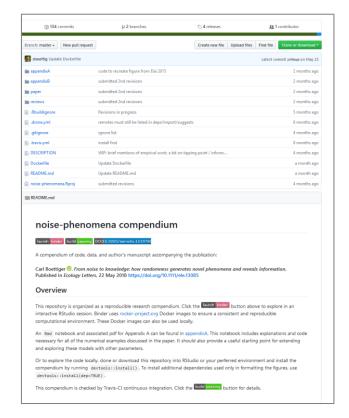
Interactive publications

New paper

(open access)



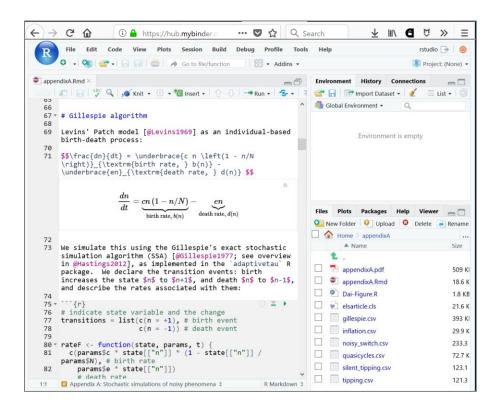
Corresponding "compendium" (with text, code, data)



https://github.com/cboettig/noise-phenomena

Interactive R Markdown notebook to explore code

(with all required files and software ready to run in Rstudio in your browser with no installation required, thanks to Binder)



https://onlinelibrary.wiley.com/doi/epdf/10.1111/ele.13085

Demo – reproduce a figure from paper on the previous slide

See the paper: https://onlinelibrary.wiley.com/doi/epdf/10.1111/ele.13085

- Note the PDF includes a link to a GitHub repo

2. Inspect the code

- Open the associated GitHub repository containing the code and data used to produce the figures for the paper
 - Repo: <u>https://github.com/cboettig/noise-phenomena</u>
 - Code for the paper: https://github.com/cboettig/noise-phenomena/blob/master/paper/paper.Rmd
- 3. Reproduce a figure without installing anything on your local computer!
 - Click the launch binder button on the main page of the repo

Interactive publications – in python too!

New paper

(in this case, a preprint)

Transparency by Design: Closing the Gap Between Performance and Interpretability in Visual Reasoning David Mascharka* Philip Tran2 Ryan Soklaski Arjun Majumdar* ¹MIT Lincoln Laboratory[†] ²Planck Aerosystems[‡] (first.last)@11.mit.edu, phil@planckaero.com Abstract Visual question answering requires high-order reason-ing about an image, which is a fundamental capability needed by machine systems to follow complex directives Recently, modular networks have been shown to be an effective framework for performing visual reasoning task While modular networks were initially designed with a de-gree of model transparency, their performance on complex visual reasoning benchmarks was lacking. Current state of-the-art approaches do not provide an effective mechanism for understanding the reasoning process. In this paper, we close the performance oan between interpretable models and state-of-the-art visual reasoning methods. We propose a set of visual-reasoning primitives which, when composed, poses a series of attention masks that allow it to correctly count two large metal cylinders in the image. manifest as a model capable of performing complex reason-ing tasks in an explicitly-interpretable manner. The fidelity and interpretability of the primitives' outputs enable an unample, in order to answer the question "What color is the paralleled ability to diagnose the strengths and weaknesses of the resulting model. Critically, we show that these primidentify which sphere is the large metal one, understand titives are highly performant, achieving state-of-the-art ac-curacy of 99.1% on the CLEVR dataset. We also show that what it means for an object to be to the right of another, and apply this concept spatially to the attended sphere. Within our model is able to effectively learn generalized representhis new region of interest, the model must find the cube and tations when provided a small amount of data containing novel object attributes. Using the CoGenT generalization determine its color. This behavior should be compositional to allow for arbitrarily long reasoning chains. task, we show more than a 20 percentage point improveposed for the VQA task [8, 12, 23, 26, 35, 37], neural module networks [2, 3, 12, 18] are among the most intuitive. Introduced by Andreas et al. [2], neural module networks 1. Introduction compose a question-specific neural network, drawing from A visual question answerine (VOA) model must be cation. This design closely models the compositional nature pable of complex spatial reasoning over an image. For exof visual reasonine tasks. In the original work, modules were designed with an attention mechanism, which allowed *Indicates equal contribution.

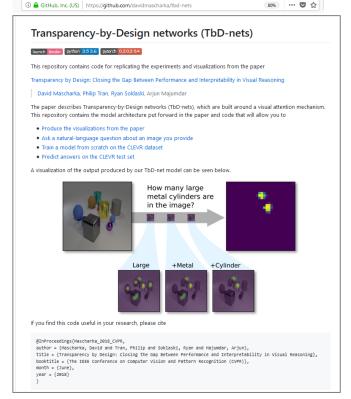
†This material is based upon work supported by the Assistant Secretary of Defense for Research and Engineering under Air Force Contract No. PA8721-05-C-0002 and/or FA8702-15-D-0001. Any opinions, findings, conclusions or recommendations expressed in this material are those of the for insight into the model's operation. However, the approach did not perform well on complex visual reasoning tasks such as CLEVR [17]. Modifications by Johnson et al. [18] address the performance issue at the cost of losing uthor(s) and do not necessarily reflect the views of the Assistant Secreta model transparency. This is problematic, because the abilf Defense for Research and Engineering.

²This work conducted while Philip was at MIT Lincoln Laboratory. ity to inspect each step of the reasoning process is crucial

https://arxiv.org/abs/1803.05268

Website explaining paper

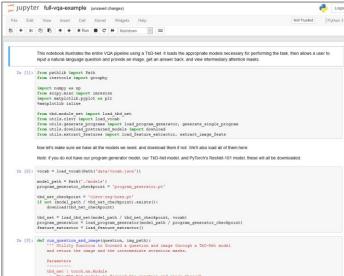
(has code to replicate experiments + plots and explicit software versions)



https://github.com/davidmascharka/tbd-nets

Interactive Jupyter notebook with code to apply their method to your own images

(with all required files and software ready to run in your browser with no installation required, thanks to Binder)



<u>https://mybinder.org/v2/gh/davidmascharka/tbd-nets/binder?filepath=full-vqa-example.ipynb</u>

What next?

UCB Prof Phillip Stark on reproducibility:

"Science is *show me*, not *trust me*"

"Perfection is impossible but improvement is easy"

There are many communities who can help!

Software Carpentry, R for Data Analysis (R4DS), RBloggers, PyData (also has R videos), RLadies, #rstats...

And we can learn a lot from each other ©

Some more R resources

R for Data Science:

https://r4ds.had.co.nz

From Excel to R:

http://rpubs.com/acolumbus/s/how-to-use-r-with-excel (includes list of common Excel functions in R)

Markdown guide:

https://bookdown.org/yihui
/rmarkdown/

Free resources aimed at beginners:

- 1. introduction to programming in R
- 2. Reproducible scientific analysis using RStudio and R

Useful but not fully free:

Datacamp - no longer recommended due to poor treatment of employees, instructors, and user community in the aftermath of sexual assault by a member of the executive team: https://www.buzzfeednews.com/article/daveyalba/datacamp-sexual-harassment-metoo-tech-startup

Bonus slides!

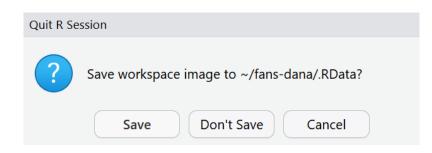
(for reference)

Three R tips you can start using today:

- here::here (use with RProject)
 - Freedom from hardcoded file paths!

```
library(here)
db <- read_csv(here("subfolder_name", "file_name.csv"))</pre>
```

- read csv
 - tidyverse version of read.csv
 - won't coerce strings to factors, outputs a dataframe (tibble)
- "Save workspace image?"
 - Don't save!



Where do we go from here?

ROpenSci's perspective:

- •Train students by putting homework, assignments & dissertations on the reproducible research spectrum
- •Publish examples of reproducible research in our field
- Request code & data when reviewing
- •Submit to & review for journals that support reproducible research
- •Critically review & audit data management plans in grant proposals
- •Consider reproducibility wherever possible in hiring, promotion & reference letters.

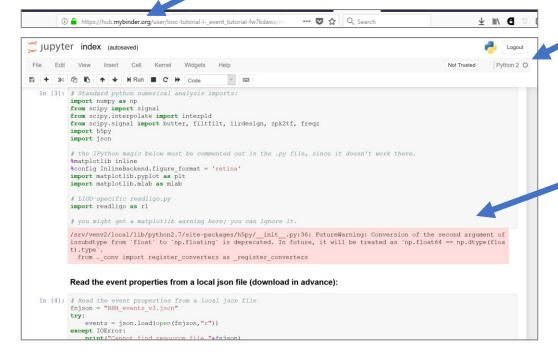
How does Binder work?

"Binder allows you to create custom computing environments that can be shared and used by many remote users"

https://mybinder.readthedocs.io/en/latest/

Visible in your browser, but running on a remote machine

Your browser

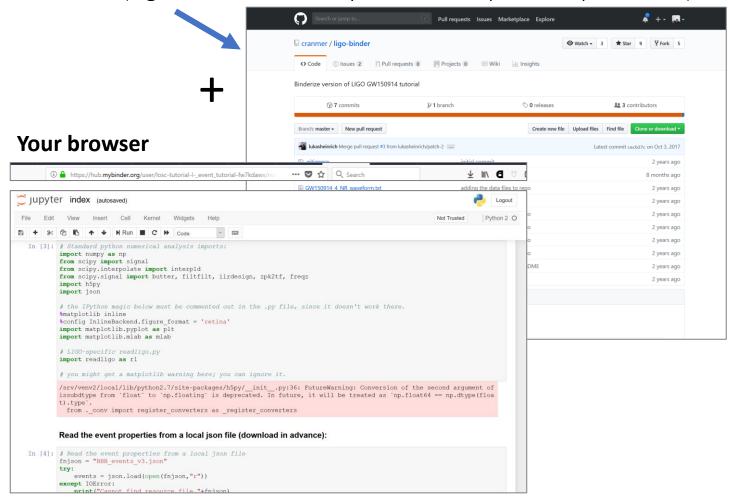


Specified version of Python (or other kernels eg R)

You see the code in the .ipynb file

How does Binder work?

Code for notebook and list of dependencies and files available on GitHub (right now Binder only works with public repositories)



How does Binder work?



builds Docker image based on repo and generates URL for public access

