Introduction to Computational Biology

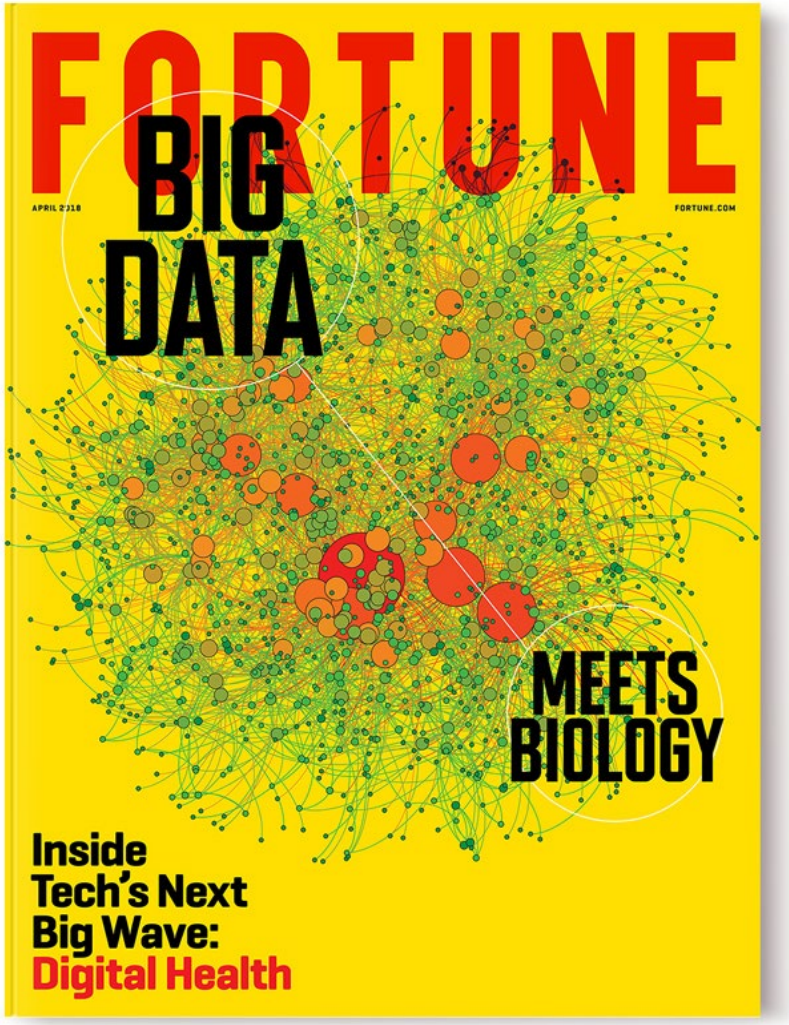
Lecture 0

BIOL 4360, BIOL 5360, MARB 6360

Dr. Chris Bird

Why are computational skills important for biologists?

- Increasing data size and complexity
- Increasing sophistication of statistical and mathematical analyses
- Transparency, reproducibility, and documentation



Why should biologists be interested in developing computational kung-fu?

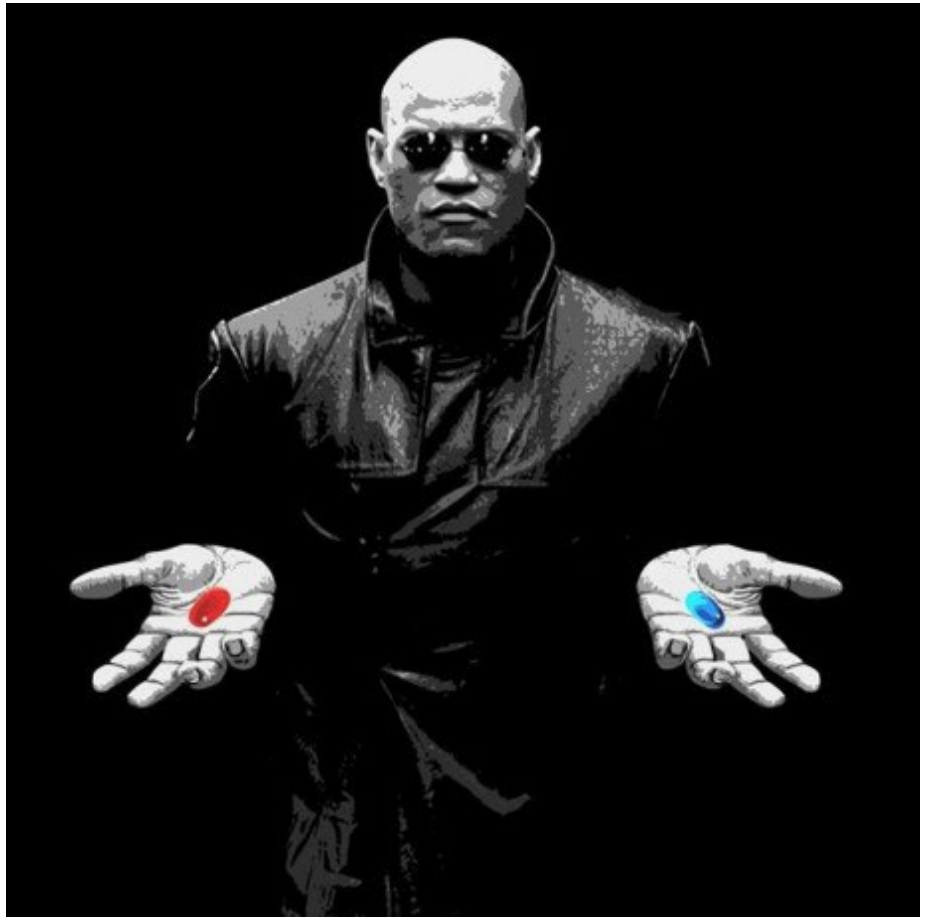
- Automate impossibly tedious, monotonous, and lengthy tasks
- Increased rate and significance of discovery
- Career success
- Maximize potential

Why did I choose to develop this course?

- Historical lack of (introductory) computational courses for biologists
- Steep learning curve
- The days of easily succeeding in biological research without computational knowledge and skill are over

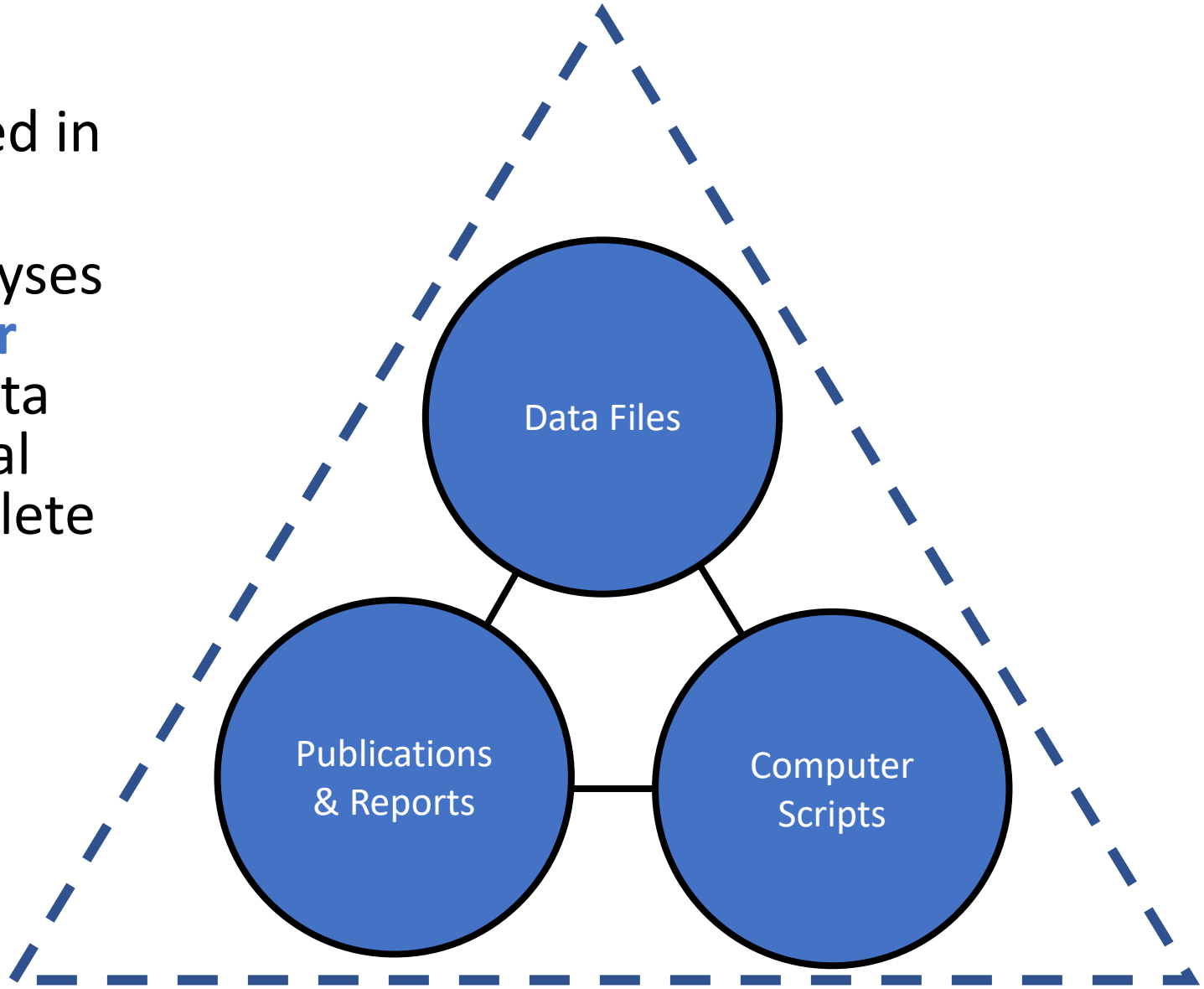
If you so choose, I will show you the philosophy of data science

- Automation
  - Interconnection
  - Modularity
- Reproducibility
  - Organization
  - Comprehension
- Openness
- Simplicity
- Correctness



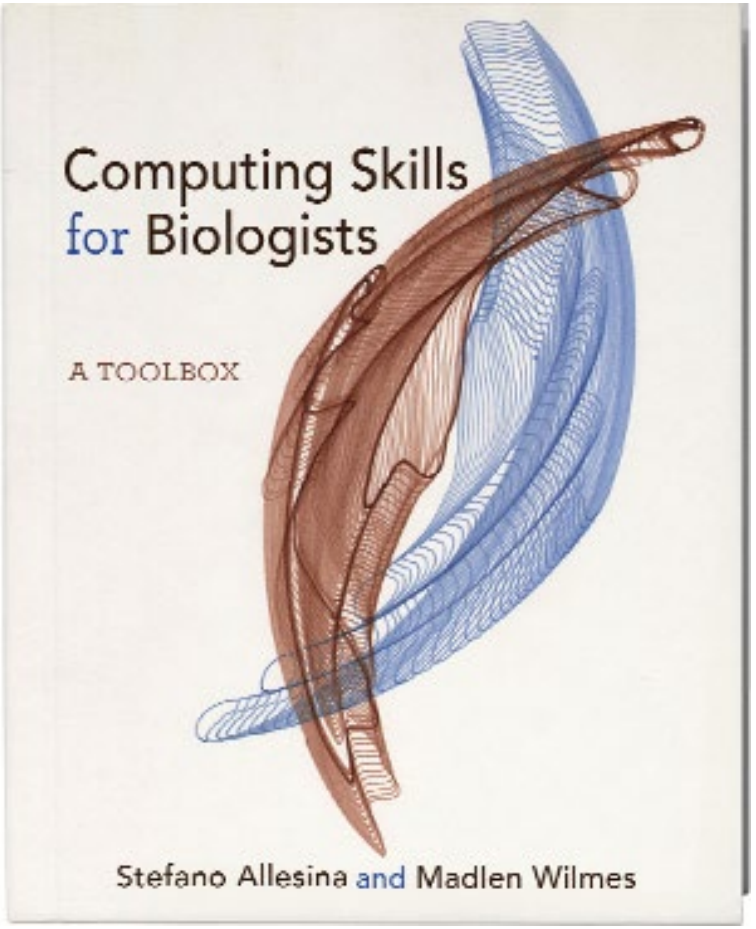
Philosophy of Data Science

- All **data is digitized** and stored in files
- Data manipulations and analyses are documented in **computer scripts** that interface with data files and require no additional human intervention to complete analysis
- Data & scripts are published with the report and **openly accessible to all**



We Used to Follow The CSB Text Book, It's a Good Resource But Not Required

- Provides you with requisite breadth of tools at the expense of depth
- Showcase of Linux, Python, R
- Organized into 10 chapters, theoretically 1 per lecture
- Goal is to flatten your learning curve

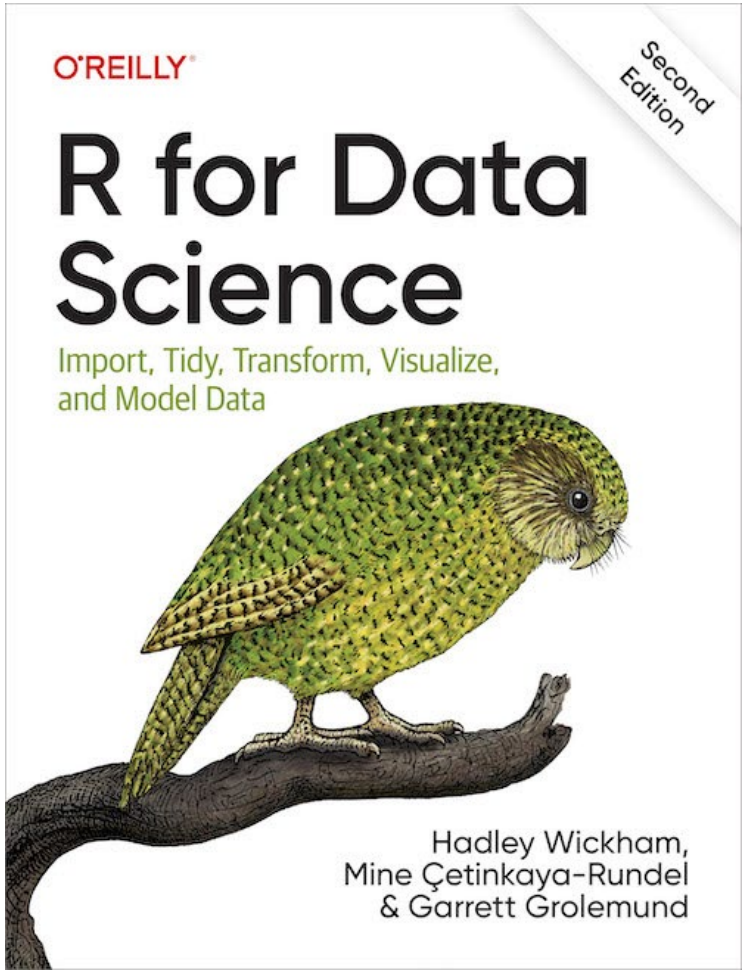


https://computingskillsforbiologists.com/

We are Going to Learn How to Use R

- You will learn core principles of R that aren't taught in other courses that expect you to use R

- You will learn to use `tidyverse`, which was masterminded by the Author of the R for Data Science book, which is free.



https://r4ds.hadley.nz/

Learning Objectives

- Recognize, describe, and organize data into standard biological data structures
- Locate scientific data repositories and extract data
- Operate UNIX/LINUX computers from command line
- Construct and modify computer programming/scripting logic structures for processing biological data
- Use version control software (git)
- Describe and use regular expressions to query data
- Typeset with LaTeX or MarkDown
- Use the most popular open-source tools for biological data manipulation
  - Shell scripting (bash)
  - Scientific computing (python)
  - Statistical computing (R)
  - Tool repositories

Syllabus & Course Organization

- Syllabus is on blackboard and github
- 3 Parts of Course
  - Linux, R, Python
- Additional skills
  - Version control with git
  - Typesetting with LaTeX, markdown

Undergraduates:¶

ACTIVITY	% of FINAL GRADE
Participation	15
Assignments	40
Exam 1	15
Exam 2	15
Final Exam	15

Graduates:¶

ACTIVITY	% of FINAL GRADE
Participation	10
Assignments	20
Exam 1	10
Exam 2	10
Final Project	BIOL 5360: 50 MARB 6360: 40
Final Presentation	MARB 6360: 10

Lectures

- Environment for you to learn new concepts
- Hands-on with computers
- Power-point & GitHub driven
  - On zoom
- Independent exercises w/ MS Forms linked in GitHub
- Note: I update the course materials prior to each lecture.
  - Don’t go ahead of where we are in the class

Assignments

- Generally due each week
  - See the schedule in our classroom repo (link in canvas)
- Scripts will be submitted through GitHub classroom
  - Starting with Assignment 2 Extra Credit
- For now, question-answer based work will be conducted with a MS Form “quiz”

SCHEDULE

SECTION 1. WELCOME TO THE MATRIX

- 08/30 Week00 Introduction & Data
  - Assignment_0 Due, 09/08
- 09/06 Week01 Unix I
  - Assignment_1, Due 09/13
  - Grad Student Course Project: Ideas, Due 09/13

Final Project (Graduate Students)

- Automate the processing and analysis of your data
  - Follow guide on [How to Organize Biological Data]
- Document work on GitHub
- Report written in LaTeX or MarkDown
  - State problem/challenge
  - Describe strategy to solve
  - Describe how code works
  - 10 min presentation during Final Exam Period (PhD students)

- Wk 3: Project idea
- Wk 5: Plan/Outline
- Wk 6: GitHub Repo
- Wk 7: Commit working function
- Wk 8: Commit 2 working functions w data input and output
- Wk 11: Draft/ progress report
- Wk 14: Final report, Working code and data on GitHub
- Final Exam: Oral pres (MARB 6360)

Questions?

Biological Data

Lecture 01

BIOL 4590, BIOL 5590

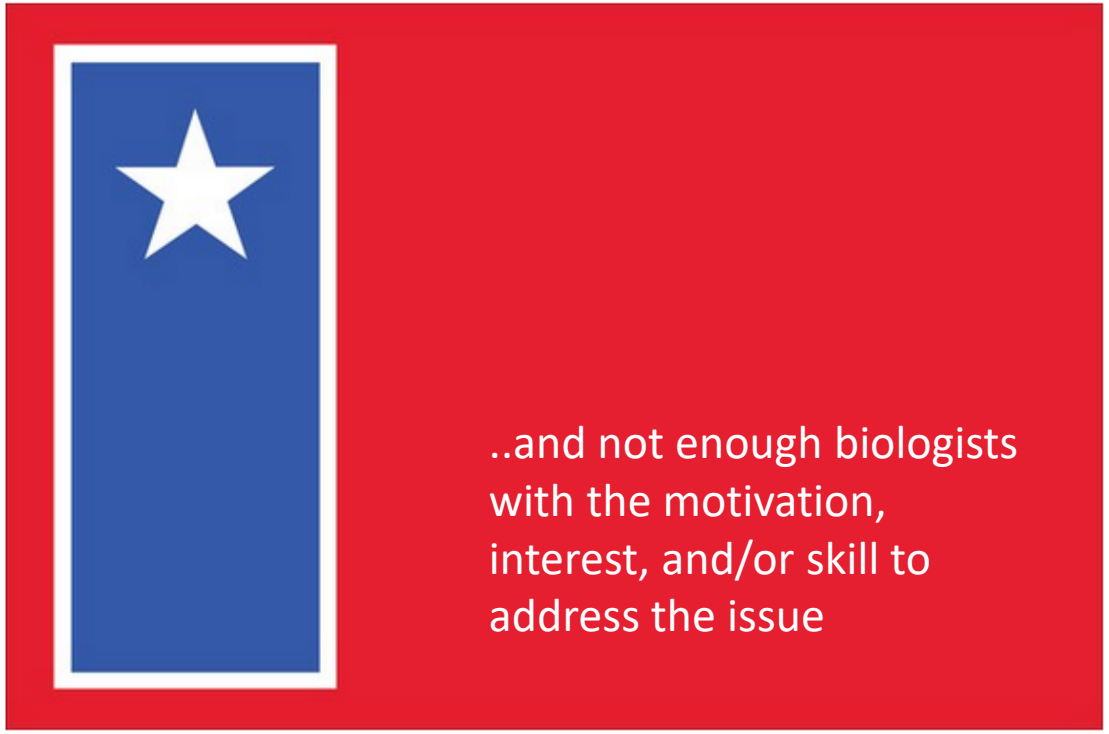
Dr. Chris Bird

Big Data Biology

- Massive amounts of data
- Associated tools, processes, procedures
- Volume, velocity, acceleration
- Goal is to tame the data
- Examples: DNA, climate, weather, remote sensing, GIS, all “omics”, populations

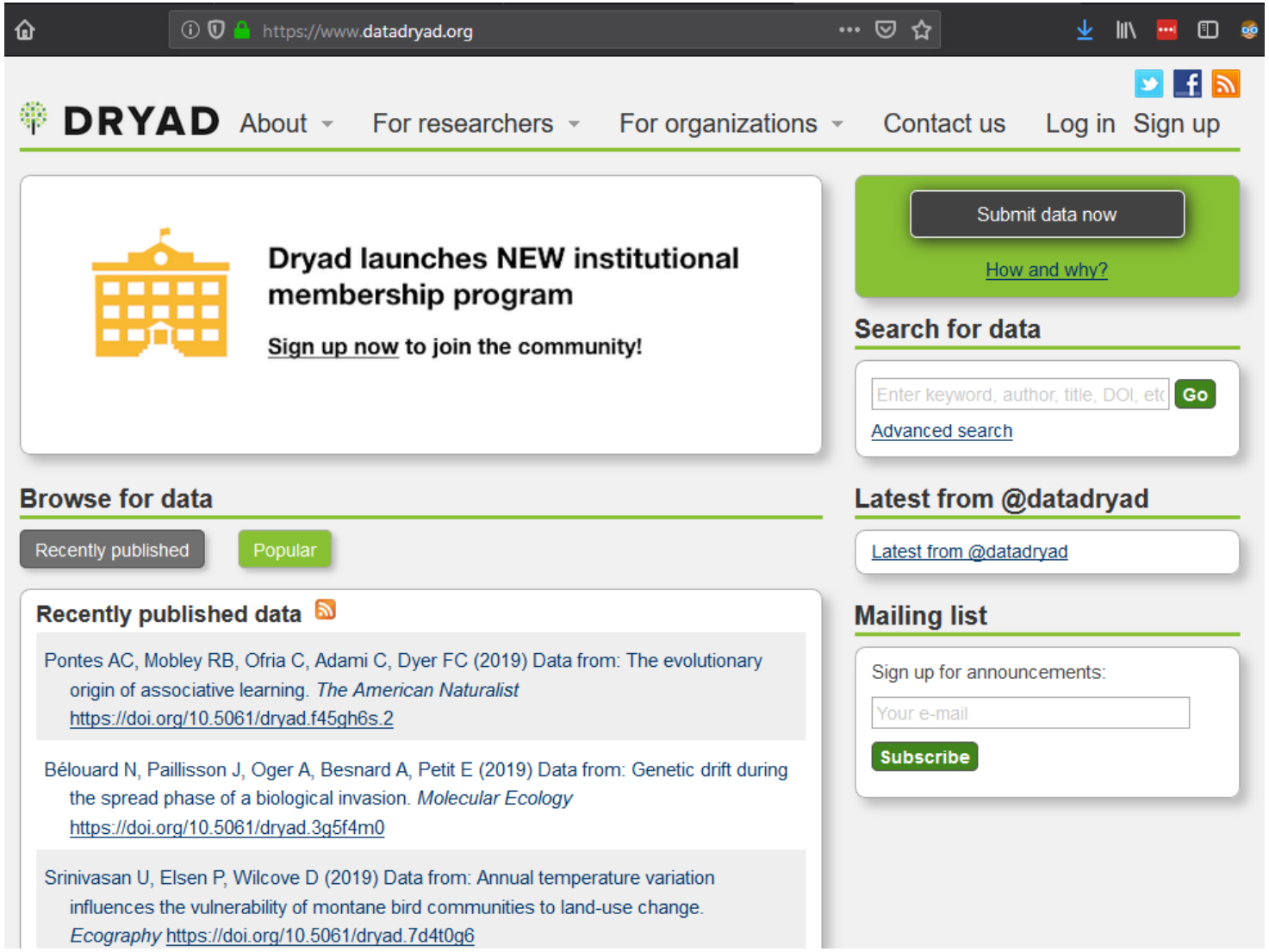
EMILY SINGER SCIENCE 10.11.13 09:30 AM

BIOLOGY'S BIG PROBLEM: THERE'S TOO MUCH DATA TO HANDLE



Repositories for Data Big and Small

- Data associated with scientific papers should be published
  - Owned by the people
  - Should be freely available
  - Promotes acceleration of knowledge generation
- All Types of Data
  - www.datadryad.com
- DNA & Proteins
  - https://www.ncbi.nlm.nih.gov/
- GIS
  - https://data.usgs.gov/datacatalog/#fq=dataType%3A(collection%20OR%20non-collection)&q=*%3A*
- Oceanographic
  - https://data.noaa.gov/datasetsearch/
- Too many to list



Let’s Explore a Data Set Published in Dryad

- www.datadryad.org
- Find Data from:
  - Direct and indirect effects of sexual signal loss on female reproduction in the Pacific field cricket (*Teleogryllus oceanicus*)
- Download the data and view it in MS Excel
  - **It is important to open files, look at data, and understand how it is organized**

Data from: Direct and indirect effects of sexual signal loss on female reproduction in the Pacific field cricket (Teleogryllus oceanicus)

Heinen-Kay J, Strub D, Balenger S, Zuk M

Date Published: August 29, 2019

DOI: https://doi.org/10.5061/dryad.v732vb1

Files in this package

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Title	**Data for Heinen-Kay et al. Sexual signal loss and female reproduction**
Downloaded	3 times
Description	Data for (1) comparison of flatwing and normal-wing homozygous female reproductive tissue, (2) offspring production of flatwing and normal-wing females, and (3) reproductive tissue comparison between populations and acoustic treatments
Download	Data for Heinen-Kay et al. Sexual signal l....xlsx (36.79 Kb)
Details	View File Details

Tidy Data (Wickham 2014)

- Each row is the "smallest unit of observation"
  - Ex: an individual fish
- Each column is a variable or dimension of information about the units of observation
  - Ex: somatic mass

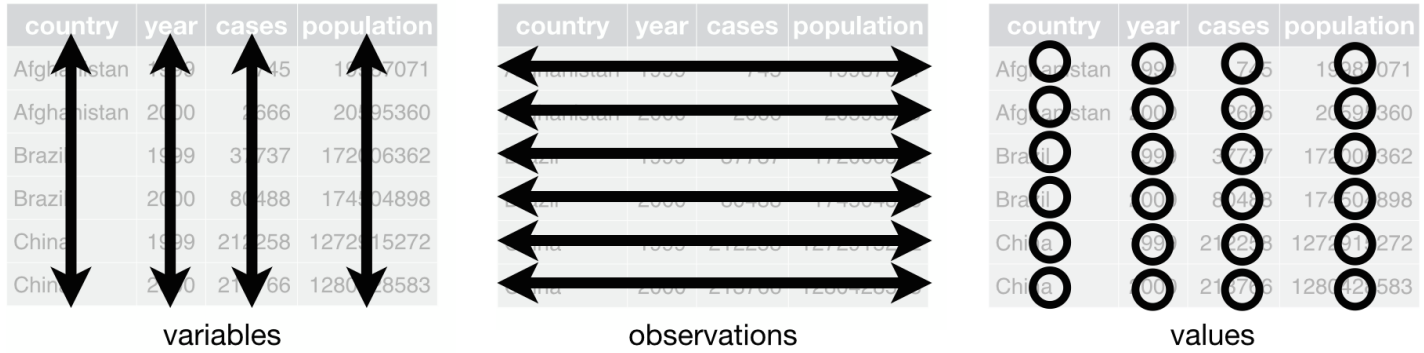
Journal of Statistical Software

August 2014, Volume 59, Issue 10. *http://www.jstatsoft.org/*

Tidy Data

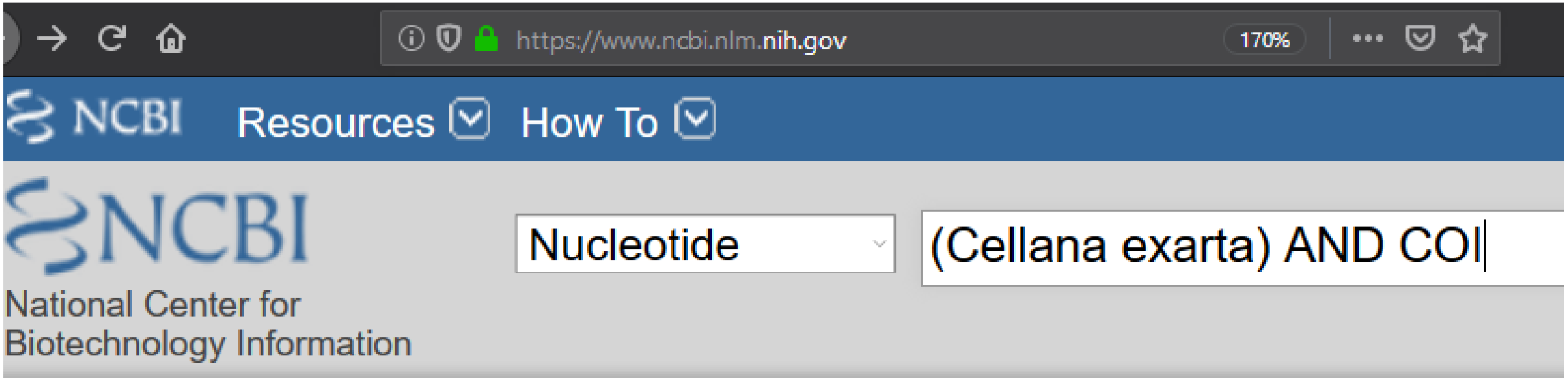
Hadley Wickham
RStudio

Abstract



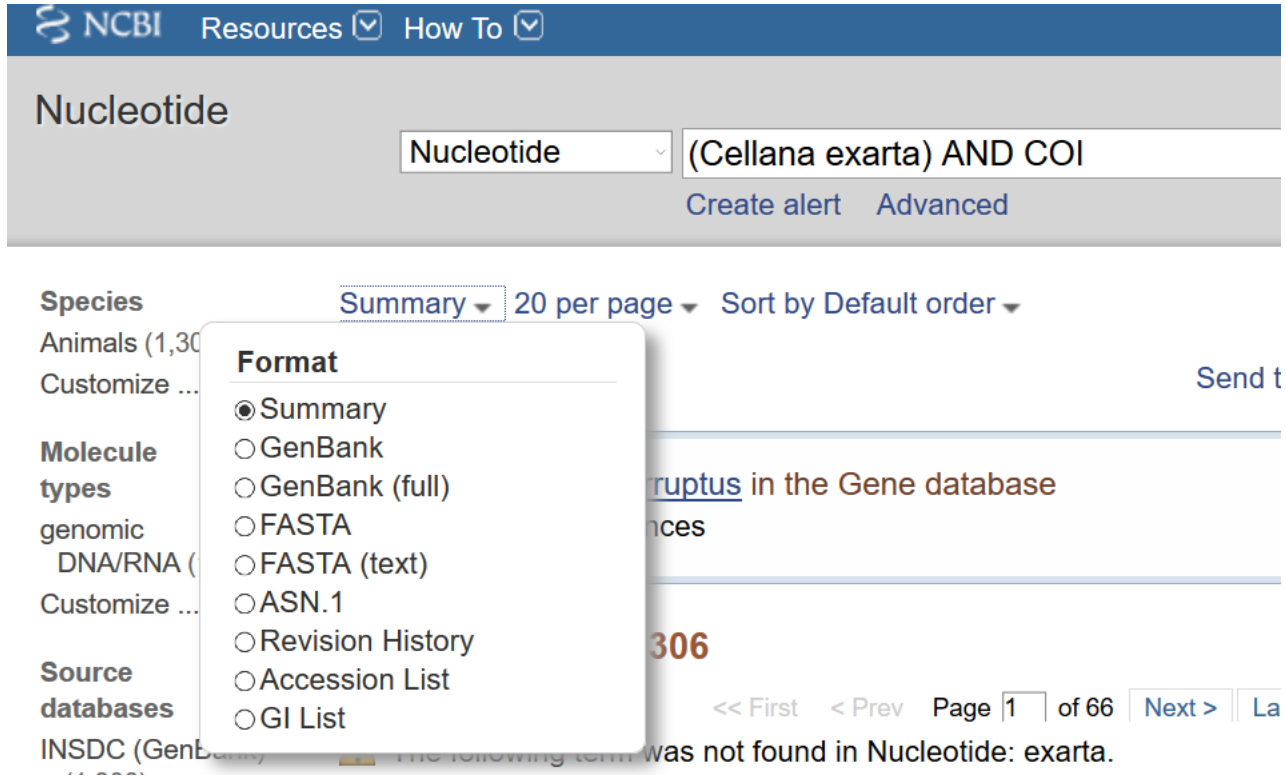
Common Data Formats & Structures are Not Always Tidy

- https://www.ncbi.nlm.nih.gov/
- Conduct the following search



GenBank Supports Several Formats, None Are Tidy

- https://www.ncbi.nlm.nih.gov/
- Switch to FASTA (text)




```
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oxidase subunit I, partial cds, specimen_voucher: NUGB-L694(Nagoya University)
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GGACCCCATTTTATATCAACATTTGTTT
```

Common DNA Data Format

- https://www.ncbi.nlm.nih.gov/
- Switch to FASTA (text)
  - Wikipedia is an excellent resource for describing data formats
- FASTA Format
  - DNA
  - Lines beginning with `>` contain the ID of the unit of observation
  - Lines that don't being with `>` contain information, each character (nucleotide) is a dimension of the unit of observation

```
>AB263731.1 Cellana radiata enneagona mitochondrial COI gene for cytochrome c
oxidase subunit I, partial cds, specimen_voucher: NUGB-L694(Nagoya University)
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GGACCCCATTTTATATCAACATTTGTTT
```

Data Formats

- I will emphasize Tidy format
- Many fields of Biology have their own particular and peculiar data formats
- There are tools available for handing and converting among data formats
- Some data formats are intimidating, at first
  - There will exist published descriptions of these
  - Duckduckgo: sam specification
    - This is a common “big data” format for next generation sequencer data
  - Take a deep breath, it’s not as intimidating as it initially seems

Repositories Can Include Scripts for Processing, Analyzing, & Visualizing Data

- www.datadryad.com
- Find Data from:
  - Meta-analyzing the likely cross-species responses to climate change
- Explore the files
  - *.xls, *.txt,
  - The extension indicates file format NOT data format
- R script
  - R is a statistical computer language
  - This file will analyze the data exactly the way it was reported in the publication

Files in this package

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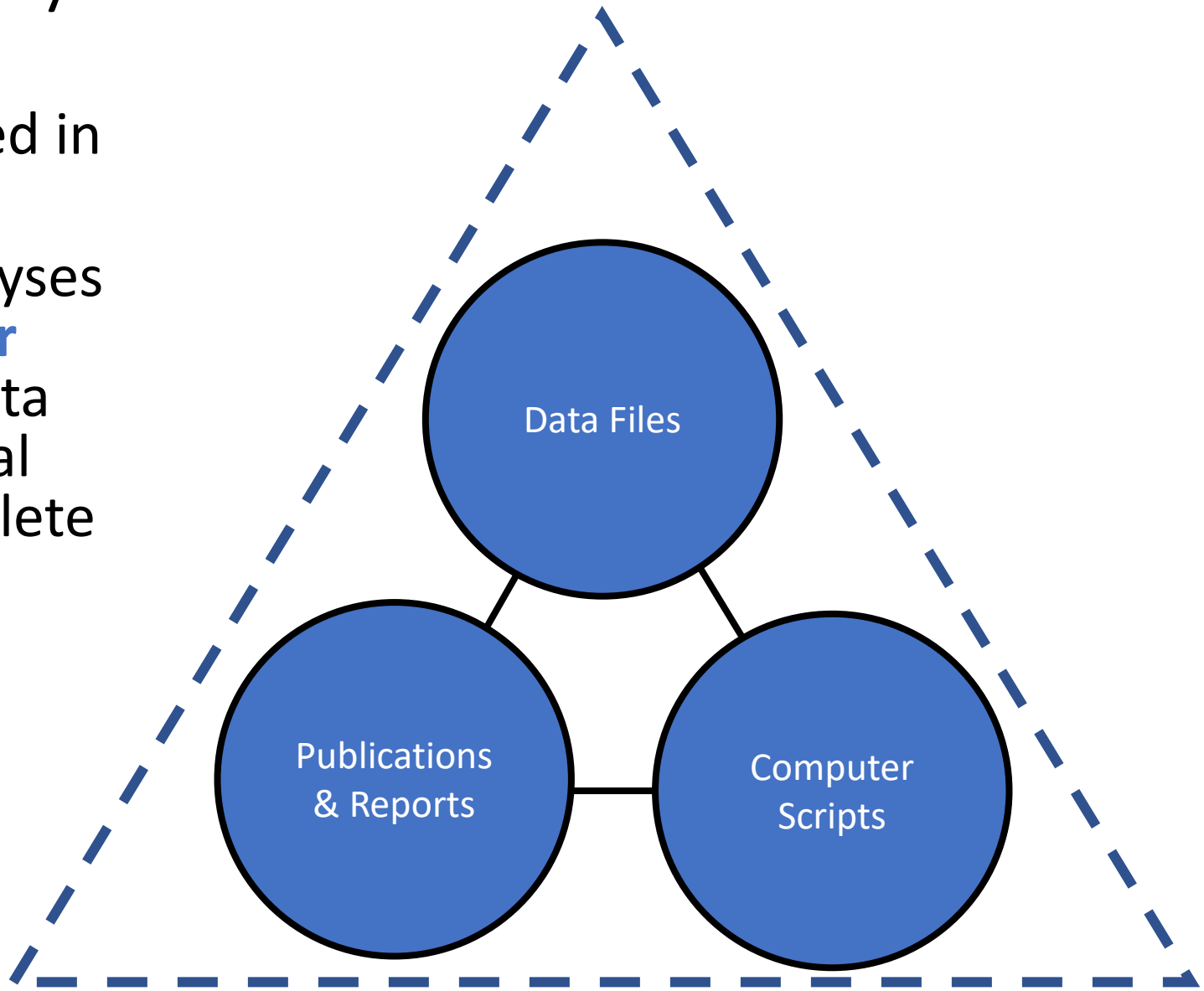
Title	**Range extent for bird species**
Downloaded	2 times
Description	This file contains the extents of occurrence (range filling) for 1205 Neotropical bird species.
Download	SM1_Metabirds.xls (2.937 Mb)
Download	README.txt (677 bytes)
Details	View File Details

Title	**R script**
Downloaded	1 time
Description	R script for effect sizes computation and data-analyses built in R version 3.5.1
Download	SM2_script_metabirds.R (5.259 Kb)
Details	View File Details

Title	**Neotropical bird consensus phylogeny**
Downloaded	1 time
Description	This Neotropical bird consensus phylogeny was estimated from 10,000 random phylogenetic trees with 'Hackett constraint' for the backbone topology from Jetz et al. (2012; Nature, 491, 444–448. https://doi.org/10.1038/nature11631) available in https://birdtree.org/. The function 'consensus.edges' of 'phytools' package (Revell, 2012; Methods in Ecology and Evolution, 3, 217–223. https://doi.org/10.1111/j.2041-210X.2011.00169.x) to build the consensus phylogeny.
Download	phy_consensus.txt (51.13 Kb)
Details	View File Details

Recall The Philosophy of Data Science

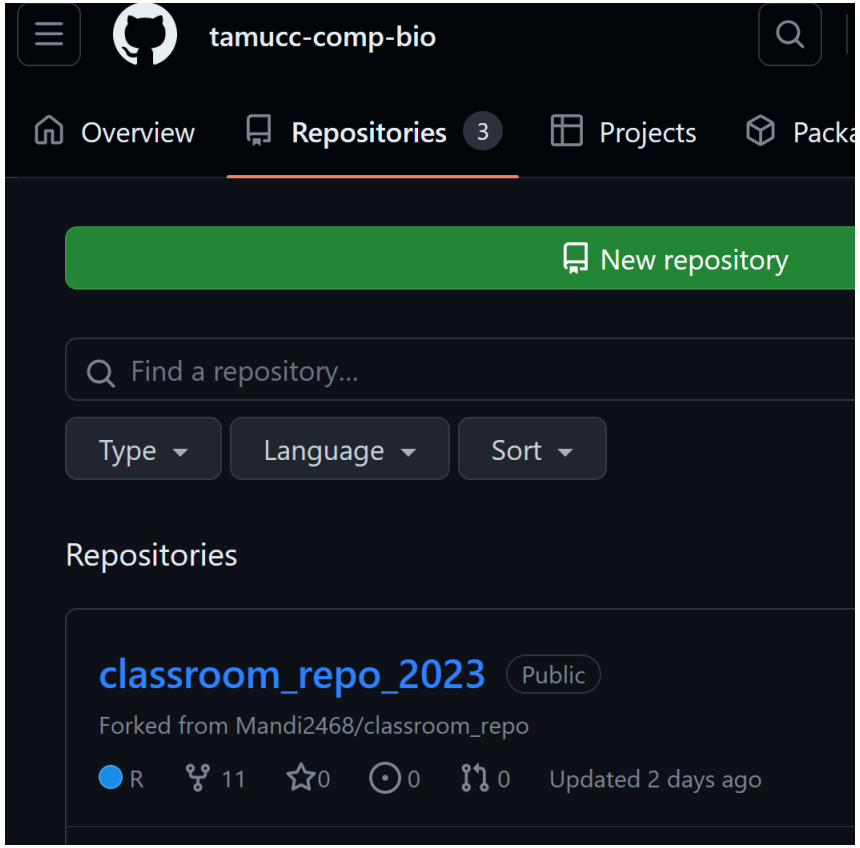
- All **data is digitized** and stored in files
- Data manipulations and analyses are documented in **computer scripts** that interface with data files and require no additional human intervention to complete analysis
- Data & scripts are published with the report and **openly accessible to all**



GitHub – A Repository of Sorts

- A company
- Website is designed to aid in developing code, like an R script
- It also serves as a repository for data, code, and scripts
- Efficient mechanism to disseminate your code to users
- Can also be used to organize a class

- https://github.com/orgs/tamucc-comp-bio/repositories



Conceptual Diagram of a GitHub Organization