

Introduction to Computational Biology

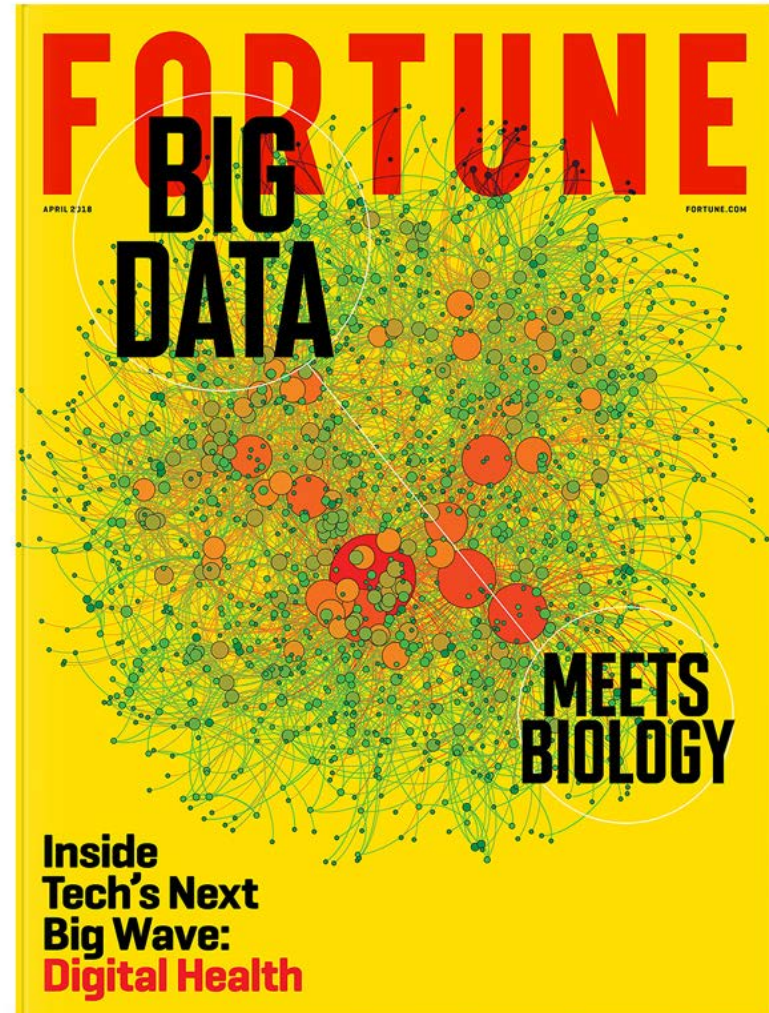
Lecture 0

BIOL 4590, BIOL 5590, MARB 6590

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



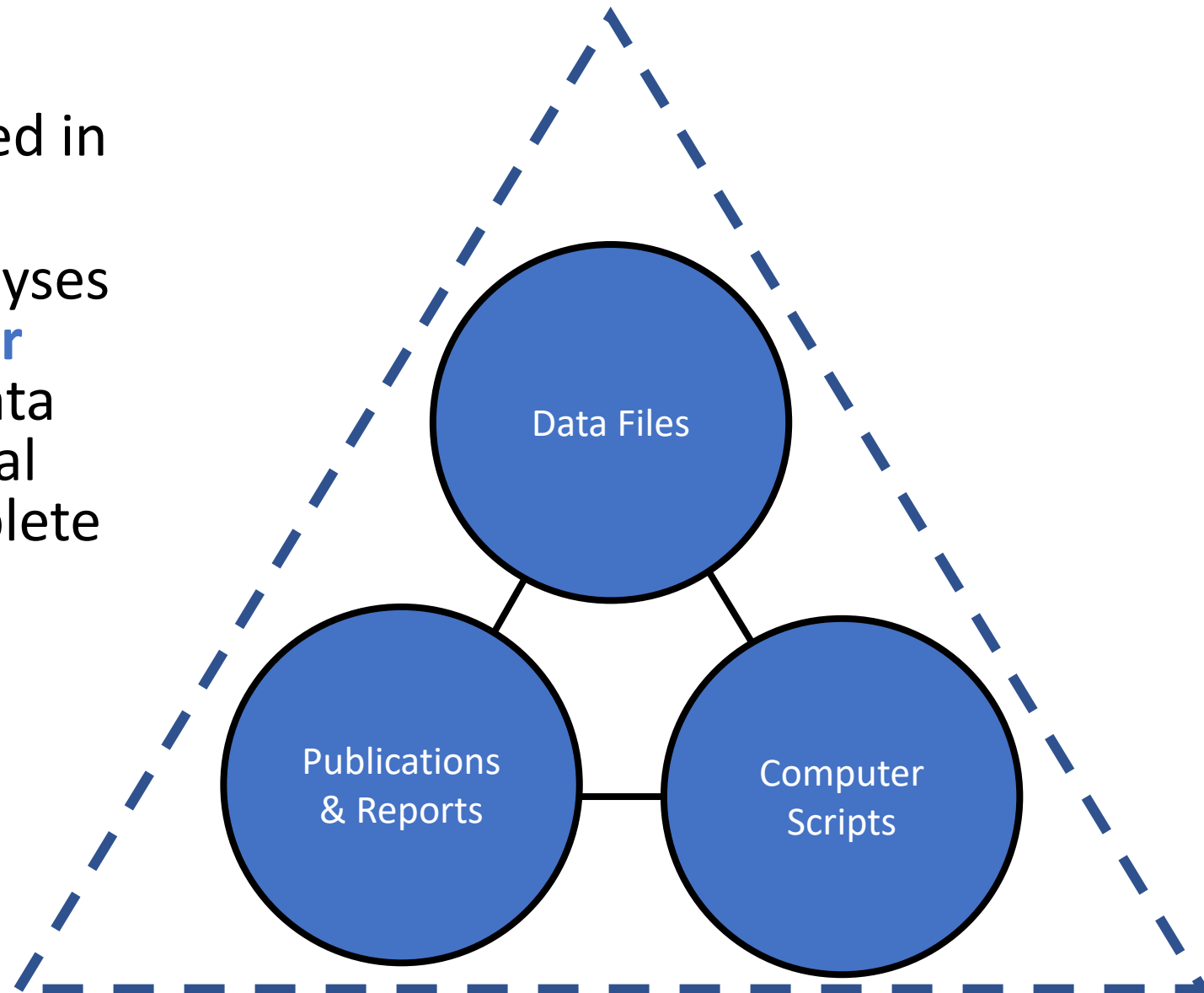
If you so choose, I will show you the philosophy of data science

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



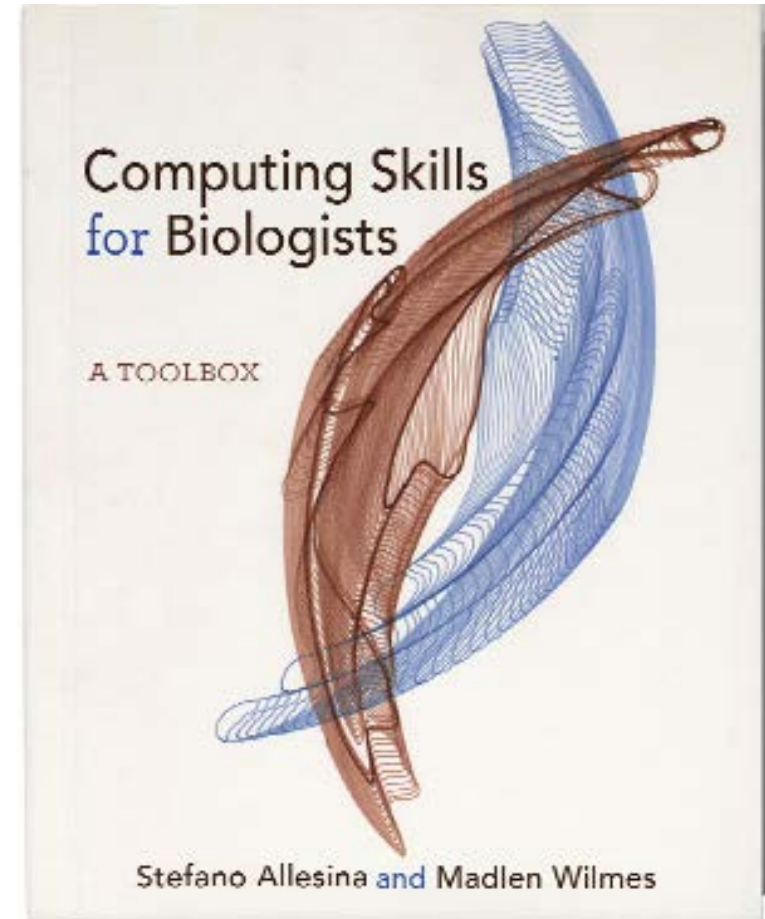
Philosophy of Data Science

- 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 Will Follow The CSB Text Book, Mostly

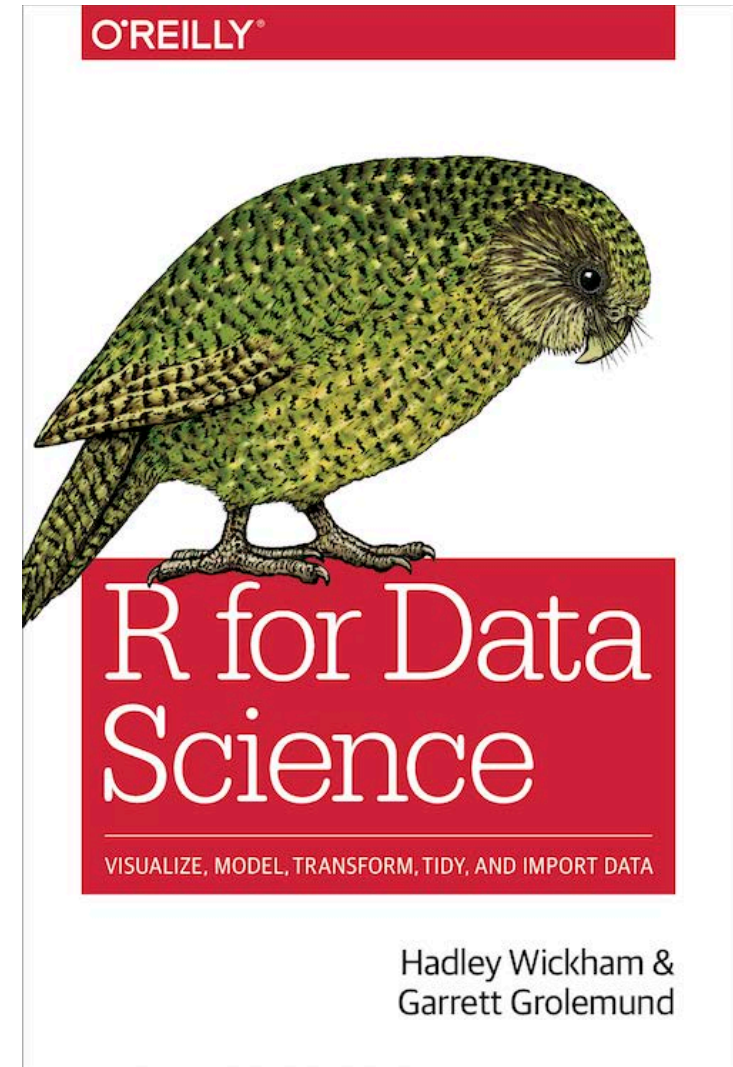
- Provides you with requisite breadth of tools at the expense of depth
- Showcase of Linux, Python, R
- Organized into 10 chapters, theoretically 1 per lecture
- Goal is to flatten your learning curve



<https://computingskillsforbiologists.com/>

This Iteration of the Course Will Include More R Than the Last

- You will learn core principles of R that aren't taught in other courses that expect you to use R, just like last year's class
- Unlike last year's class, you will learn to use `'tidyverse'`, which was masterminded by the Author of the R for Data Science book, which is free.
 - This will be used to supplement the CSB book's cursory treatment of `'tidyverse'`



<https://r4ds.had.co.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
 - Unix, Python, R
- Additional skills
 - Version control with git
 - Typesetting with LaTeX, markdown

Undergraduates:

ACTIVITY	% of FINAL GRADE
Participation	15
Assignments	40
Exam 1	12.5
Exam 2	12.5
Final Exam	20

Graduates:

ACTIVITY	% of FINAL GRADE
Participation	10
Assignments	20
Exam 1	10
Exam 2	10
Final Project	50*

Lectures

- Environment for you to learn new concepts
- Hands-on with computers
- Power-point & github driven
 - On webex
- Independent exercises w/ MS Forms through GitHub

Assignments

- Generally due each week
 - See syllabus
- Scripts will be submitted through GitHub classroom
- For now, question-answer based work will be conducted with a MS Form “quiz”

Final Project (Graduate Students)

- Automate the processing and analysis of your 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
- 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

Questions?

Biological Data

Lecture 0.1

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

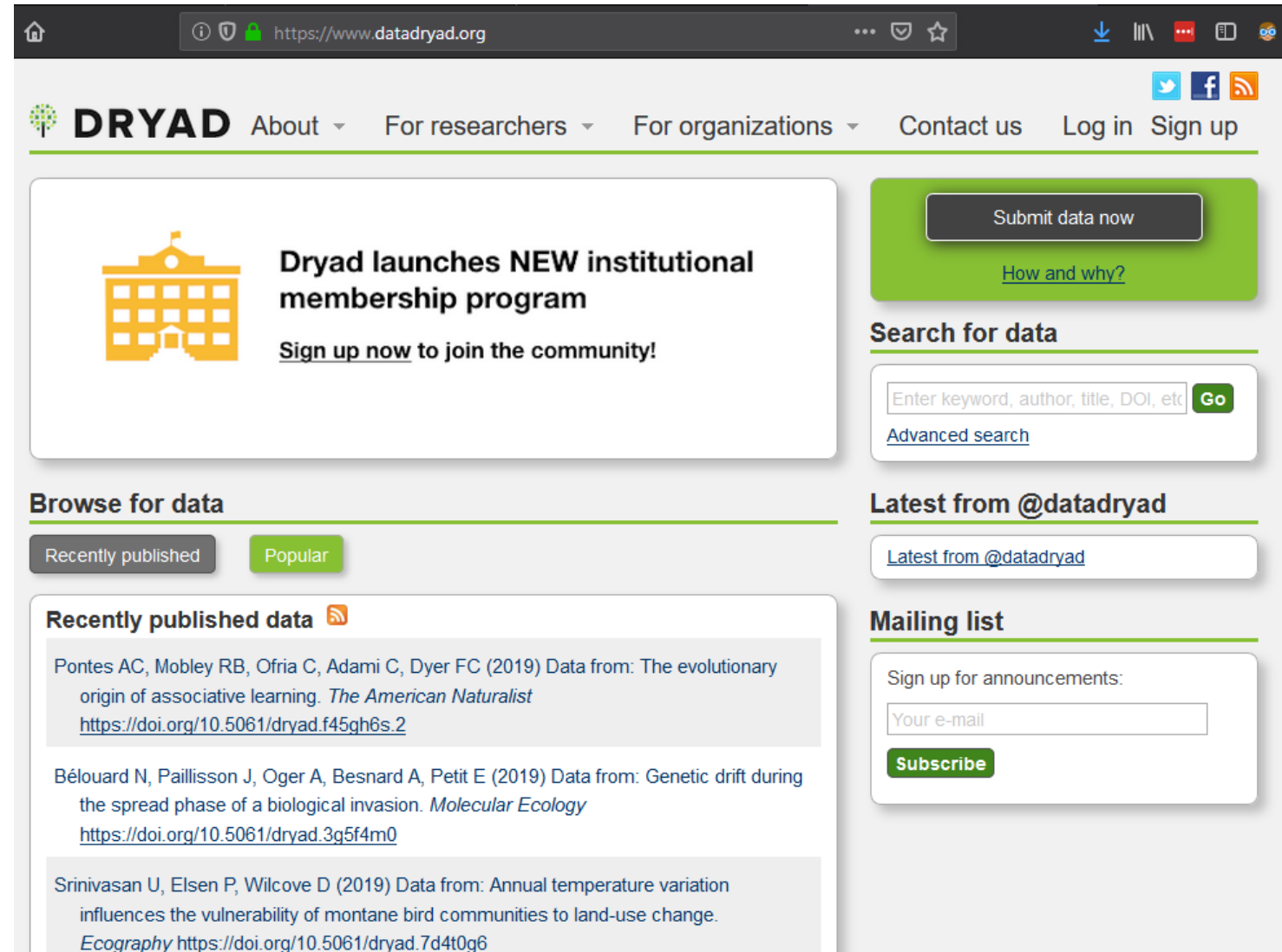
BIOLOGY'S BIG PROBLEM: THERE'S TOO MUCH DATA TO HANDLE



..and not enough biologists
with the motivation,
interest, and/or skill to
address the issue

Biological Data 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\(collection%20R%20non-collection\)&q=%3A*](https://data.usgs.gov/datacatalog/#fq=dataType%3A(collection%20R%20non-collection)&q=%3A*)
- Oceanographic
 - <https://data.noaa.gov/datasetsearch/>
- Too many to list



The screenshot shows the Dryad website homepage. The browser address bar displays <https://www.datadryad.org>. The website features a navigation bar with links for 'About', 'For researchers', 'For organizations', 'Contact us', 'Log in', and 'Sign up'. A prominent green button labeled 'Submit data now' is accompanied by a link 'How and why?'. A central announcement states 'Dryad launches NEW institutional membership program' with a 'Sign up now' link. Below this, a 'Browse for data' section offers 'Recently published' and 'Popular' filters. The 'Recently published data' section lists three entries with their titles and DOIs. On the right, there is a 'Search for data' box with a 'Go' button and a link to 'Advanced search'. Below that, a 'Latest from @datadryad' section shows a link to the latest tweets. At the bottom right, a 'Mailing list' section includes a sign-up form for announcements and a 'Subscribe' button.

DRYAD About ▾ For researchers ▾ For organizations ▾ Contact us Log in Sign up

Dryad launches NEW institutional membership program
Sign up now to join the community!

Submit data now
[How and why?](#)

Search for data
Enter keyword, author, title, DOI, etc **Go**
[Advanced search](#)

Browse for data
Recently published Popular

Recently published data

- Pontes AC, Mobley RB, Ofria C, Adami C, Dyer FC (2019) Data from: The evolutionary origin of associative learning. *The American Naturalist*
<https://doi.org/10.5061/dryad.f45gh6s.2>
- Bélouard N, Paillisson J, Oger A, Besnard A, Petit E (2019) Data from: Genetic drift during the spread phase of a biological invasion. *Molecular Ecology*
<https://doi.org/10.5061/dryad.3g5f4m0>
- Srinivasan U, Elsen P, Wilcove D (2019) Data from: Annual temperature variation influences the vulnerability of montane bird communities to land-use change. *Ecography* <https://doi.org/10.5061/dryad.7d4t0g6>

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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>

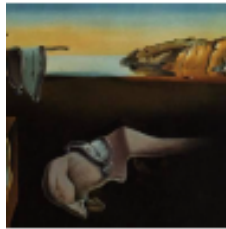


Files in this package

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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 loss and female reproduction.xlsx (36.79 Kb)
Details	View File Details

Tidy Data ([Wickham 2014](#))



Journal of Statistical Software

August 2014, Volume 59, Issue 10.

<http://www.jstatsoft.org/>

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

Tidy Data

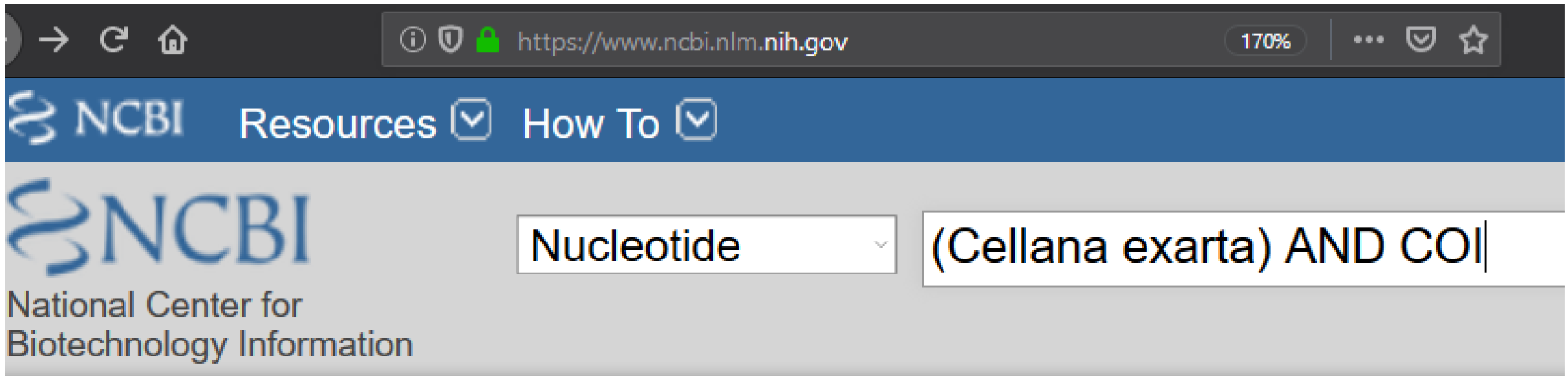
Hadley Wickham
RStudio

Abstract

A huge amount of effort is spent cleaning data to get it ready for analysis, but there has been little research on how to make data cleaning as easy and effective as possible. This paper tackles a small, but important, component of data cleaning: data tidying. Tidy datasets are easy to manipulate, model and visualize, and have a specific structure: each variable is a column, each observation is a row, and each type of observational unit is a table. This framework makes it easy to tidy messy datasets because only a small set of tools are needed to deal with a wide range of un-tidy datasets. This structure also makes it easier to develop tidy tools for data analysis, tools that both input and output tidy datasets. The advantages of a consistent data structure and matching tools are demonstrated with a case study free from mundane data manipulation chores.

Common Data Formats & Structures are Not Always Tidy

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



The screenshot shows the NCBI (National Center for Biotechnology Information) website. The browser's address bar displays the URL <https://www.ncbi.nlm.nih.gov/> with a 170% zoom level. The NCBI logo and navigation links "Resources" and "How To" are visible. The search interface includes a dropdown menu set to "Nucleotide" and a search box containing the query "(Cellana exarta) AND COI".

GenBank Supports Several Formats, None Are Tidy

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

NCBI Resources ☒ How To ☒

Nucleotide

Nucleotide (Cellana exarta) AND COI

Create alert Advanced

Species Summary 20 per page Sort by Default order

Animals (1,300) Customize ...

Molecule types

genomic

DNA/RNA (1,300) Customize ...

Source databases

Format

- ☒ Summary
- ☐ GenBank
- ☐ GenBank (full)
- ☐ FASTA
- ☐ FASTA (text)
- ☐ ASN.1
- ☐ Revision History
- ☐ Accession List
- ☐ GI List

Send to

306

<< First < Prev Page 1 of 66 Next > La

The following term was not found in Nucleotide: exarta.

```
>AB263731.1 Cellana radiata enneagona mitochondrial COI gene for cytochrome c
oxidase subunit I, partial cds, specimen voucher: NUGB-L694 (Nagoya University)
TACATTATACATTATTATAGGAGTTTGATCTGGATTGGCAGGTACTGGTTAAGTATGTTAATTCGGGCT
GAATTAGGTCAACCTGGTCTTTGCTAGGAGATGATCAGCTATATAACGTGATTGTTACTGCGCAGCCTT
TTGTTATGATTTTCTTTTAGTAATACCAATGATAATTGGGGGTTTGGAAATTGGTTGGTTCCTCTTAT
ACTTGGGGCTCCAGATATGGCTTTTCCTCGTTTAAATAATATGAGGTTTGGTTACTGGTTCCTCTTTA
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CTAGAAATGTGGCCCATTCCTGGTCTTCTGTTGATTGGCTATTTTCTCTTCATTGGCTGGTATTTTC
TTCAATTCTTGGGGCTGTTAATTTTATTACTACAGTGGTAAACATTTCGTTGGCGAGGTCTTCAGTTTGAA
CGGCTACCTTTGTTTGTATGATCTGTTAAGATTACAGCTATTTTACTTCTTCTTCTCTCTCTGTGTGG
CTGGGGCTATTACTATGCTTTTAACTGACCGTAATTTTAATACCTGTTTTTTGACCTGGAGGAGGAGG
GGACCCCATTTTATATCAACATTGTTT
```

```
>AB263730.1 Cellana radiata enneagona mitochondrial COI gene for cytochrome c
oxidase subunit I, partial cds, specimen voucher: NUGB-L693 (Nagoya University)
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```

```
>AB263729.1 Cellana radiata enneagona mitochondrial COI gene for cytochrome c
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```

```
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TTCAATTCTTGGGGCTGTTAATTTTATTACTACAGTGGTAAACATTTCGTTGGCGAGGTCTTCAGTTTGAA
CGTCTACCTTTGTTTGTATGATCTGTTAAGATTACAGCTATTTTACTTCTTCTTCTCTCTCTGTGTGG
CTGGGGCTATTACTATGCTTTTAACTGACCGTAATTTTAATACCTGTTTTTTGACCTGGAGGAGGAGG
GGACCCCATTTTATATCAACATTGTTT
```

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 begin 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)
TACATTATACATTATTATAGGAGTTTGATCTGGATTGGCAGGTACTGGTTTAAAGTATGTTAATTCGGGCT
GAATTAGGTCAACCTGGTTCCTTGCTAGGAGATGATCAGCTATATAACGTGATTGTTACTGCGCACGCTT
TTGTTATGATTTTCTTTTAGTAATAACCAATGATAATTGGGGGTTTGGAAATTGGTTGGTTCCTCTTAT
ACTTGGGGCTCCAGATATGGCTTTTCCTCGTTTAAATAATATGAGGTTTGGTTACTGGTTCCTTCTTTA
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CTAGAAATGTGGCCCATTCCTGGTCTTCTGTTGATTGGCTATTTTTCTCTTCATTGGCTGGTATTTTC
TTCAATTCTTGGGGCTGTTAATTTTATTACTACAGTGGTAAACATTTCGTTGGCGAGGTCTTCAGTTTGAA
CGGCTACCTTTGTTTGATGATCTGTTAAGATTACAGCTATTTTACTTCTTCTTCTCTTCTGTGTTGG
CTGGGGCTATTACTATGCTTTTAACTGACCGTAATTTTAAACCTGTTTTTTTGACCCTGGAGGAGGAGG
GGACCCCATTTTATATCAACATTTGTTT
```

```
>AB263730.1 Cellana radiata enneagona mitochondrial COI gene for cytochrome c
oxidase subunit I, partial cds, specimen_voucher: NUGB-L693 (Nagoya University)
TACATTATACATTATTATAGGAGTTTGATCTGGATTGGCAGGTACTGGTTTAAAGTATGTTAATTCGGGCT
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CTGGGGCTATTACTATGCTTTTAACTGACCGTAATTTTAAACCTGTTTTTTTGACCCTGGAGGAGGAGG
GGACCCCATTTTATATCAACATTTGTTT
```

```
>AB263729.1 Cellana radiata enneagona mitochondrial COI gene for cytochrome c
oxidase subunit I, partial cds, specimen_voucher: NUGB-L692 (Nagoya University)
TACATTATACATTATTATAGGAGTTTGATCTGGATTGGCAGGTACTGGTTTAAAGTATGTTAATTCGGGCT
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TTCAATTCTTGGGGCTGTTAATTTTATTACTACAGTGGTAAACATTTCGTTGGCGAGGTCTTCAGTTTGAA
CGGCTACCTTTGTTTGATGATCTGTTAAGATTACAGCTATTTTACTTCTTCTTCTCTTCTGTGTTGG
CTGGGGCTATTACTATGCTTTTAACTGACCGTAATTTTAAACCTGTTTTTTTGACCCTGGAGGAGGAGG
GGACCCCATTTTATATCAACATTTGTTT
```

```
>AB263728.1 Cellana radiata enneagona mitochondrial COI gene for cytochrome c
oxidase subunit I, partial cds, specimen_voucher: NUGB-L691 (Nagoya University)
TACATTATACATTATTATAGGAGTTTGATCTGGATTGGCAGGTACTGGTTTAAAGTATGTTAATTCGGGCT
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TTGTTATGATTTTCTTTTAGTAATAACCAATGATAATTGGGGGTTTGGAAATTGGTTGGTTCCTCTTAT
ACTTGGGGCTCCAGATATGGCTTTTCCTCGTTTAAATAATATGAGGTTTGGTTACTGGTTCCTTCTTTA
TTTTTACTTCTTGCTTCTTCTGCTGTTGAAAGAGGAGTAGGTACAGGTTGGACAGTATACCCCCCTCTTT
CTAGAAATGTGGCCCATTCCTGGTCTTCTGTTGATTGGCTATTTTTCTCTTCATTGGCTGGTATTTTC
TTCAATTCTTGGGGCTGTTAATTTTATTACTACAGTGGTAAACATTTCGTTGGCGAGGTCTTCAGTTTGAA
CGTCTACCTTTGTTTGATGATCTGTTAAGATTACAGCTATTTTACTTCTTCTTCTCTTCTGTGTTGG
CTGGGGCTATTACTATGCTTTTAACTGACCGTAATTTTAAACCTGTTTTTTTGACCCTGGAGGAGGAGG
GGACCCCATTTTATATCAACATTTGTTT
```


Data Formats

- I will emphasize Tidy format
- Many fields of Biology have their own particular 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 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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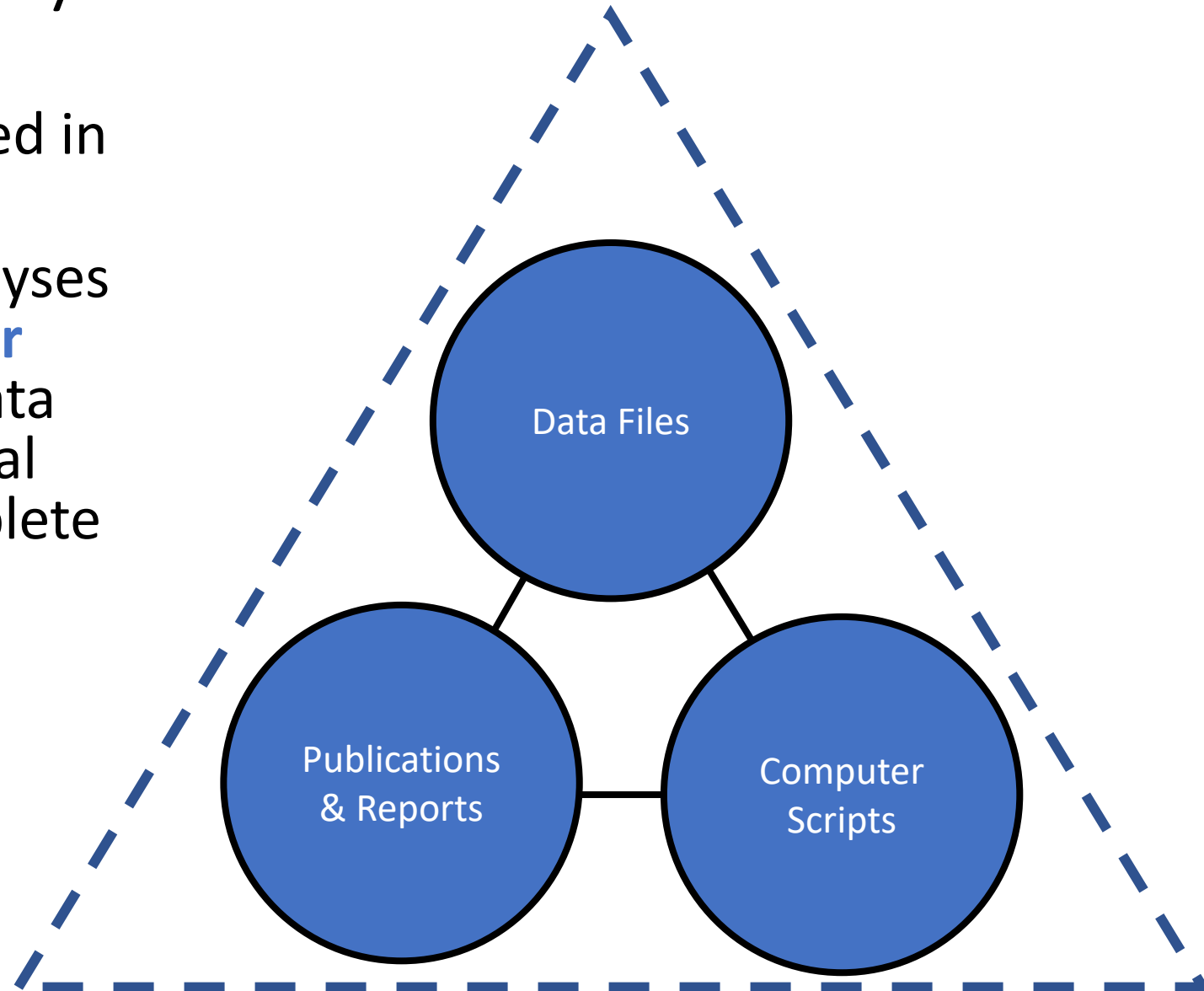
Title	Range extent for bird species
Downloaded	2 times
Description	This file contains the extents of occurrence (range filling) for 1205 Neotropical bird species.
Download	SM1 Metabirds.xls (2.937 Mb)
Download	README.txt (677 bytes)
Details	View File Details

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**

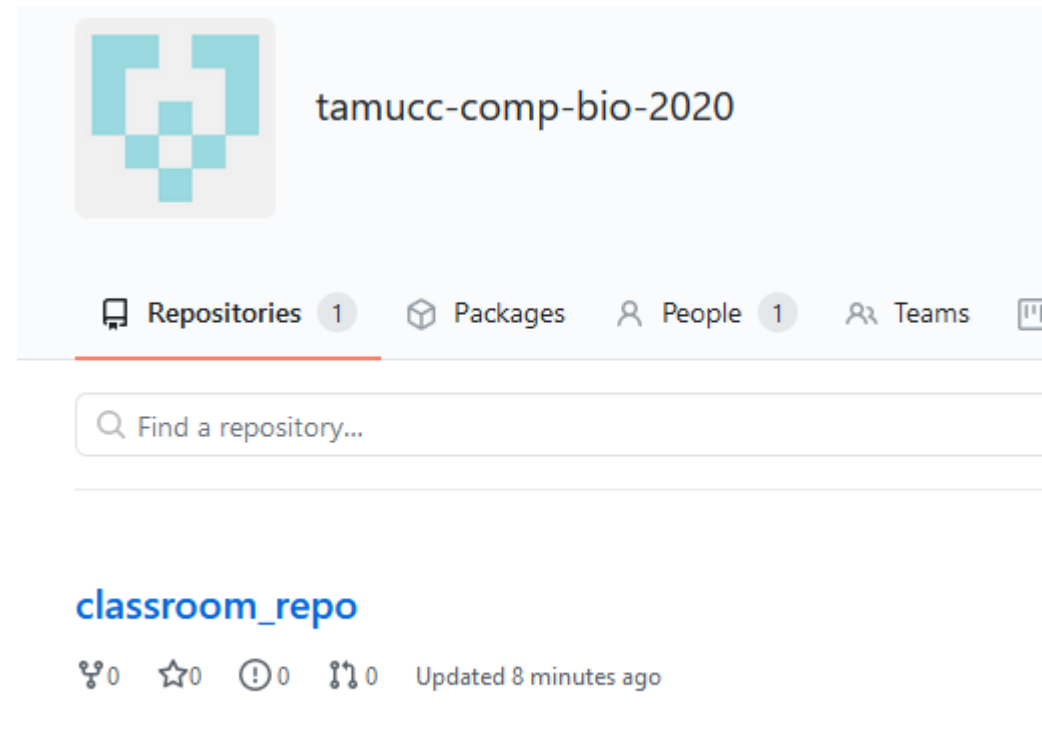




GitHub – A Repository of Sorts

- 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/tamucc-comp-bio-2020>



Conceptual Diagram of a GitHub Organization

