

Welcome to **BILD62**

Dr. Juavinett
jah-vah-nett
(or, Dr. J)



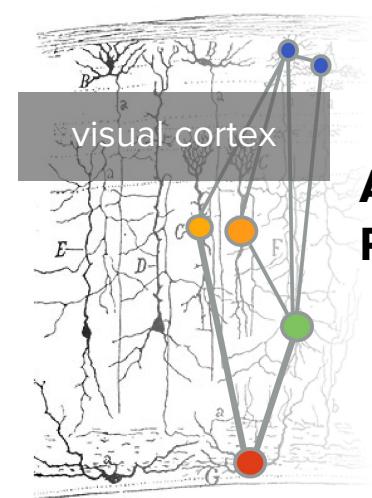
Image: [garetsworkshop/Shutterstock](#)

Objectives for today

- Introduce the teaching staff, students, and class
 - Motivate learning how to code as a biology student
 - Discuss course logistics, expectations, & tools
 - Start coding!
-

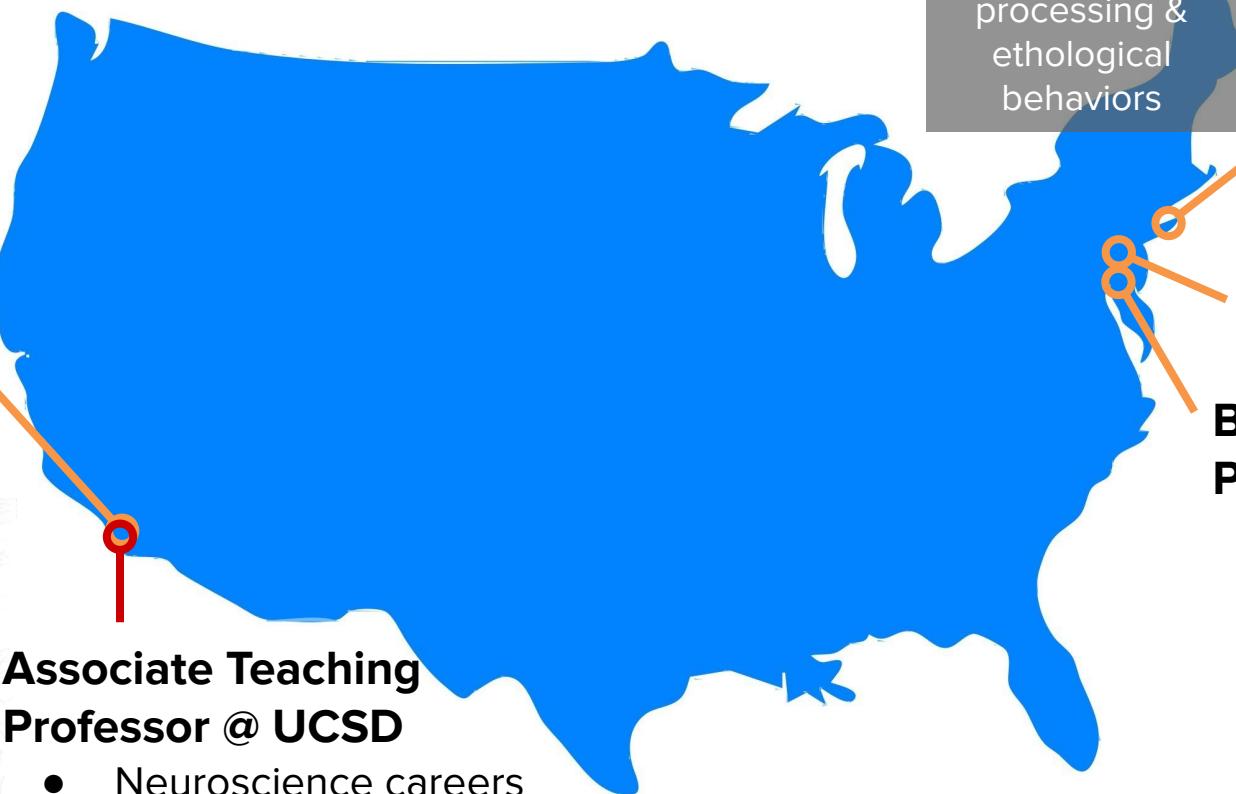


PhD in
Neuroscience
@ UCSD



Associate Teaching Professor @ UCSD

- Neuroscience careers & education
- Open-source data

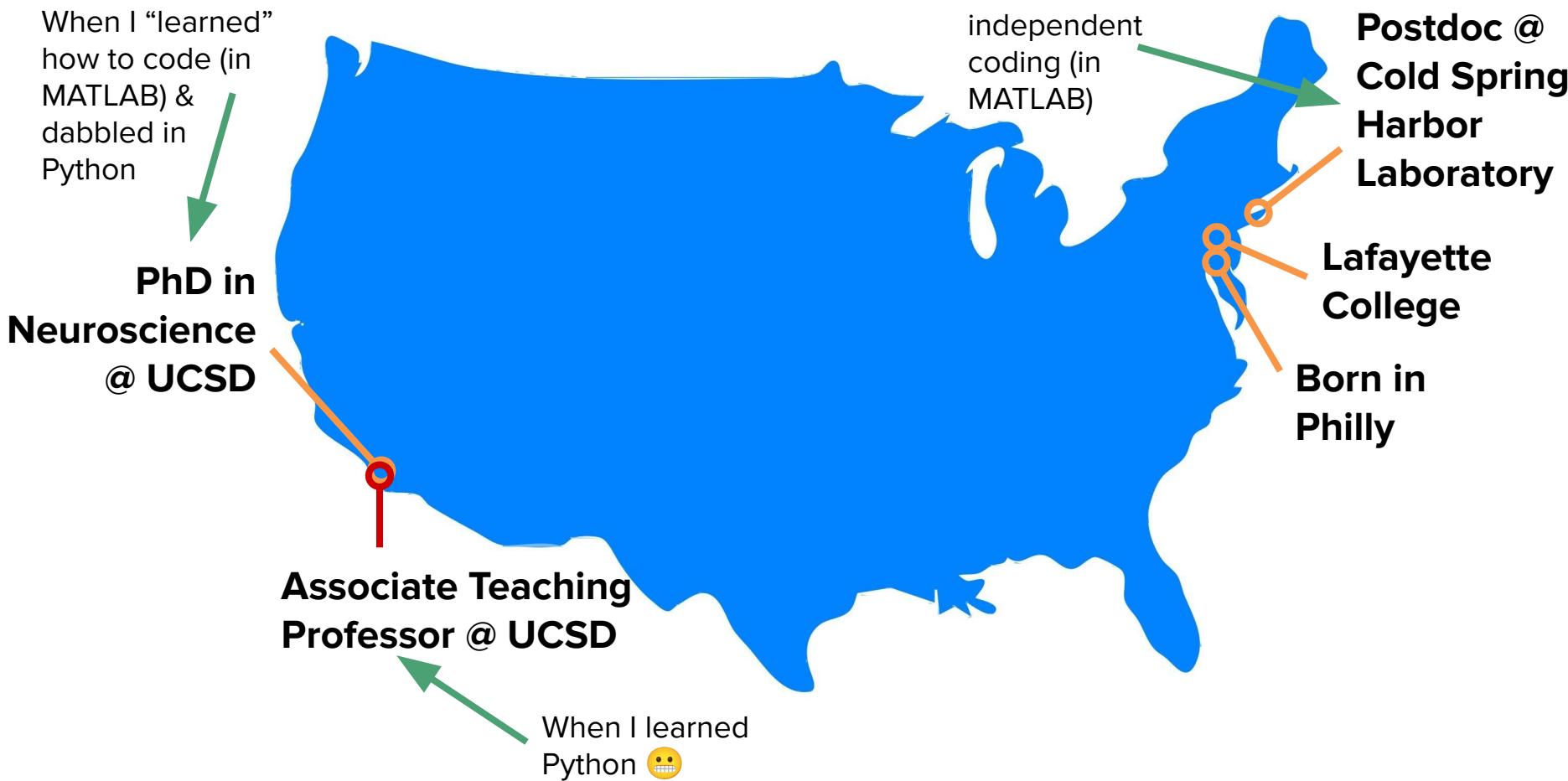


multisensory
processing &
ethological
behaviors

**Postdoc @
Cold Spring
Harbor
Laboratory**

Lafayette
College

Born in
Philly



Introduction to our teaching staff!



Abhishek Gupta
a8gupta@ucsd.edu



Marina Hu
mlhu@ucsd.edu

Let's be human,
for just a second.

With the folks next to you,
share:

- Your name, major, and preferred pronouns
- Something that brought you joy over the break
- Why you're taking this course



Objectives for today

- Introduce the teaching staff, students, and class
 - **Motivate learning how to code as a biology student**
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-

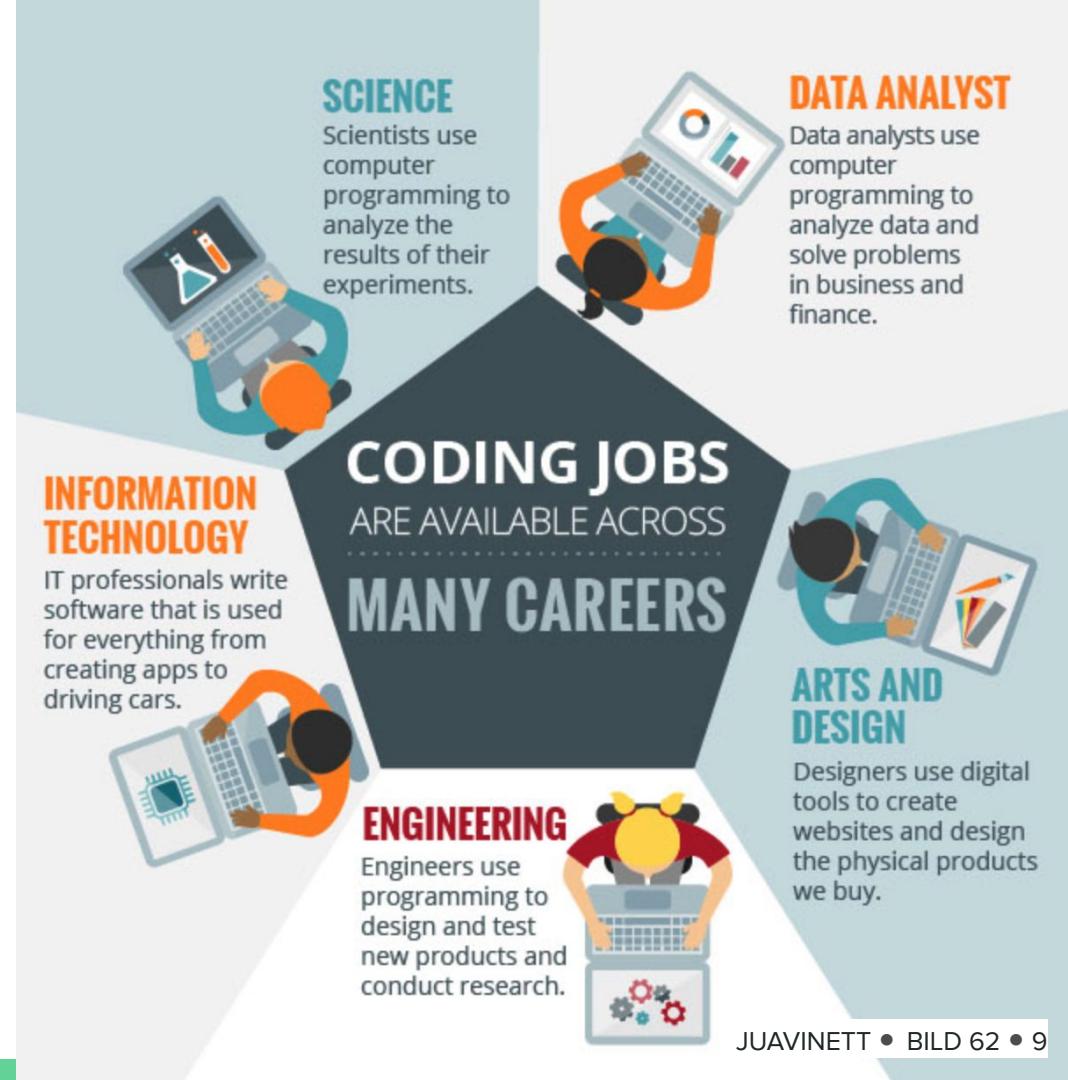
What does coding have to
do with *biology*?

Why *you*, right now?



Why should I learn how to code?

- Coding is useful for:
 - Data acquisition (controlling hardware, image acquisition, etc)
 - Data analysis & visualization
 - Computational modeling
- Beyond research, there are more and more jobs for software engineers, and they pay well
(see report by Burning Glass:
<https://www.burning-glass.com/research-project/coding-skills/>)

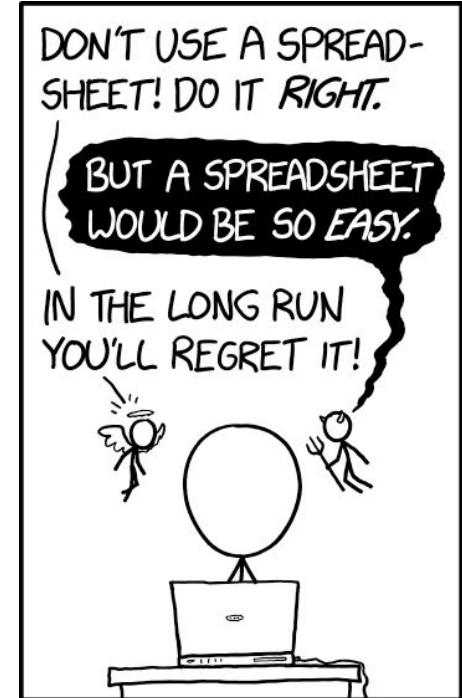


Excel can only handle datasets with **“1 million rows, and 16,000 columns** — many datasets in biology are much larger than this!

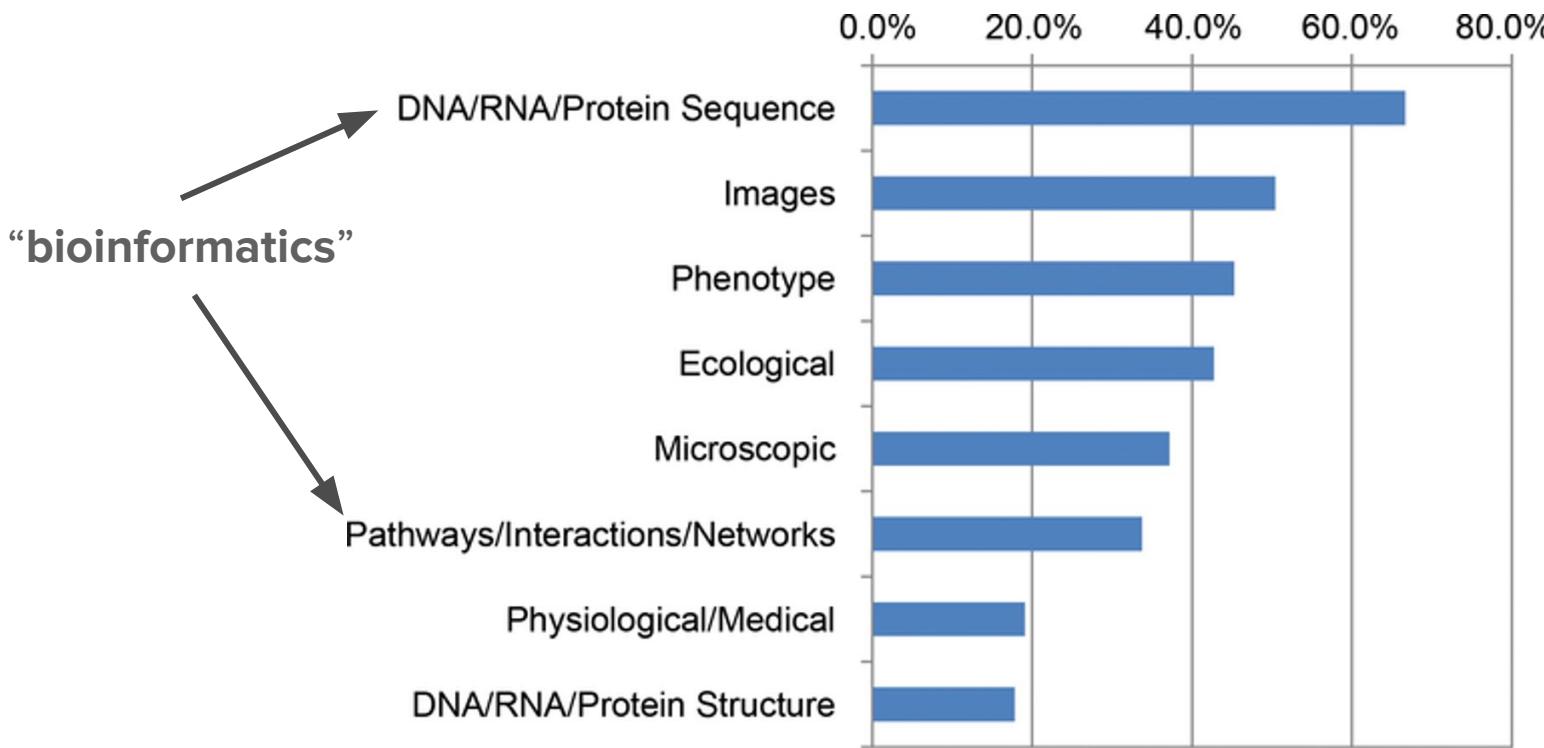
You can automate analyses in Excel, but this is quite limited.

There are also specialized biological data analysis software programs, but often these are limited in how much they can be customized.

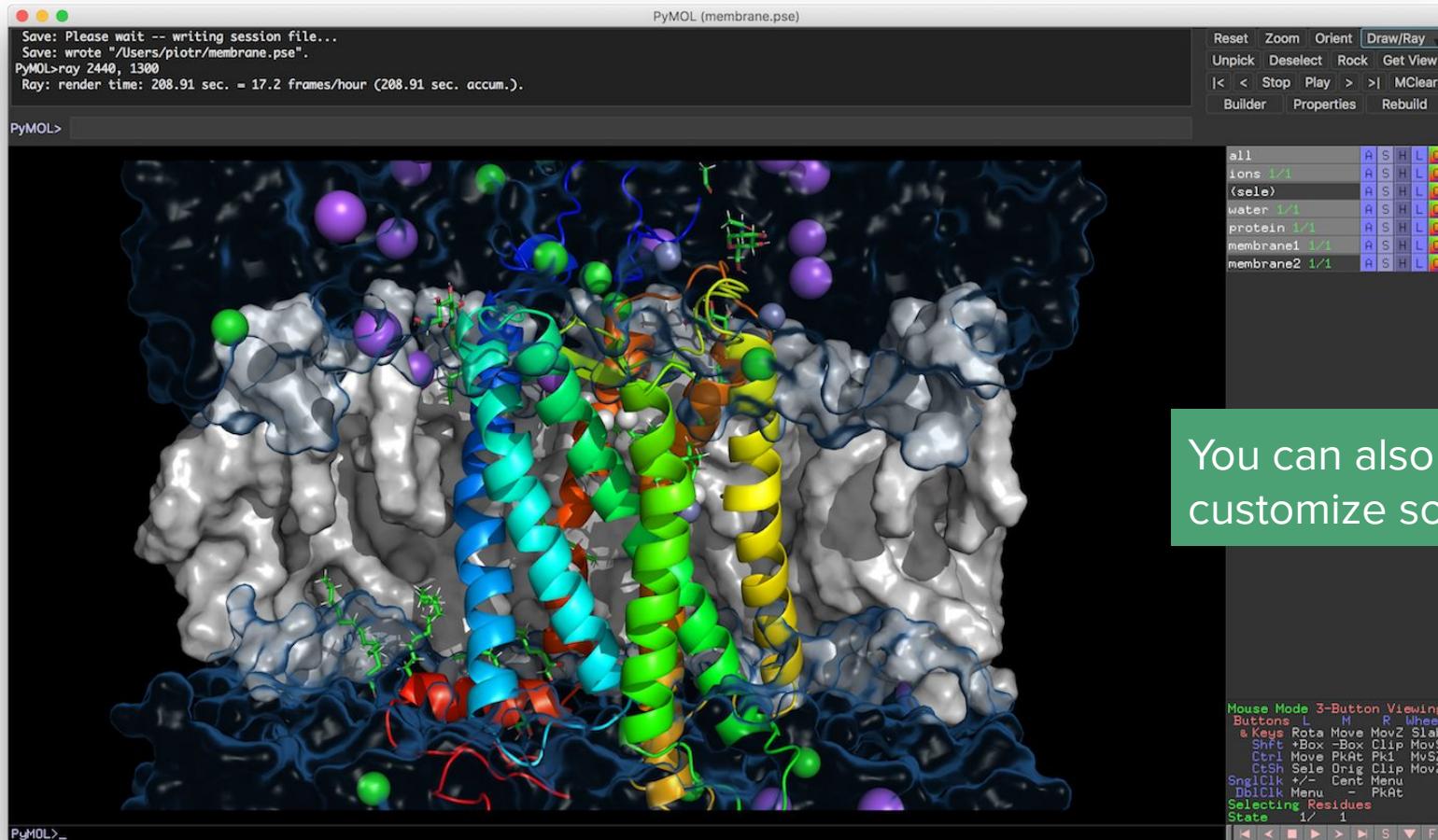
Code is *infinitely* customizable.



<https://xkcd.com/2180/>



Major data types used by National Science Foundation (NSF)
Biological Sciences Directorate principal investigators (PIs).



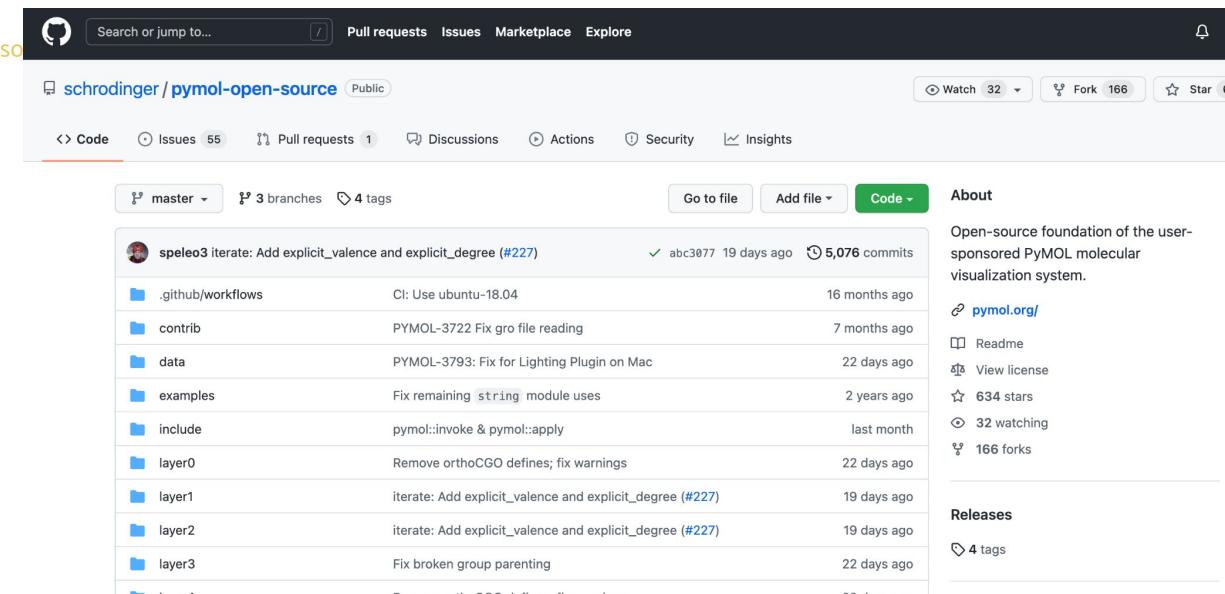
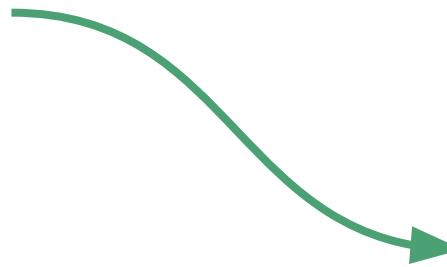
Open-Source Philosophy

PyMOL is a commercial product, but we make most of its source code freely available under a permissive license. The open source project is maintained by [Schrödinger](#) and ultimately funded by everyone who purchases a PyMOL license.

Open source enables open science.
This was the vision of the original PyMOL author Warren L. DeLano.

[Visit the Open-Source Project](#)

[Become a sponsor](#)



The screenshot shows the GitHub repository page for `schrodinger/pymol-open-source`. The repository is public and has 5,076 commits. The main page displays a list of recent commits, including:

- speleo3 iterate: Add explicit_valence and explicit_degree (#227) - 19 days ago
- .github/workflows CI: Use ubuntu-18.04 - 16 months ago
- contrib PYMOL-3722 Fix gro file reading - 7 months ago
- data PYMOL-3793: Fix for Lighting Plugin on Mac - 22 days ago
- examples Fix remaining string module uses - 2 years ago
- include pymol::invoke & pymol::apply - last month
- layer0 Remove orthoCGO defines; fix warnings - 22 days ago
- layer1 iterate: Add explicit_valence and explicit_degree (#227) - 19 days ago
- layer2 iterate: Add explicit_valence and explicit_degree (#227) - 19 days ago
- layer3 Fix broken group parenting - 22 days ago

On the right side of the page, there are sections for **About**, **Releases**, and **Code**. The **About** section describes it as the open-source foundation of the user-sponsored PyMOL molecular visualization system. The **Releases** section shows 4 tags. The **Code** section includes links for Go to file, Add file, and Code.

AND many software packages for biologists can be modified... if you know how to code!

By taking this class, you're ahead of the game!

Many researchers learn to code really informally, and relatively late in their careers



ashley, ahem, dr. juavinett
@analog_ashley



Neuroscientists of Twitter, when did you learn* how to code?

*Let's say, when you felt reasonably capable writing your own simple code (e.g. reading data and plotting, or communicating with an Arduino)

19% High school or earlier

30% College

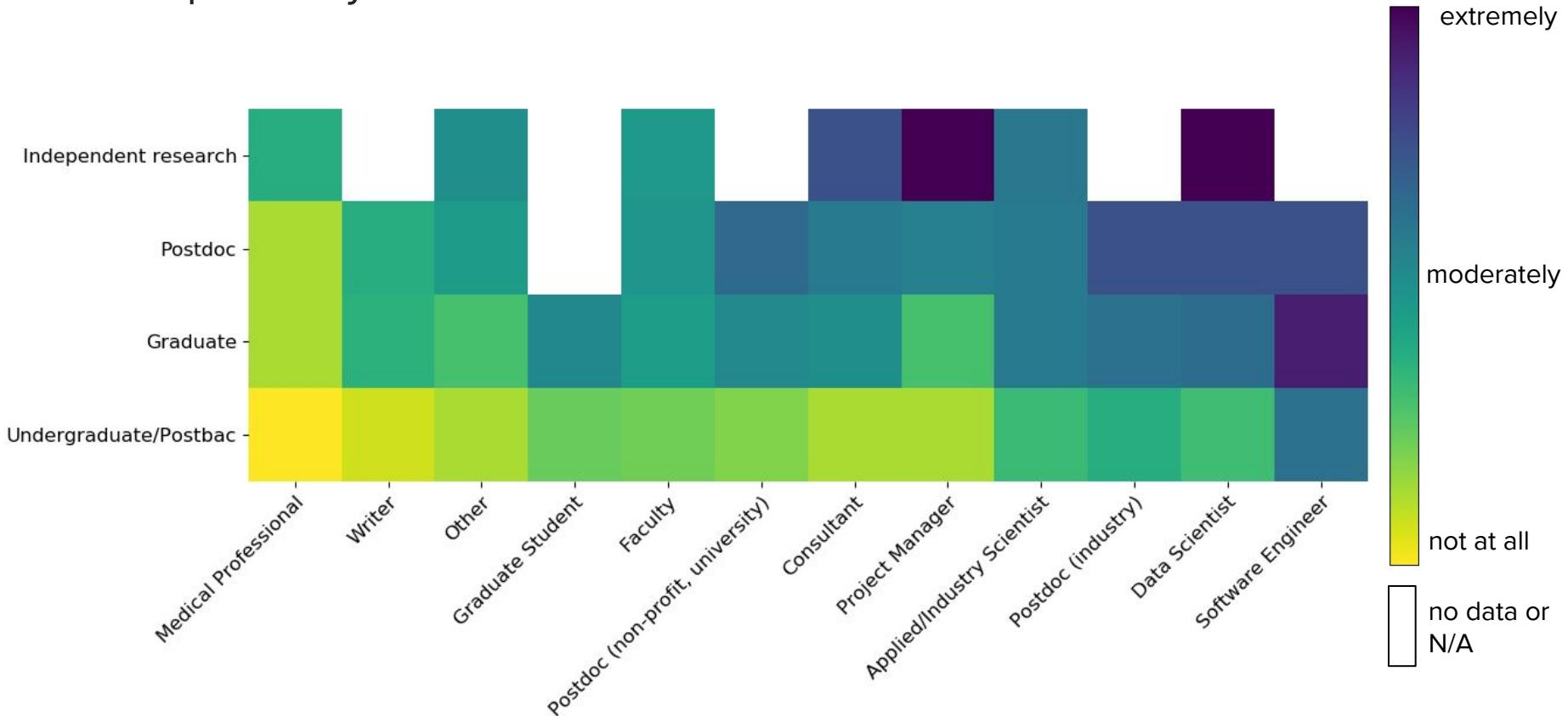
36% Graduate school

15% After graduate school

313 votes • Final results

+ many comments that they *still* hadn't learned how, and wanted to!

How comfortable did/do you feel working with code at this point in your career?



Objectives for this morning

- Introduce the teaching staff, students, and class
- Motivate learning how to code as a biology student
- **Discuss course logistics, expectations, & tools**
- Start coding!

First step: let's drop our ideas of what it means to be a *coder*.

Programming, like learning a language, *takes time*.



Your language brain matters more for learning programming than your math brain

New research contradicts long held assumptions about coding



Amy Nippert

Neuroscience

University of Minnesota

May 12, 2020



2 peer comments



Christina Morillo on Wikimedia Commons.

<https://massivesci.com/articles/programming-math-language-python-women-in-science/>,
summarizes this article: <https://www.nature.com/articles/s41598-020-60661-8>

Previous studies have shown that math and logic problems seem to rely mainly on the multiple demand regions in the left hemisphere, while tasks that involve spatial navigation activate the right hemisphere more than the left. The MIT team found that reading computer code appears to activate both the left and right sides of the multiple demand network, and ScratchJr activated the right side slightly more than the left. This finding goes against the hypothesis that math and coding rely on the same brain mechanisms.

<https://news.mit.edu/2020/brain-reading-computer-code-1215>
about this study: <https://elifesciences.org/articles/58906>

What will help you succeed in this course?

Things that predict success:

- How successful you *think* you'll be
- Completing assignments on time
- Asking questions when you have them
- Attending discussion sections & office hours

Things that **do not** predict success:

- Gender
- Age
- Personality
- Math ability



29A



@StuxnetStudios · 14h



New programming student:

"I'm not very good at this. When I type out the code, I have to fix lots of errors. And I have to look up how to do most of it."

Instructor:

"You're doing it right."

29

275

1.4K



Historical sidenote: why is it called a bug?

In 1947, computer scientist & legend **Grace Hopper** found a *literal* bug in their computer, causing it to produce many errors.



Interview with Grace Hopper:
<https://www.youtube.com/watch?v=QA33wW5LaNY>

Photo # NH 96566-KN (Color) First Computer "Bug", 1947

92	
9/9	
0 800	Anton started
1 000	stopped - Anton ✓
	13' UC (032) MP - MC
	(033) PRO 2
	cosack
	{ 1.2700 9.037 847 025 9.037 846 995 cosack
	2.130476415 (23) 4.615925059 (-)
	2.130476415
	Relays 6-2 in 033 failed several speed test
	in relay " 10.00 test .
1 100	Relays changed
1 525	Started Cosine Tape (Sine check) Started Mult + Adder Test.
1 545	Relay #70 Panel F (moth) in relay.
1 600	First actual case of bug being found.
1 700	Closed down .

<https://www.nationalgeographic.org>thisday/sep9/worlds-first-computer-bug/>

What is programming, anyway?

- Programming is the way humans communicate with **computers**
 - It's a language!



Wait, what's a computer?

Hardware: the physical parts of the computer (CPU, hard drive, etc.)

Memory:

Primary: fast, temporary storage

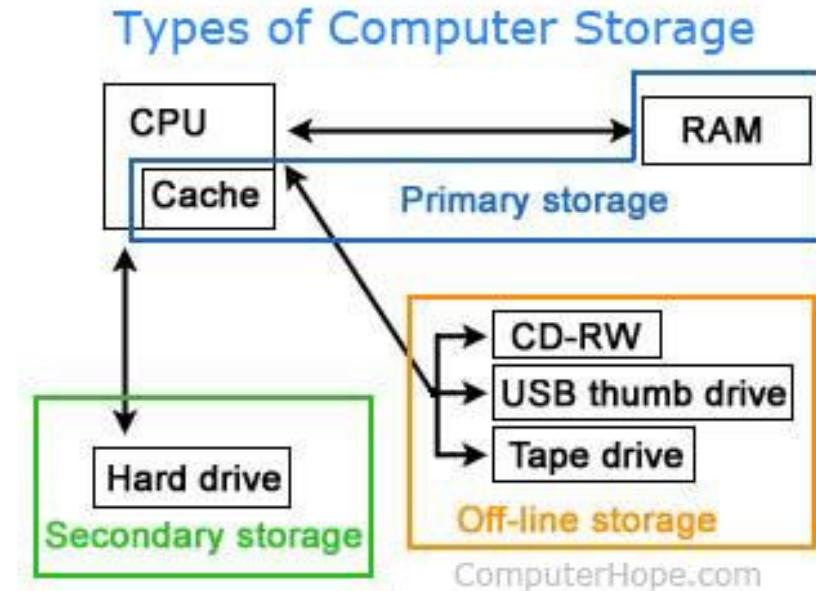
Secondary: slower, long-term storage

Tertiary: cloud storage

All computer memory is stored in **binary**.

[More information about memory](#)

[Great explainer about binary memory](#)



Wait, what's a computer? (continued)

Interface: software, the operating system,
what you see

File structure

cats = files

Each has their own name.

boxes = folders/directories

Where you store the cats.

You can put a box into another box,
but you can't put a box into a cat.

This is a copy
of a cat, *not*
an actual cat



What is programming, anyway?

- Programming is the way humans communicate with computers
 - It's a language!
- The instructions we give the computer are taken **literally** and **sequentially**

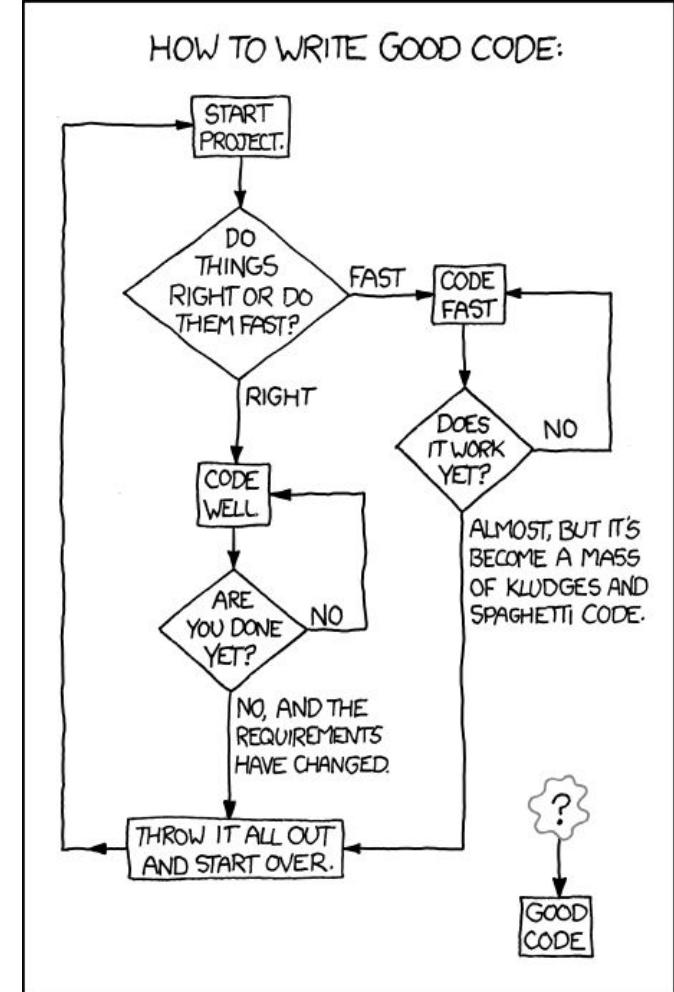
Capitalization matters:
print() ≠ **Print()**

b = a * 2
a = 2

computer: what is a?

The path to writing good, efficient code

1. Make it **work**
2. Make it **right**
3. Make it **fast**



XKCD, <https://xkcd.com/844/>

The path to writing good, efficient code

1. Make it **work**
2. Make it **right**
3. Make it **fast**

Our goal is to get to this step

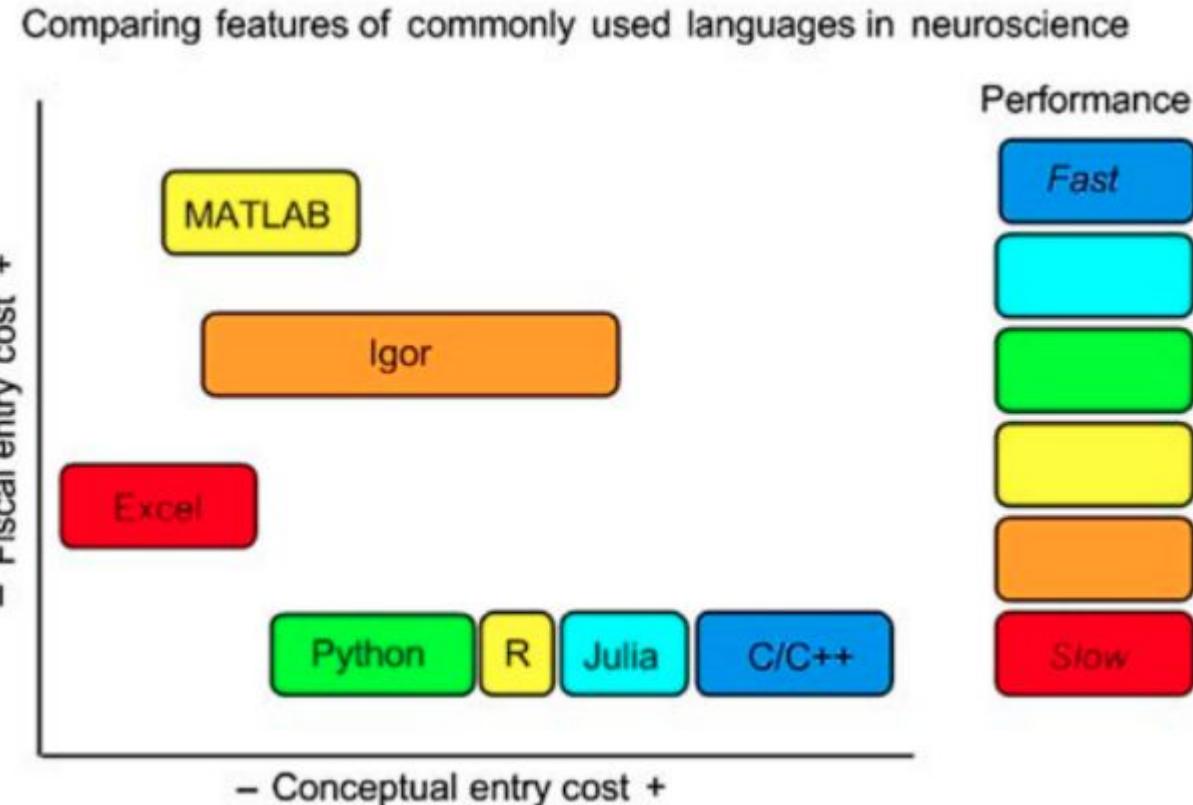
If you ultimately became a ***full-time, professional developer***,
you'd care about step 3.

For most problems biologists face,
step 3 isn't paramount.



Considerations for choosing a programming language

- Fiscal & conceptual entry
- Usage in particular field or profession



From Wallisch (2017)

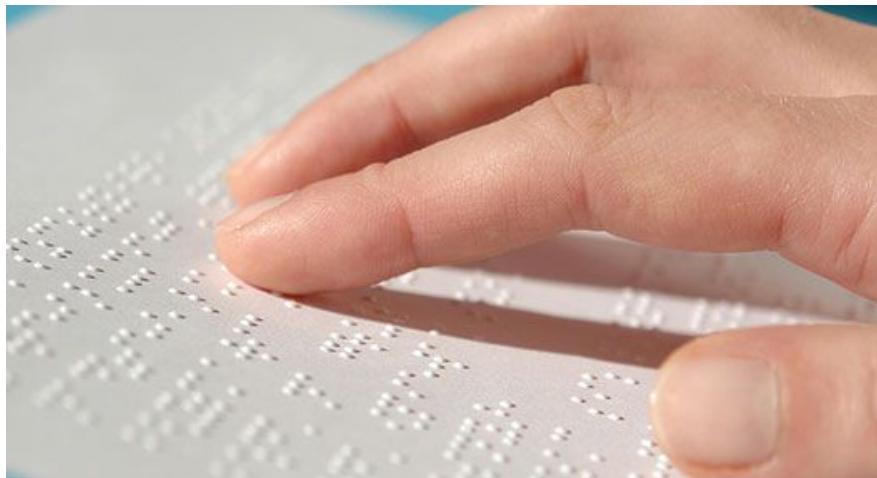
All coding languages eventually need to talk to the computer in binary:

01001000 01100101 01101100 01101100 01101111 00100001

(hello)

[Learn How To Write Your Name In Binary Code](#)

There are many types of binary code, beyond computers



Braille

<https://www.afb.org/blindness-and-low-vision/braille/what-braille>

A • -	J • - - -	S • • •
B - • • •	K - • -	T -
C - • - •	L • - • •	U • • -
D - • •	M --	V • • • -
E •	N - •	W • - -
F • • - •	O - - -	X - • • -
G - - •	P • - - •	Y - • - -
H • • • •	Q - - • -	Z - - • •
I • •	R • - -	

Morse code

https://www.discoveryworld.org/about/blog/discover_at_home/morse-code/

In this class, we'll use Python

- Programming language, development led by Python Software Foundation (www.python.org)
- Uses concise structure & wording similar to human language
- A “high-level language”



Assembly language vs. high-level language

```
section .text
global _start
_start:
    mov ecx, 10
    mov eax, '0'
    l1:
    mov [num], eax
    mov eax, 4
    mov ebx, 1
    push ecx
    mov ecx, num
    mov edx, 1
    int 0x80
    mov eax, [num]
    inc eax
    pop ecx
    loop l1
    mov eax, 1
    int 0x80
section .bss
    num resb 1
```

```
for num in range(10):
    print(num)
```

Inspired by Porter & Zingaro,

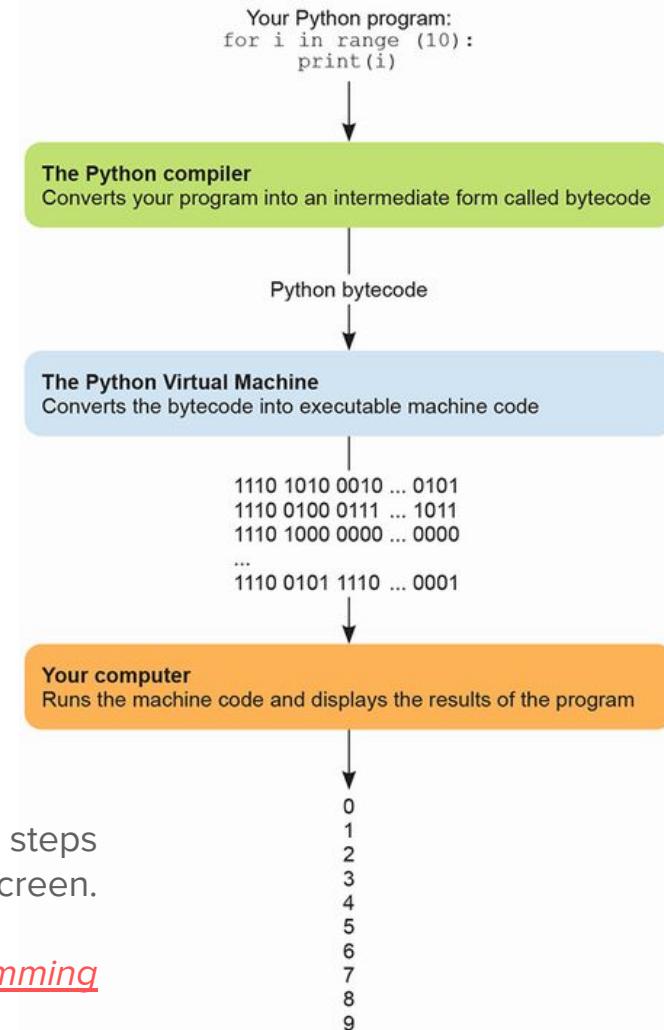
[Learn AI-Assisted Python Programming](#)

In this class, we'll use Python

- Python can be used for many purposes, from web programming, to creating games, to analyzing & visualizing data
 - Extension: '.py'
- We'll also work in **Jupyter Notebooks**
 - Extension '.ipynb'

Your Python program goes through several steps before you see the output on your screen.

From Porter & Zingaro, [Learn AI-Assisted Python Programming](#)



Course Objectives

- Read and run basic Python programs, recognizing the structures used and explaining how they work
- Manipulate and create objects in Python
- Write, edit, and execute Python code in Jupyter Notebooks as well as the command line
- Visualize and run hypothesis-testing on simple datasets in Python
- Implement common algorithms for analyzing biological data and determine when such computations are appropriate

And, we're going to do all of this in a world with AI assistants (i.e. chatGPT):

It's still important to be able to read Python code to gain an overall understanding of what it does.

Grading breakdown

In-class work & participation (15%)

Assignments (30%)

Quizzes (30%)

Final project (25%)

Assignments & project components

lose 10% each day they are late.

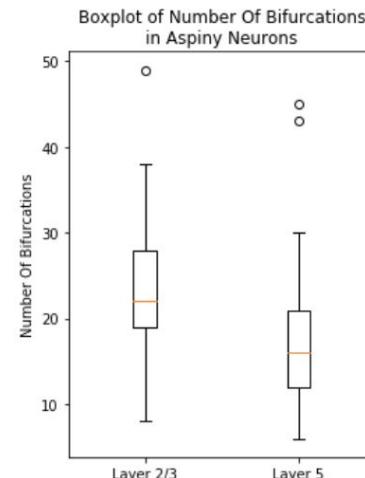
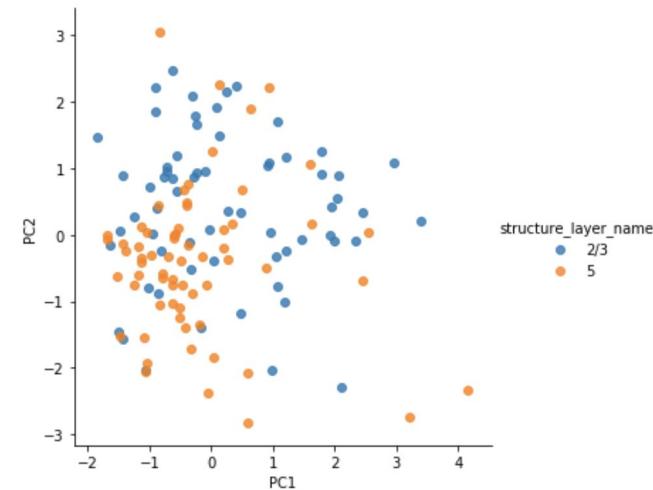


Assignments

- Due **every Friday at 5 pm**
- Worth 5% each
- Completed individually
- Programmatically graded (via Datahub/NBGrader)
- In discussion, you'll cover how to submit these. There are also written instructions on Canvas.

Project, groups of 2-3

- Includes the project proposal, code, and presentation.
- Your final project will either:
 - Write a program to complete a task
 - Analyze & visualize data of your choosing
- We will discuss possibilities for your project as we move through the course.



END OF YEAR SALE - SAVE 50%

0 1
Days0 6
Hours1 1
Minutes0 6
Seconds[VIEW PLANS](#)

DATAQUEST

[COURSES](#)[STUDENT STORIES](#)[WE'RE HIRING](#)[BLOG](#)[START LEARNING](#)[LOG IN](#)

Learn Data Science

Whether you're new to the field or looking to take a step up in your career, Dataquest can teach you the data skills you'll

Take a FREE course!

 Email Password

You can also sign up for **Stepik** (<https://stepik.org/course/56730/>) or **DataQuest** (free!) & complete lessons in parallel with our course.

Python Basics for Data Analysis (Skill Path) or Data Scientist in Python (Career Path)

Office hours

Vote on the entry survey!

Why should you come to office hours?

- You have clarifying questions about the course or its content
- You have concerns about the course and your progress
- You'd like to talk about career paths in biology or neuroscience



Course Tools



“Tutoring” and project help;
more on this later.



Sharing public course materials
<https://github.com/BILD62>

Interacting with course materials



You can find all of our course materials on either Canvas or the course GitHub: https://github.com/BILD62/BILD62_WI25

Lectures

In other words, PDF slides shown during class.

Hosted on GitHub in the Lectures folder

If I use both a PDF and a Jupyter Notebook during lecture, these numbers will match

Materials

Jupyter Notebooks

You can pull these locally or to DataHub, or look at them online via GitHub or Colab/ Binder



Assignments

Jupyter Notebooks, submitted through **Assignments** tab

Answers posted in the Assignments folder on Github





THE MAGIC LINK FOR THIS COURSE:

Sync with your datahub:



[https://datahub.ucsd.edu/hub/user-redirect/
git-sync?repo=https://github.com/BILD62/BILD62_WI25](https://datahub.ucsd.edu/hub/user-redirect/git-sync?repo=https://github.com/BILD62/BILD62_WI25)



*Where our course
content lives*

To clone Materials to DataHub:

1. Click on the magic link.
2. Log in to DataHub as prompted.
3. You'll be in our course folder now!
4. Save your own copy by adding your initials to the end of the file name. **DO NOT DO THIS FOR ASSIGNMENTS!**
5. Next time you click the link, you'll have a fresh copy, plus your copy.

Introduction to the UCSD DataHub & Jupyter Notebooks

A screenshot of a Jupyter Notebook interface. At the top, there's a navigation bar with icons for file operations, a Python logo, 'Logout', and 'Control Panel'. Below it is a toolbar with icons for file, edit, view, insert, cell, kernel, widgets, help, and various cell execution and validation buttons. The main area shows the title 'jupyter ProgrammingFundamentals' and the status 'Last Checkpoint: 11/05/2019 (autosaved)'. The bottom right corner shows 'Not Trusted' and 'Python 3'.

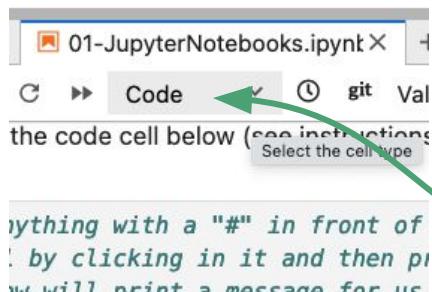
About Jupyter Notebooks

- Jupyter is a loose acronym for Julia, Python, and R
- Run in a web browser but it's not *necessarily* online
(it is when we use the DataHub)
- Usefully, it will show plots directly in the notebook as you work your way through, performing analyses in real-time
(this is why it is used by many scientists!)
- **If you change anything in the cell, you need to re-run it.**



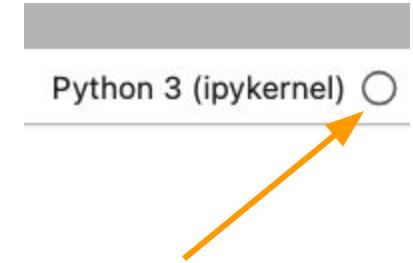
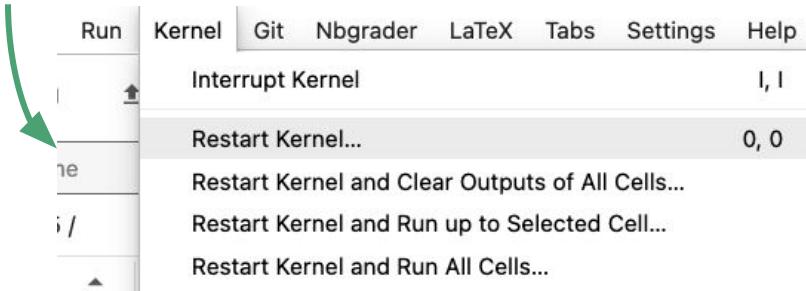
Using Jupyter Notebooks

- **Cell:** the main organizational structure of the notebook
 - Use **Shift+Enter** to run a cell (or press Run)
 - You can run cells out of order, and move cells around!
 - Cells can be **code** (the default) or **markdown** (descriptive text or images)
 - Code cells have [] :
 - If there is a star ([]* :), that means your cell is running
 - Change between code & markdown using **Code** menu (or keyboard shortcuts)



Kernel: the engine that runs the code

- You can clear your **namespace** and get a fresh start by restarting the kernel
- Use **Kernel** menu to interrupt and/or restart if it gets stuck!



You can tell if the kernel is busy by whether or not the circle next to Python 3 (upper right corner) is filled or not. (filled = busy)

Expressions describe
how to combine pieces of
data (e.g., add them!)

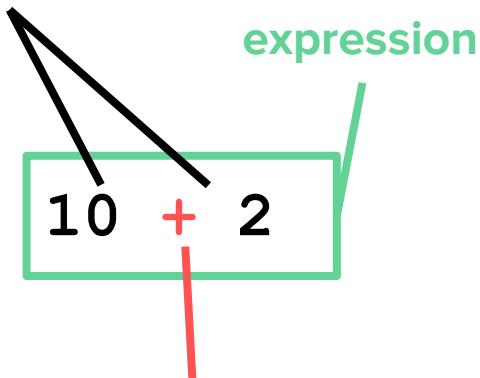
SYMBOLS YOU WILL ENCOUNTER IN THIS COURSE

Symbol	Name	Sample Usage
=	Equal sign	Assign variable
#	Pound sign; hashtag	Line comments
[]	Brackets	Indexing & Slicing
()	Parentheses	Using functions
{ }	Curly Brackets	Defining dictionary
' '	Single quotes	Creating string
" "	Double quotes	Creating string
_	Underscore	In variable names
!	Explanation point	To test not equal (!=)
\	Back slash	Delineate line break
:	Colon	Indexing

Basic arithmetic operators in Python

Symbol	Operation	Usage
+	Addition	$10+2$
-	Subtraction	$10-2$
*	Multiplication	$10*2$
/	Division	$10/2$
**	Exponent	$10**2$
%	Modulo	$10\%2$

inputs



operand

If you want a whole number (floor division), use `//` instead.

Let's get into a Jupyter notebook!
Use the magic link (on Canvas
and these slides) to sync up your
DataHub with our folder, and
open notebook 01.

Before next class...

- Access Canvas (canvas.ucsd.edu) & DataHub (datahub.ucsd.edu)
- Fetch your first assignment — instructions in discussion section
- (Optional) Sign up for Stepik and/or DataQuest
- (Optional) Install VS Code or Anaconda

You only *really* need access to the DataHub, but having the ability to use Python & Jupyter Notebooks on your local computer *may* be useful (especially for final projects)!

To interact with Jupyter Notebooks on your computer using VS Code *OPTIONAL*

1. Install VS Code for your operating system.
2. If you're using Windows, [download git](#).
3. In Terminal (Mac) or the Anaconda Prompt (Windows), clone the repository by running the following command:
`git clone http://www.github.com/BILD62/BILD62_WI25.git`
4. File > Open Folder > Find the BILD62_WI25 folder you just created
5. Install ipykernel when prompted

To interact with Jupyter Notebooks on your computer using Anaconda **OPTIONAL**

1. Install Anaconda with Python 3.7 for your operating system.
2. If you're using Windows, [download git](#).
3. In Terminal (Mac) or the Anaconda Prompt (Windows), clone the repository by running the following command:
git clone http://www.github.com/BILD62/BILD62_WI25.git
4. Open Jupyter Notebook. There are two ways to open:
 - o In Terminal (Mac) or the Anaconda Prompt (Windows), type **jupyter notebook**
 - o Open Anaconda Navigator and launch jupyter notebook
5. On the Jupyter landing page, navigate to the notebook and open it.
 - o It will open in a browser but is *not* using an internet connection.