PSY 4219 / 6219 Scientific Computing for Psychological and Brain Sciences

Mon/Wed 2:30-3:35pm Kissam Center C214

> Thomas Palmeri 507 Wilson Hall

thomas.j.palmeri@vanderbilt.edu

Office Hours: Mon 11am-12pm (or by appointment)

Grader

Jason Chow jason.k.chow@vanderbilt.edu

Help Session:

Mondays 3:50-5:00

this room (or WH 113)

except for next week, which will be Wed after class

Office Hours:

by appointment (on Zoom or in person)

Brightspace

PSY 4219-01 Sci Computing Psy and Brain (2022F)







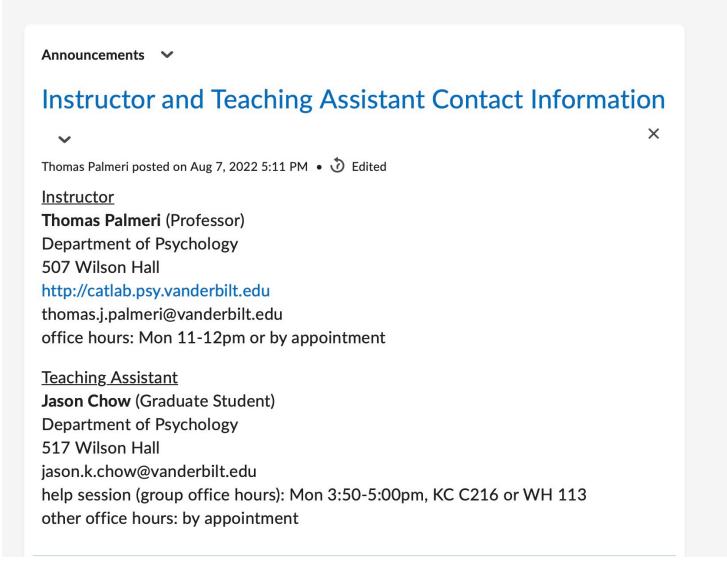


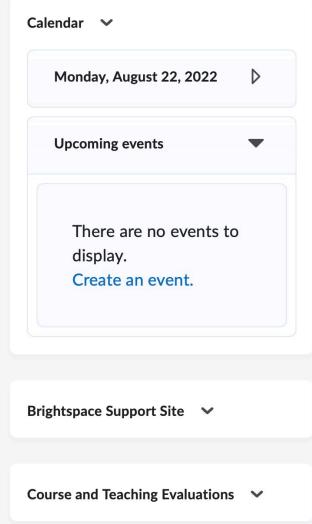






Content Activities & Assessments > Classlist Grades Course Admin Help >





Course Goals

 for students to develop proficiency designing, coding, and debugging computer programs to control experiments, perform data analyses, and simulate neural or psychological mechanisms in Python

programming methods
how to debug programs
computational linear algebra
scientific computing methods
image processing
optimization

algorithms and data structures best practices graphing and visualization data science methods signal processing simulation

- some prior programming experience required
- no prior knowledge of Python required
- recommend some psychology or neuroscience

Course Goals

the first several weeks will cover Python basics at a fairly brisk pace - this will be review for some

(if you have had a ton of experience with Python, scientific computing, data science, image and signal processing, talk with me about whether this is the right course for you)

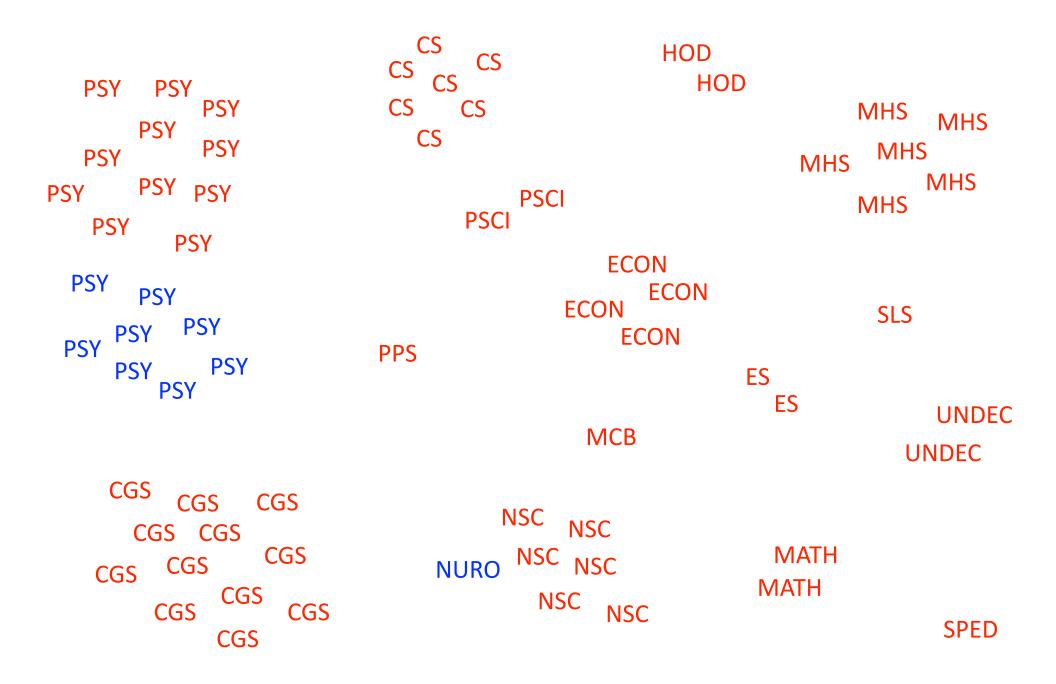
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- some prior programming experience required
- no prior knowledge of Python required
- recommend some psychology or neuroscience concepts and techniques are relevant to those in other disciplines

grad undergrad

distribution of majors in this course



Best Practice

 Throughout the course I will try to emphasize "best practices" for programming specifically and also for any use of computers (data collection, data storage, computation, analyses, modeling) in science generally.

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Our first **Best Practice**

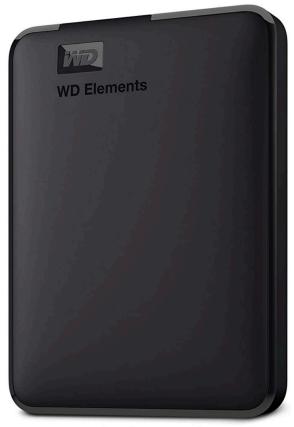
- Back up your computer every day.
- Ideally have two backups in two different places.
- Use external hard drives and/or servers.
- If in a lab, talk to your advisor about backing up.

external hard drive

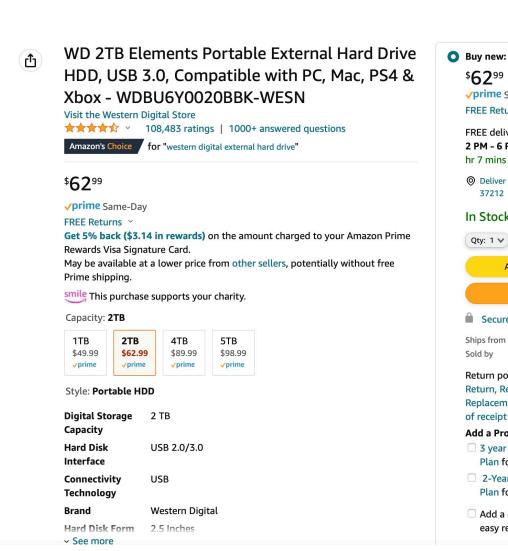








Roll over image to zoom in



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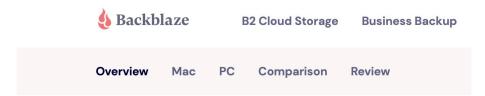
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Backblaze Unlimited Backup

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https://www.nytimes.com/wirecutter/reviews/best-online-backup-service/

Best Practices

be careful about upgrading your operating system (obviously, you want to install things like security patches)

apps often do not work right after a major OS upgrade

more generally, specialized applications and programs often break when an OS changes

also, be careful about upgrading Python or its packages - some programs may not work in an upgraded version

Best Practices

be careful about upgrading your operating system

please, never upgrade in the middle of the semester

Best Practices

be careful about upgrading your operating system

in fact, laboratory computers can have operating systems years (if not decades old) that run specialized equipment or perform important analyses (that have not been translated to new platforms)

one of our monkey neurophysiology labs on the ground floor had a computer running Windows XP to control a physiology rig and its instruments

others have had computers running MS DOS

Hardware

- chipsets, monitors, CPU vs. GPU

O/S

Mac OS, Windows, Linux

Programing Languages

- Python, MATLAB, R, C++, Java, Javascript, Scheme

Why will we focus on Python programming? What are some differences between programming languages?

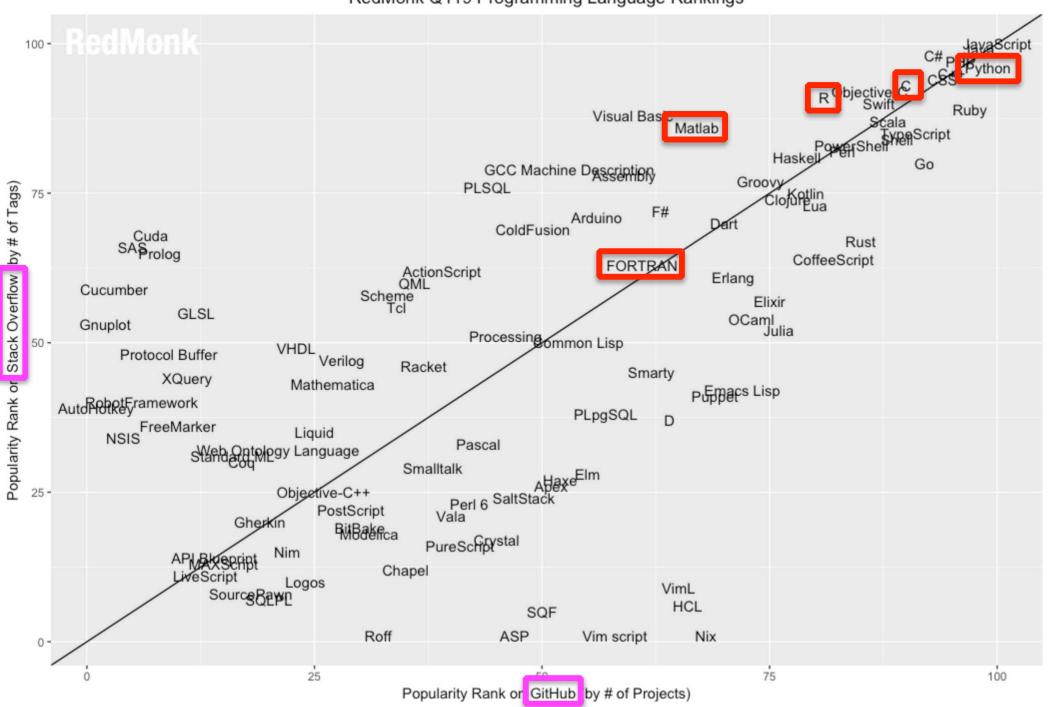
- Your statistics course requires R.
- Another requires SAS.
- Your lab uses Matlab.
- Or E-Prime.
- Or a custom system.
- CS1101 teaches Java.
- CS/DS1100, CS1104, and CS2204 use Python.
- This courses uses Python.

over the course of a career programming, you may change languages several times I went from Basic & Pascal, to C and Lisp and Fortran, to Matlab, to Python

How do languages differ? Popularity

- Popularity means lots of code/tools that are shared.
- Popularity means many other users who can help.
 - Python, MATLAB, R
 - most popular languages in psychology and neuroscience
 - Java– Javascript
 - widely used in industry
 runs much of the web
 - C / C++ (the "assembly language" of the 21st century)
 - used for certain critical applications where speed is critical
 - Fortran, Pascal, LISP, BASIC
 - widespread usage in the 70s and 80s
 - Fortran still used extensively in numeric computing tools

RedMonk Q119 Programming Language Rankings



Free

- Python, R, C++, Octave (Matlab clone)
- IDEs may be commercial products (free for education)

Expensive

- Matlab (commercial product)
- "free" with Vanderbilt site license
- without site license, \$2000+ per user in year one, \$500-1000 per year per user every year after (10x that much in industry)

Programming Environment

- IDE (Integrated Development Environment)
 - write and edit computer programs
 - debug computer programs

• Python, R, C++

- variety of paid and free solutions, some outstanding
- some are language-specific (R Studio, PyCharm, Spyder)
- some work with many languages (Eclipse, VS Code)

MATLAB

outstanding, you get what you pay for

Programming

In The Old Days

- IDE (Integrat
 - write and ed
- use an editor program to write code
- debug com
 use a compiler to create object files
- Python, R, Q
 - variety of p

 - some work

- use a linker to connect object files with libraries and create an executable program
- some are la debug using print statements
 - debug using a standalone debugger program

MATLAB

outstanding, you get what you pay for

Programming Environment

- Notebooks
 - Jupyter (Python and R)
 - Google Colab (Python)
 - we will use primarily at the start of class

Programming Environment

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 - Google Colab (Python)
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Toolboxes, Libraries, and Extensions

 What functions and tools are available above and beyond the core programming language?

Python and R

 1000s of free routines created, shared, and supported by scientists and statisticians in standard repositories

Matlab

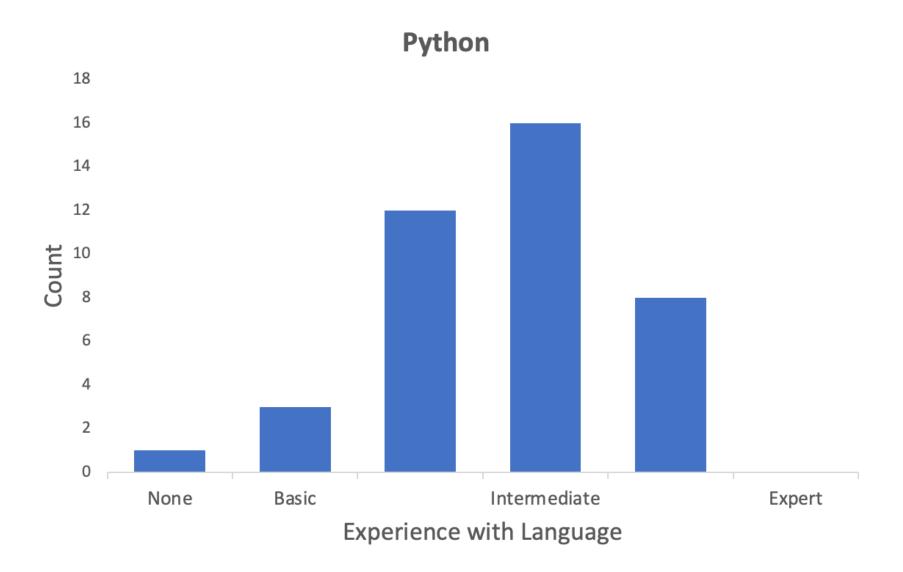
- 100+ toolboxes (not free) by Mathworks
- 1000s of free routines created by users (matlabcentral)
- free Psychophysics Toolbox

Functionality

What can the language and toolboxes do for you?

Python

- complete programming language
- computer scientists love it
- mathematics and graphing comparable to Matlab and R
- object-oriented
- designed to interface well with other languages
- widely used in data science and machine learning
- growing popularity in psychology and neuroscience

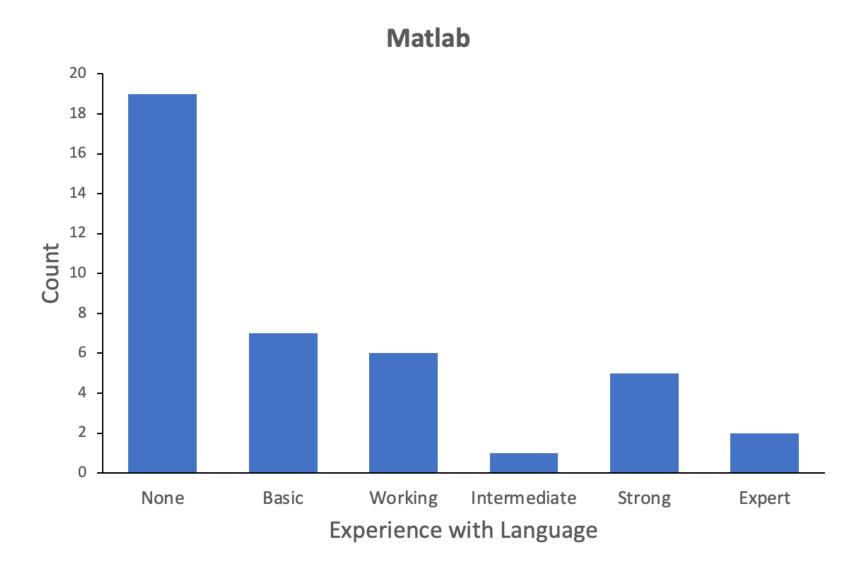


Functionality

What can the language and toolboxes do for you?

MATLAB

- designed for numeric operations (Matlab = Matrix Laboratory)
- outstanding graphing capabilities
- difficult to implement non-numeric data structures
- object-oriented capabilities are tacked on
- lean but quirky syntax
- many computer scientists hate Matlab
- widely used in engineering (and psychology and neuroscience)

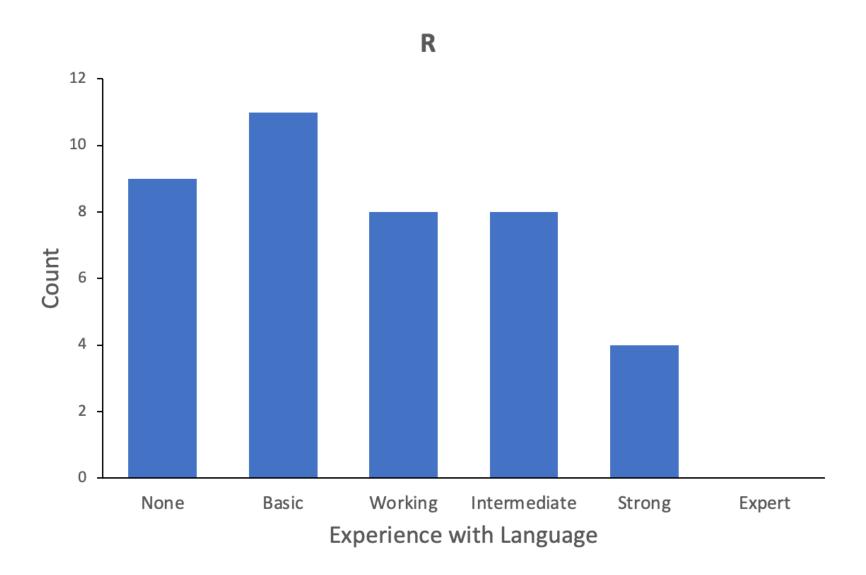


Functionality

What can the language and toolboxes do for you?

• R

- designed from the ground up for statistical analyses
- not designed by computer scientists
- great for analyses and simulation
- excellent graphing capabilities
- more general than scripting languages like SAS or SPSS
- not used as a general purpose programming language
- widely used in psychology for statistical analyses and computational modeling

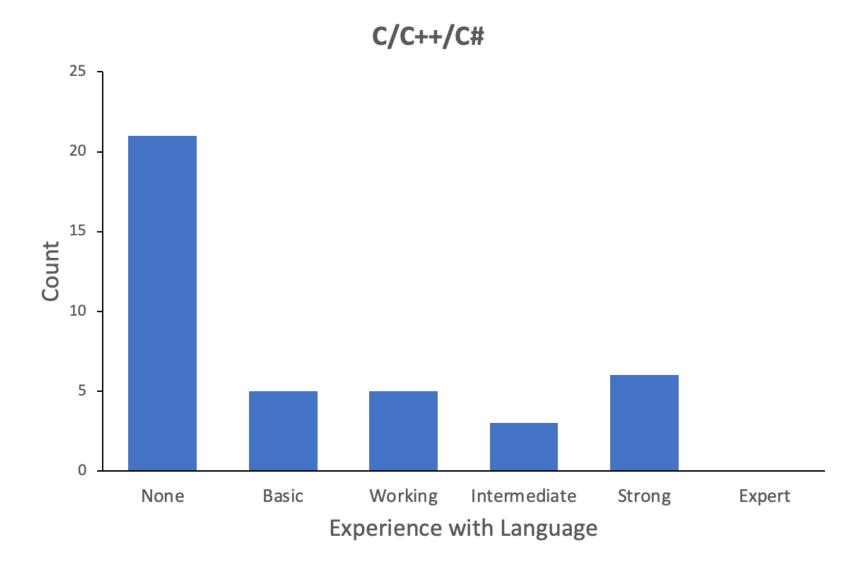


Functionality

What can the language and toolboxes do for you?

• C++

- full object-oriented language
- "assembly language" of the 21st century
- few standard or centralized libraries for science
- powerful tools for applications development
- some specialized, powerful libraries
- Python and Matlab are "written in" C/C++
- libraries/packages are written in C/C++ or Fortran



Interpreted vs. Compiled Language

Matlab, Python, R

- interpreted language
- lines of a program are interpreted one at a time, as if you were typing them in by hand (only a bit faster)
- programs run inside Matlab or Python or R

C++, Fortran

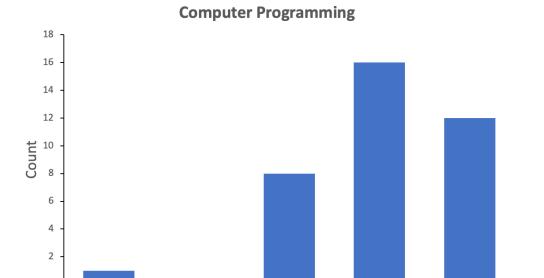
- programs compiled and then linked to libraries
- executable programs (.exe) files (or equivalent)
- most programs you run are compiled
- the operating system on your computer is compiled
- can call compiled C/Fortran from Python (or Matlab)

Matlab, Python, R

- slow, because it is interpreted (vectorized can be fast)
- these languages became popular for real applications only in the past 10 years as computer speeds have increased
- make gpu/parallel programmer easy(er)

• C/C++, Fortran

- blazingly fast
- a C++ program can run 100x faster than Python program
- core R, Matlab, Python functions are in C/C++ or Fortran
- doing simulations sometimes requires (some) C/C++ code
- gpu/parallel programming hard



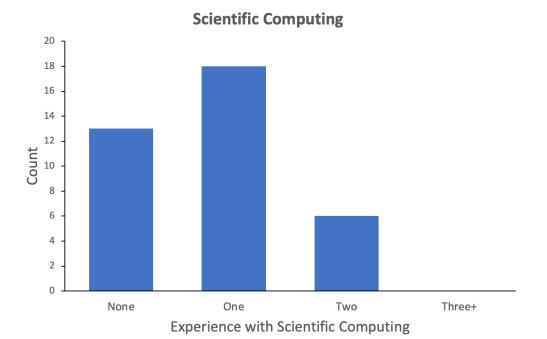


Two

Three+

Online

None



Course Logistics

Syllabus is on Brightspace

PSY 4219-01 Sci Computing Psy and Brain (2022F)



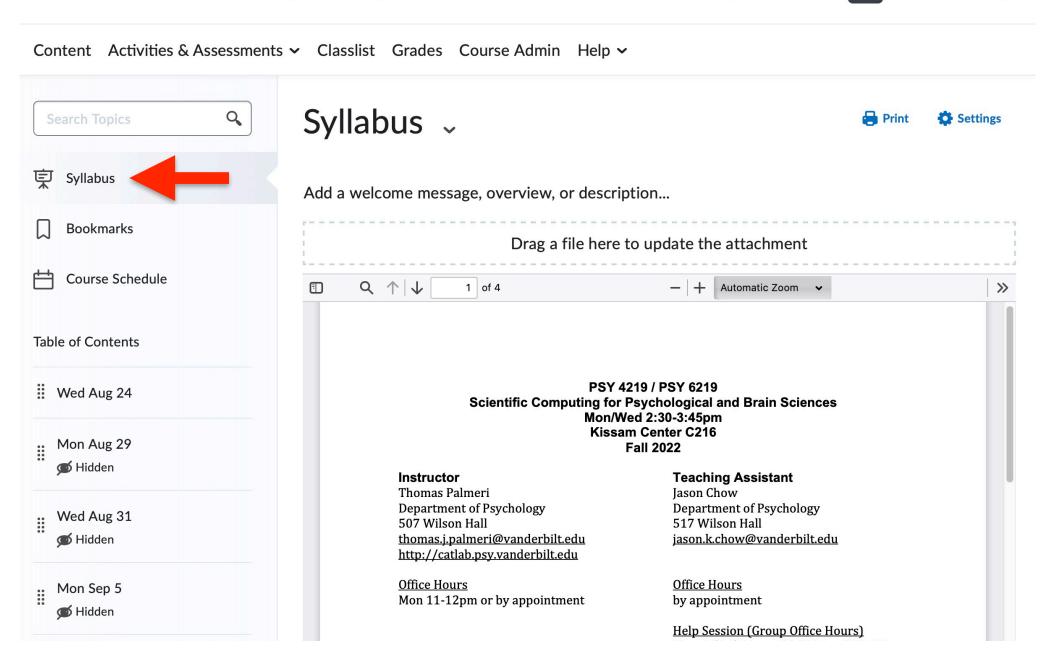












Office Hours

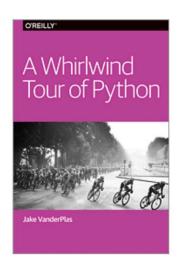
- Palmeri (507 Wilson Hall)
 Mon 11am-12pm or by appointment (office or Zoom)
- Chow (517 Wilson Hall)
 Mondays 3:50-5:00,* this room (or WH 113)
 or by appointment (office or Zoom)

^{*} the first one will be next Wednesday (August 31)

Optional Textbooks

- A Whirlwind Tour of Python by Jake VanderPlas <u>https://jakevdp.github.io/WhirlwindTourOfPython/</u>
- Python Data Science Handbook, also by Jake VanderPlas https://jakevdp.github.io/PythonDataScienceHandbook/
- Introduction to Computation and Programming in Python, by John V. Guttag
- plus other readings / web sites on Brightspace

Versions on Google CoLab we'll talk about later



https://colab.research.google.com/github/jakevdp/WhirlwindTourOfPython/blob/master/Index.ipynb



Course Requirements

Weekly Homework Assignments

- assignment will vary in the number of points
- turn in assignments on Brightspace
- multiple files (when necessary) should be ZIPed together
- Jason will read and run your code
- the code should work, it must be commented, it must be general, it must use good programming style
- I encourage students to help each other out (esp on Piazza), but you need to do the assignments on your own
- come to Jason's help sessions, ask questions
- come to our offices

Course Requirements

for graduate students

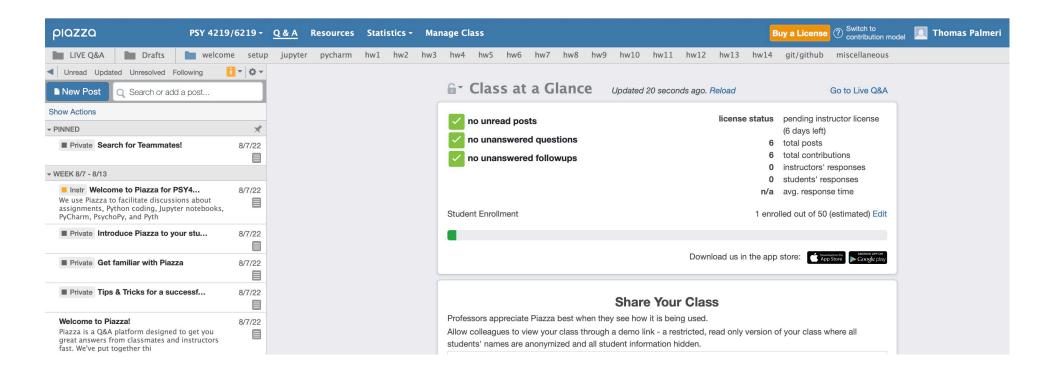
- being a mezzanine course (undergrad and grad) I am required from time-to-time to have some additional work (questions on assignments) for graduate students (required by the college and graduate school)
- undergrads will be able to complete these questions for some extra credit

Laptops in Class

- following along with code (I upload before class)
- download pdf of slides and bringing them to class (note that slides uploaded before class may differ a bit from notes uploaded after class)
- please avoid non-class-related activities

piazza.com/vanderbilt/fall2022/psy42196219

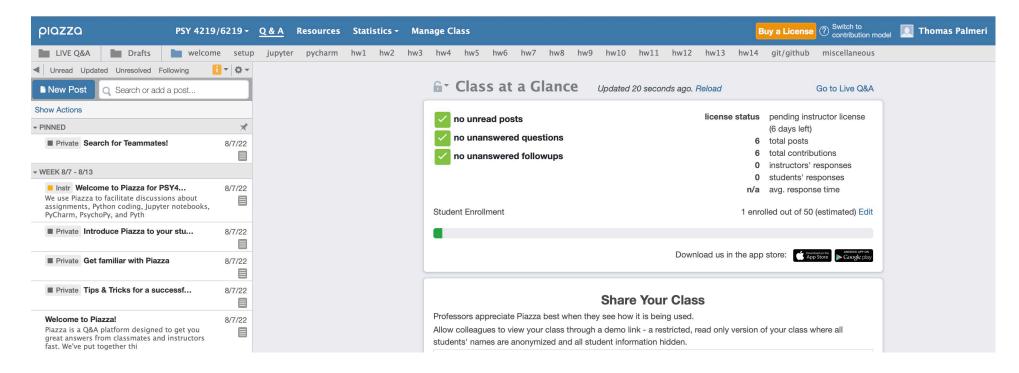
facilitate discussions about assignments, Python coding, Jupyter notebooks, PyCharm, and Python setup - can learn from each other



piazza.com/vanderbilt/fall2022/psy42196219

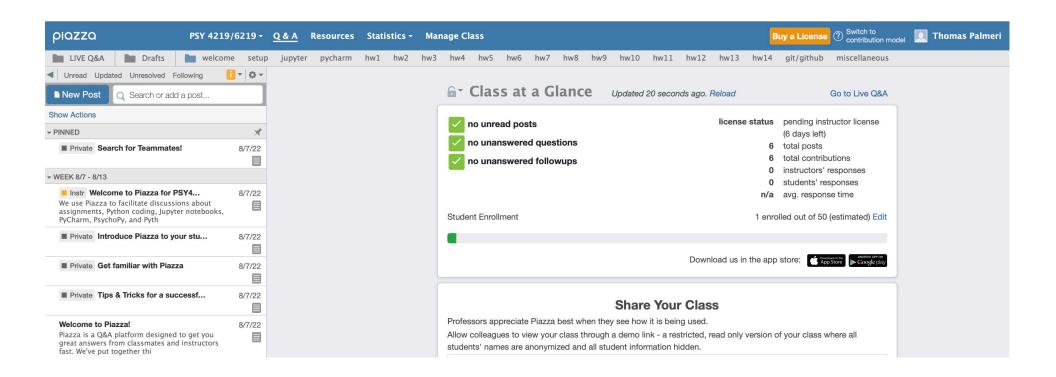
you can share code snippets with specific questions, but please do not share a full swath of code (especially if they are for completing assignments)

you can post privately to me and Jason, but try to post publicly



piazza.com/vanderbilt/fall2022/psy42196219

from syllabus: We also encourage students to help other students on Piazza – doing so will not only help you learn the material more deeply, but may earn you a bit of extra credit at the end of the semester if you're at the borderline between two final grades.



Homework 1

- I will try to have most assignments due on a Wednesday, allowing for you to post questions on Piazza over the weekend and see Jason during his help session after class on Monday.
- The first homework assignment will be due Wednesday September 7th by class time (submitting on Brightspace).
- There will be some "checkmark" parts as well as a bit of coding. I will post the full assignment soon, but until then I will give a few pieces in the slides.

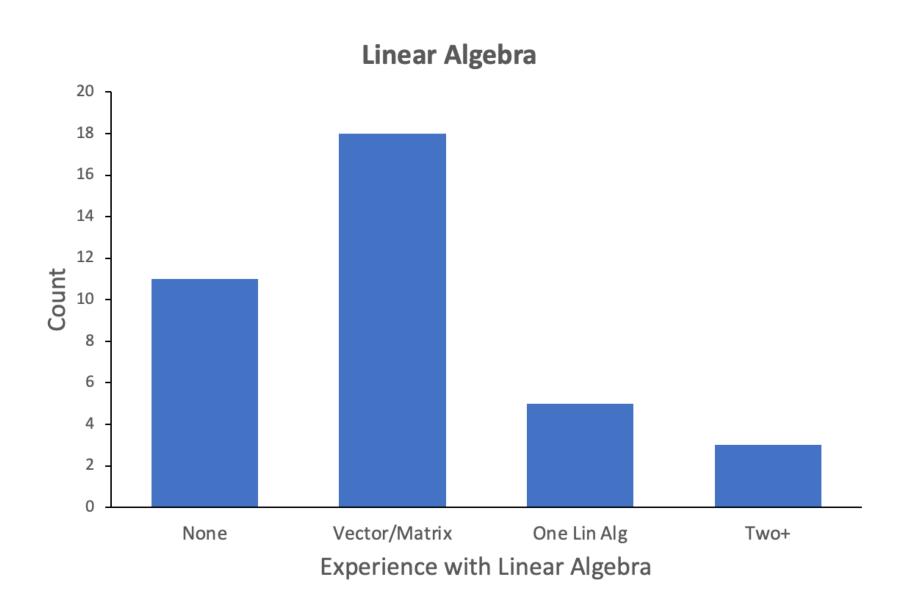
piazza.com/vanderbilt/fall2022/psy42196219

(part of) HOMEWORK 1:

Create a Post and Respond to a Post on Piazza (under the "welcome" tag) - share something about yourself (your interests and hobbies, or your future plans, or what you hope to learn in the class, or really anything you're willing to share)

I shared a (long) post with a bit about myself - after you create a post for yourself, you can respond to the one I wrote or respond to another post

linear algebra



videos on linear algebra

The Essence of Linear Algebra series (<u>3blue1brown</u>) linked below is an excellent resource for reviewing (or learning) basic concepts of linear algebra. The most important concepts to review are vectors (Chapter 1-2), linear transformations and matrices (Chapter 3), matrix multiplication (Chapter 4), non-square matrices as transformations between dimensions (Chapter 8), and dot products (Chapter 9).

Please review these over the next few weeks.

https://www.youtube.com/playlist?list=PLZHQObOWTQDPD3MizzM2xVFitgF8hE_ab

statistics background

