Syllabus

Syllabus for CHBE 5838-002: Quantitative Approaches for Chemical and Biological Engineers: Fall 2025

Lecture Times: Monday/Wednesday 1:55 p.m.-3:10 p.m.

Location: JSCBB B115

Lecturer: Prof. Michael Shirts

Office: JSCBB C123

Email: michael.shirts@colorado.edu

Office hours: Thurs, 3-4 or Friday, 3-4 (as announced)

Topics

This class is intended to cover quantitative methods that are highly helpful for chemical and biological engineering. The focus on the class is numerical approaches, specifically implemented in Python, including important numerical, data science, and visualization libraries. The goal is to get you to a point that you feel confident in learning and going further afterwards. **A detailed course schedule (https://canvas.colorado.edu/courses/122214/pages/schedule-of-topics)** is posted on the course Canvas website, and will likely be tweaked during the semester, as I gauge the interests of the class and the progress we make.

Course Communication

Canvas will be used to communicate class information. You are responsible for all the information that is posted here! For most routine administrative questions you can email me, or send a question to the Slack workspace. Email is **not** a good way to clarify questions on the material; those questions should be answered in office hours or Slack. If you have questions on any administrative topic (typos in materials, scheduling questions, etc.), email or Slack works very well. I will make every effort to return emails within 24 hours.

(https://canvas.colorado.edu/courses/122214/files/80165604/download?wrap=1)

Slack Workspace

The course will have a Slack workspace that you will be invited to after the first class, and can be useful for asking questions and discussion that the whole class can participate in.

Attendance policy

Attendance at the lecture sessions of class is required, and will be included in the grade. There is a significant amount of interactive programming during the class. Emergencies requiring missing the classes can be excused with special arrangements.

Course Materials

The class will be taught using Python. For Python, I recommend using with the free Miniconda or Anaconda packages, which can be used on Windows, Linux, and OS X. **See the Canvas web site on how to install Miniconda or Anaconda (https://canvas.colorado.edu/courses/122214/pages/important-for-first-day-software-for-the-course)** , and **additional coding resources (https://canvas.colorado.edu/courses/122214/pages/readings-and-resources)** .

We will be using a variety of resources for the course. All of the subjects in this class are covered in many different ways in a number of online resources, and it makes the most sense to point you to the best resource for each topic. Links to each of these will be posted as we go through the course, though may be updated (no less than one week before).

Learning Activities

This class will operate on a mix of learning modes. It will include lectures and in-class learning activities in the flipped classroom model, both alone and working together in breakout sessions, as well as weekly homework assignments.

I will solicit feedback regularly to make sure we are maximizing learning!

Assessment

Points will be given for course participation, weekly homework

- Course Participation: 32.5%
- Homework 67.5% (7.5% for each of 9 assignments)

There is no set curve in the class; I'm happy to give all A's if everyone demonstrates that they have mastery of the material.

Course Participation

As we will be using a student-directed learning and flipped classroom model to large extent, course participation becomes very important part of the course. **It will be vital that you spend some time on the homework and play around with Python outside of class**. Lectures will include short mini-lectures on difficult topics, working through Python notebooks to demonstrate concepts, and working on assignments in groups. Ways to demonstrate participation are:

- Asking and answering questions in class.
- Posting questions to ask before class in Slack (must be asked by 10:00 pm the night before lecture for credit).
- Identifying additional resources to share with the class.
- Pointing out typso in materials I distribute.
- Providing feedback on how the class could be better.
- Coming to office hours or other meeting with the professor at least once in the first couple of weeks.
- Working collaboratively on the labs/assignments given during class.
- Continuing to explore the material if you finish early.

Homework

There will be regular homework assignments in this class, due on Thursday at midnight, posted at least a week before. Homework should be submitted via the course's Canvas web site. No late homework will be accepted without prior arrangement (though if there's some technical difficulties with the website and it gets submitted 30 minutes late, I don't care). However, I am fairly understanding of conflicts if you inform me ahead of time, or if there is something entirely outside of your control. Not all homework problems can be solved solely by information presented in class, and will often require spending time on the reading.

Homework will be graded on a check-plus / check / check-minus basis.

- 0: no effort made, any problems not attempted, or no homework turned in.
- check-minus: all problems attempted, some progress made, lack of basic understanding
- check: perhaps some conceptual problems, but most of the problems solved mostly correctly, and effort to explore the problem.
- check-plus: all problems basically correct, no major conceptual issues, provides evidence that the programmed solutions are indeed correct, but there may be some minor math errors on some problems.

In general, a student with more check-pluses than checks and almost no check-minuses would be on target to get an A in the class. More checks than check-pluses, and not too many check minuses, would be would be more like an A-. **Once** during the semester, you may resubmit a homework after grading for an improved score, if it is submitted within a week of being returned. All problems that are incorrect/incomplete must be substantially improved to get regrade credit.

Pair Programming

In class, we will use pair programming in break out sessions. In these sessions, you will go into a break out room and work through the problems together. Pair programming means one person writes, while the other person comments and provides suggestions, rather than just two people working through simultaneously. **The wikipedia page on "Pair Programming"**

(https://en.wikipedia.org/wiki/Pair_programming) has a good description of the principles. You should take turns being the "driver" and the "observer" - take turns on each exercise or every 15 min or so on homework.

You can work on your homework either alone, or with a pair-programming partner. **If you choose to work using pair-programming, you must submit the same file, and indicate at the top of the file that you pair-programmed, meaning you worked on the program together, with both people present.** You may turn in only one pair programming assignment, as long as it is clearly labeled at the top the two people it belongs to. **You should actually use pair programming, so should be working on the homework at the *same* time, not dividing up tasks.** Cheating would be copying or using someone else's code other than in pair-programming. You may discuss homework with anyone, as long as you do not look at what they are typing or copy their files.

Policy on ChatGPT, Gemini and Other AI Programming Assistants

We are entering a brave new world - we don't entirely know to what extent AI will change what it means to write computer code or solve computational problems in the future. There are two important facts about AI and coding. The first is that AI can, in fact, write useful code. The second is that it can get completely lost and produce absolutely unusable garbage, or worse yet, produce answers to the wrong question, or include subtle errors. I have yet to use ChatGPT to write or program any code of moderate length that did not have at least one serious bug.

Given that:

- You may use AI assistance for coding.
- You are heavily advised to write a version of your code first; use AI as an assistant to fix code or suggest alternatives.
- All code must be well-documented. You may NOT use AI to write the documentation.
- You **must** disclose all use of AI assistance in your homework and how you used it in moderate detail (i.e 1-2 paragraphs per problem).
- **Regardless of using AI or not**, you must describe what you did in order to validate that your code actually does what it is intended to do in the way it is intended to do it.

How to Succeed in the Course

- One could learn almost everything in this course on one's own. There is no lack of Python tutorials and math explainers out there! I will be expecting people to put in a moderate amount of effort (10 or so hrs/week, including class time) during the 10 weeks we have together. If people are putting in the work, then I hope to give essentially all A's and A-'s.
- You are expected to take responsibility for learning! You should read the suggested materials, work through the problems in detail, and seek out other resources as necessary to aid your understanding.
- Learn to use online resources. Virtually any question you can think of in this course has been thought of before and asked online. By the end of the course, you should be able to find those answers, and will be set for continuing to do so afterwards!
- Be an independent learner. Work on problems by yourself first. Try to resolve difficulties by taking different approaches, working on different but related examples, or reading other texts. Then, consult your peers for discussion of the best approach. Working jointly on homework from the get-go tends to let things you don't understand slip by unnoticed.
- Don't worry about struggling. Some people take easily to programming and math, some don't, but you **will** be able to get to a useful level for whatever your research is! A very common problem is to get stuck on a bug in a program for quite some time. There's always an answer, and the key is to figure out what the program is actually doing at any point - we'll talk about this some more over the course of the module.

Classroom Behavior

Students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in person, remote, or online. Failure to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed, religion, sexual orientation, gender identity, gender expression, veteran status, marital status, political affiliation, or political philosophy. For more information, see the **Student Classroom and Course-Related Behavior Policy**

(https://www.colorado.edu/compliance/policies/student-classroom-course-related-behavior) , the (https://www.colorado.edu/sccr/student-conduct) **Student Code of Conduct** (https://www.colorado.edu/sccr/student-conduct) , and the (https://www.colorado.edu/oiec/) **Office of Institutional Equity and Compliance** (https://www.colorado.edu/oiec/) .

Policies for Infectious Diseases

Members of the campus community should **follow CDC guidelines for physical distancing, masking, and/or staying home if they are sick or test positive for all respiratory illnesses** (https://www.cdc.gov/respiratory-viruses/prevention/precautions-when-sick.html) . Stay home and away from others (including people you live with who are not sick) if you have respiratory virus symptoms that aren't better explained by another cause. These symptoms can include fever, chills, fatigue, cough, runny nose, and headache, among others. You can go back to your normal activities when, for at least 24 hours, both are true 1) Your symptoms are getting better overall, **and** 2) You have not had a fever (and are not using fever-reducing medication). When you go back to your normal activities, take added precaution over the next 5 days, such as masking and avoiding crowded spaces.

Preferred Student Names and Pronouns

CU Boulder recognizes that students' legal information doesn't always align with how they identify. If you wish to have your preferred name (rather than your legal name) and/or your preferred pronouns appear on your instructors' class rosters and in Canvas, visit the **Registrar's website** (https://www.colorado.edu/registrar/students/records/info/preferred) for instructions on how to change your personal information in university systems.

Honor Code

All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the **Honor Code** (https://www.colorado.edu/sccr/students/honor-code-and-student-code-conduct) . Violations of the Honor Code may include, but are not limited to: plagiarism (including use of paper writing services or technology such as essay bots), cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty of others. Understanding the course's syllabus and what the requirements are for course work is a vital part in adhering to the Honor Code.

All incidents of academic misconduct will be reported to the Student Conduct & Conflict Resolution office (**StudentConduct@colorado.edu** (mailto:StudentConduct@colorado.edu)). Students found responsible for violating the Honor code will be assigned resolution outcomes from Student Conduct & Conflict Resolution as well as academic sanctions from the faculty member. Visit the **Honor Code website** (https://www.colorado.edu/sccr/students/honor-code-and-student-code-conduct) for more information on the academic integrity policy.

Any discovered incidents of academic dishonesty will be reported to the departmental disciplinary committee who will recommend an academic sanction. Sanctions can range from an F for the particular assignment and a lowering of your grade at least a full letter grade to an F for the course. In addition, all confirmed incidents will be reported to the University Honor Code where further nonacademic disciplinary action can be taken. The following list includes some of the examples of dishonest acts (not all of them) for which a hearing will result:

1. Talking to each other during a class individual exam or bringing any information into the exam.
2. Any alteration, forgery, or falsification of official records (such as modification of graded homework problems or exams for which you are seeking additional credit).
3. Allowing another person to take an exam for you (false identification).
4. Knowingly providing material of your own or of others to a fellow student.
5. Possession of or observation of examinations or solutions to examinations prior to the date and time of the exam.
6. Allowing another person to answer clicker questions for you, or answering clicker questions for someone else.

Mental Health and Wellness

The University of Colorado Boulder is committed to the well-being of all students. If you are struggling with personal stressors, mental health or substance use concerns that are impacting academic or daily life, please contact **Counseling and Psychiatric Services (CAPS)** (https://www.colorado.edu/counseling/) located in C4C or call (303) 492-2277, 24 hours /7 days a week.

Schedule of Topics

Below is the preliminary schedule of topics for the course, with applicable readings.

- "Python for Computational Scientists and Engineers", available both as **PDF** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf) , and as **Jupyter notebooks, one for each chapter** (https://github.com/fangohr/introduction-to-python-for-computational-science-and-engineering/tree/master/book)
- **SL** (http://scipy-lectures.org/) is Scipy-lectures.org
- ISL is James et al. "An Introduction to Statistical Learning", the Python version. You can download a pdf copy **from the book's webpage** (https://www.statlearning.com/) .

Date	Topic	Some readings
Aug 25th	Class 1: Class introduction, Jupyter notebooks, and python basics	**PCSE** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf) , Chapters 1, 2
Aug 27th	Class 2: Lists, dictionaries and flow control	**PCSE** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf) , Chapters 3, 4, 6
Sep 3th	Class 3: Functional Programming	**PCSE** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf) , 5, 7, 8, **SL: Python Language** (http://scipy-lectures.org/intro/language/python_language.html) , All Code Academy lessons
Sep 8th	Class 4: Numpy, arrays, matrices, and linear algebra	**PCSE** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf) , chapters 13,14, (chapter 10 "From MATLAB to Python" may be interesting if you have MatLab background)
Sep 10th	Class 5: Making it pretty and fast: data formatting and code vectorization	**pyformat.info** (https://pyformat.info/) , a few blog posts, like **this post** (https://medium.com/pythoneers/vectorization-in-python-an-alternative-to-python-loops-2728d6d7cd3e) and **this post** (https://blog.paperspace.com/numpy-optimization-vectorization-and-broadcasting/) , and **this one** (https://realpython.com/numpy-array-programming/) .
Sep 15th	Class 6: Matplotlib: a picture is worth 1000 Words	**PCSE** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf) , chapter 15.1, **SL: Plotting in Python** (http://scipy-lectures.org/intro/matplotlib/index.html) , **SL: 3D plotting in Python** (http://scipy-lectures.org/packages/3d_plotting/index.html) , see also videos and tutorials posted in: **Class 6: Plotting and Visualization** (https://canvas.colorado.edu/courses/122214/pages/class-6-plotting-and-visualization?wrap=1)
Sep 17th	Class 7: SciPy and solving differential equations	**SL: SciPy,** (http://scipy-lectures.org/intro/scipy.html) **PCSE** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf) , chapter 16
Sep 22rd	Class 8: Numerical linear algebra: solutions, spans and null spaces	See class notes posted on **Class 8: Matrices and Linear Algebra** (https://canvas.colorado.edu/courses/122214/pages/class-8-matrices-and-linear-algebra?wrap=1) , see also the linked **matrix review** (https://online.stat.psu.edu/statprogram/reviews/matrix-algebra) , the **Khan academy introduction** (https://www.khanacademy.org/math/linear-algebra) to linear algebra is also good

Sep 24th	Class 9: Eigenvalues and eigenvectors	See Class 8
Sep 29th	Class 10: Systems of initial value differential equations	**SL: SciPy,** (http://scipy-lectures.org/intro/scipy.html) **PCSE** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf), chapter 16
Oct 1st	Class 11: Optimization and solving nonlinear equations	**SL: Optimization** (https://scipy-lectures.org/advanced/mathematical_optimization/)
Oct 6th	Class 12: More complex optimization and solving nonlinear systems of equations	**SL: Optimization** (https://scipy-lectures.org/advanced/mathematical_optimization/)
Oct 8th	Class 13: Pandas, statistical tools and more plotting	**SL: Pandas in statistics** (http://scipy-lectures.org/packages/statistics/index.html), **PCSE** (https://fangohr.github.io/introduction-to-python-for-computational-science-and-engineering/book.pdf), Chapter 17
Oct 13th	Class 14: Linear regression and model fitting	ISL: Reading is ISL, Chapters 1, Chapter 2.1-2.3, Chapters 3.1-3.2
Oct 15th	Class 15: Nonlinear regression and model fitting	Class Notes
Oct 20th	Class 16: Linear algebra transformations. PCA, and SVD	Class notes
Oct 22nd	Class 17: Error analysis, error bars, and bootstrapping	**The importance of being uncertain** (https://www.nature.com/articles/nmeth.2613) (*Nature Methods* **10**, 809–810 (2013)) **Error bars** (https://www.nature.com/articles/nmeth.2659) (*Nature Methods* **10**, 921–922 (2013)) **Visualizing samples with box plots** (https://www.nature.com/articles/nmeth.2813) (*Nature Methods* 11, 119-120 (2014)) ISL, chapters 5.1 and 5.2
Oct 27th	Class 18: Hypothesis testing	• Read over **https://online.stat.psu.edu/statprogram/reviews/statistical-concepts** (https://online.stat.psu.edu/statprogram/reviews/statistical-concepts). Reviewing your own corresponding textbook on the subject is great, too. This should mostly be review! • **Significance, P-values and tests** (https://www.nature.com/articles/nmeth.2698) (*Nature Methods,* **10**, 1041–1042 (2013)) • **Power and sample size** (https://www.nature.com/articles/nmeth.2738) (*Nature Methods* **10**, 1139–1140 (2013)) • **Comparing Samples - Part 1** (https://www.nature.com/articles/nmeth.2858) (*Nature Methods* **11**, 215–

		216 (2014)) •
Oct 29th	Class 19: Hypothesis testing	• **Comparing samples—part II** (http://www.nature.com/doifinder/10.1038/nmeth.2900) - (*Nature Methods* **volume 11**, pages355–356 (2014) • **Nonparametric tests** (http://www.nature.com/doifinder/10.1038/nmeth.2937) (*Nature Methods* **volume 11**, pages 355–356 (2014))

Accommodation for Religious Obligations

Campus policy requires that faculty provide reasonable accommodations for students who, because of religious obligations, have conflicts with scheduled exams, assignments or required attendance. Please notify me well before any conflict so we can arrange proper accommodation. See the **campus policy regarding religious observances (http://www.colorado.edu/policies/observance-religious-holidays-and-absences-classes-andor-exams)** for full details.

Accommodation for Disabilities, Temporary Medical Conditions, and Medical Isolation

If you qualify for accommodations because of a disability, please submit your accommodation letter from Disability Services to your faculty member in a timely manner so your needs can be addressed. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the **Disability Services website. (https://www.colorado.edu/disabilityservices/)** You can reach out Disability Services at 303-492-8671 or **dsinfo@colorado.edu (mailto:dsinfo@colorado.edu)** for further assistance.

If you have a temporary medical condition or required medical isolation for which you require accommodation, please notify me before any missed class, so we can arrange the proper accommodations. Also see **Temporary Medical Conditions (http://www.colorado.edu/disabilityservices/students/temporary-medical-conditions)** on the Disability Services website.

Sexual Misconduct, Discrimination, Harassment and/or Related Retaliation

CU Boulder is committed to fostering an inclusive and welcoming learning, working, and living environment. University policy prohibits **protected-class (https://www.colorado.edu/oiec/policies/protected-class-nondiscrimination-policy/protected-class-definitions)** discrimination and harassment, sexual misconduct (harassment, exploitation, and assault), intimate partner violence (dating or domestic violence), stalking, and related retaliation by or against members of our community on- and off-campus. The Office of Institutional Equity and Compliance (OIEC) addresses these concerns, and individuals who believe they have been subjected to misconduct can contact OIEC at 303-492-2127 or email **cureport@colorado.edu (mailto:cureport@colorado.edu)**. Information about university policies, **reporting options (https://www.colorado.edu/oiec/reporting-resolutions/making-report)**, and **OIEC support resources (https://www.colorado.edu/oiec/support-resources)** can be found on the **OIEC website (https://www.colorado.edu/oiec/)**.

Please know that faculty and graduate instructors are required to inform OIEC when they are made aware of incidents related to these policies regardless of when or where something occurred. This is to ensure the person impacted receives outreach from OIEC about resolution options and support resources. To learn more about reporting and support resources for a variety of issues, visit the **Don't Ignore It (https://www.colorado.edu/dontignoreit/)** page.