CHE 305: Numerical and Statistical Analysis for Chemical Engineers Fall 2023

Note: All times are in Pacific Time; PDT prior to November 5 and PST after November 5

Lectures

Mondays and Wednesdays, 10:00-11:50 AM, VHE 217

Instructor
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(or by appointment)

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(or by appointment)

Course Description and Learning Objectives

This course is an introduction to numerical algorithms, computational tools, principles of probability and statistics, and their application to chemical engineering problems. After successfully completing this course, a student should be able to:

- 1. Explain the mathematics underlying common numerical algorithms
- 2. Apply numerical methods including linear systems analysis, regression, curve fitting, root finding, optimization, numerical integration, and solution of differential equations
- 3. Apply concepts from probability and statistics including error propagation, hypothesis testing, and parameter estimation
- 4. Write MATLAB programs to implement numerical and statistical methods
- 5. Apply built-in MATLAB tools to solve chemical engineering problems
- 6. Prepare written reports and technical illustrations summarizing numerical and statistical methods and interpretation of results

Required Software and Materials:

All commercial computer software used in this course must be properly licensed. Use of unlicensed commercial software is not allowed and it may result in a failing grade. MATLAB and Microsoft Office licenses are available for free to students through USC.

- Microsoft Office, available through USC ITS, https://itservices.usc.edu/office/
- MATLAB, available through USC ITS, https://itservices.usc.edu/matlab/
- A computer capable of running this software (ideally a laptop that can be brought to inperson lectures)
- The textbook *Numerical and Statistical Methods for Bioengineering: Applications in MATLAB* by Michael R. King and Nipa A. Mody (2011); ISBN 9780521871587

USC Technology Support Links

<u>Blackboard help for students</u> <u>Software available to USC Campus</u>

Lecture structure

Lectures will consist of two 110-minute sessions per week, except in instances where university holidays are observed. The theoretical concepts underlying numerical and statistical methods will be introduced by the instructor, and then there will be interactive coding and calculation exercises

to demonstrate application of the methods. For quiz days, students will be permitted 30 minutes of in-class time at the end of lecture to complete quizzes.

Students are expected to attend lectures in person. Students may be able to attend lectures via Zoom or have access to prerecorded lectures during extenuating circumstances at the discretion of the instructor.

Lecture Schedule

This is a tentative schedule. The exact material covered within a certain week is subject to change, with notice.

- Week 1: Course Introductions and MATLAB basics (Ch. 1)
- Week 2: Programming Control Structures in MATLAB (Appendix A)
- Week 3: MATLAB Function files. (Appendix A)
- Week 4: Linear algebra Systems of linear equations, LU factorization. (Ch. 2.1-2.7)
- Week 5: Iterative methods. Linear regression. (Ch. 2.8-2.10)
- Week 6: Polynomial regression. General linear least squares. Interpolation (Ch. 2.11-2.13)
- Week 7: Review and Midterm Exam
- Week 8: Root finding. Bracketing and open methods. (Ch. 5)
- Week 9: Numerical quadrature. (Ch. 6)
- Week 10: Ordinary differential equations. Initial value problems. Adaptive methods. (Ch. 7.1-7.4)
- Week 11: Stiff systems. Boundary value problems. Nonlinear regression. (Ch. 7.6, Ch. 8)
- Week 12: Elementary probability and statistics. Discrete and continuous probability distributions. (Ch. 3.1-3.5)
- Week 13: Confidence intervals. Hypothesis testing. (Ch. 3.6, Ch. 4.1-4.3)
- Week 14: Parametric and non-parametric hypothesis testing. ANOVA. (Ch. 4.4-4.12)
- Week 15: Propagation of error and review for final exam

Grading

Grades will be based on projects, quizzes, a midterm examination, and a final examination.

Projects: 50%
Quizzes: 10%
Midterm Exam: 20%
Final Exam: 20%

Final letter grades will follow the scale below. However, a grading curve may be implemented at the instructor's discretion. Curves for my courses are typically implemented if the average course grade is below 80%.

Α	A-	B+	В	C+	С	D	F
<u>></u> 93%	[93%,90%)	[87%,90%)	[80,87%)	[77%,80%)	[70%,77%)	[60%,67%)	< 60%

Projects

You can think of Projects as homework, but slightly more in depth (hence the extended due dates). Each programming project will test the implementation of numerical and statistical methods in MATLAB. Students will be provided with a short description of a chemical engineering problem and will be expected to solve this problem using material taught in the course. The emphasis of these projects will be successful implementation of methods and interpretation of results, rather than the efficiency of the coding.

Programming project reports must be submitted electronically via Blackboard as a single submission that contains the following:

- 1. MATLAB program files (i.e., m-files) written to solve the assigned problem, as well as any additional necessary files (i.e., excel files). Each MATLAB code must include a comment at the top of the m-file with the student's name and USC ID number.
- 2. A report in PDF format that uses plain, descriptive language to describe:
 - a. the mathematical or algorithmic strategy used to solve the assigned problem.
 - b. how this strategy was implemented in MATLAB.
 - c. the graphical and textual output (as appropriate) from this program. If the assigned problem requires running the program with several input conditions, the output corresponding to each input must be provided.
 - d. how the program output should be interpreted as a solution to the problem

Assignments e-mailed to the TA or the instructor will not be accepted.

There will be 5 programming projects assigned throughout the semester, each worth 10 points. The general scoring for projects is provided below. Partial credit will be given where appropriate.

- 0 points: No evidence that concepts were understood. No competent code or project submission.
- 5 points: Some evidence for understanding of fundamental concepts. Code has major flaws and/or project report does not adequately address algorithmic strategies.
- 10 points: Clear understanding of the fundamental concepts. Code accomplishes all numerical tasks, returns the correct answer(s), and report clearly describes numerical methods.

Quizzes

There will be 6 in-person quizzes assigned, each worth 4 points. The lowest of the 6 scores will be dropped and only 5 quiz scores will count towards your final grade. Quizzes will receive a score of 0, 1, 2, 3, or 4 points. The scoring for quizzes is provided below.

- 0 points: No significant effort, no evidence that numerical or programming concepts were understood.
- 1 point: Minimal effort; not close to correct answer
- 2 points: Significant effort, some evidence of fundamental concepts; serious flaws in code
- 3 points: Understands fundamental concepts and had correct approach, but made a mistake along the way that resulted in incorrect answer
- 4 points: Perfect submission; answer is correct with correct steps.

Quizzes will be assigned in class and students will have a ~30-minute window to complete and submit the quiz in class. Any students that are unable to complete the quizzes in class or require additional time may use the remainder of the day to complete the quiz at their leisure. However, all quizzes must be submitted by 11:59PM to Blackboard on the day that they are assigned. Quizzes that are emailed to professor/TA or submitted late will not be accepted.

Exams

Exams will either be in-person or take-home. If in-person, the time limit of the exam will be the length of the class period. If an exam is take-home, students must return the exam by the specified date and time (usually 24-hour window). Students will have access to notes, books, and computers for all exams (in-person or take home). Exams will be graded according to a rubric that will be made available after the exams are graded. Exams cannot be rescheduled unless there are genuine extenuating circumstances.

Special Dates

This is a tentative schedule. Project due dates and quiz/exam dates are subject to change, with notice. Note that Wednesday November 29 is the last day of lecture.

Holidays:

Monday September 4: No class, Labor Day

Wednesday November 22: No class, Thanksgiving Break

Quizzes:

Wednesday September 6: Quiz 1
Wednesday September 20: Quiz 2
Wednesday October 18: Quiz 3
Wednesday November 1: Quiz 4
Wednesday November 15: Quiz 5
Wednesday November 29: Quiz 6

Project Due Dates:

Wednesday September 13: Project 1 Wednesday September 27: Project 2 Wednesday October 26: Project 3 Wednesday November 8: Project 4 Wednesday November 29: Project 5

Exams:

Wednesday October 4: Midterm Exam (10:00-11:50 AM)
Monday December 11: Final Exam (8:00-10:00 AM)

Collaboration Policy

Students are encouraged to discuss and work together on projects, but the work each student hands in must be their own. It is not acceptable to merely copy another student's effort; each student must be capable of fully understanding and describing everything they have submitted in the project assignment. If you have any doubts regarding whether a certain instance of collaboration is acceptable at any point in the semester, ask the instructor for clarification.

Work on guizzes and exams will be completely independent.

We will be using plagiarism detection software to verify that each student submits their own code. Identical code includes code for which the only difference is the name of the variables. Any students submitting work that contains substantial runs of identical code or report text will receive zero points for the assignment and reported to USC Office of Academic Integrity (OAI).

Artificial Intelligence (AI) Programs

Since creating, analytical, and critical thinking skills are part of the learning outcomes of this course, all assignments should be prepared by the student working individually or in groups. Students may not have another person or entity complete any substantive portion of the assignment. Developing strong competencies in these areas will prepare you for a competitive workplace. Therefore, using Al-generated tools is prohibited in this course, will be identified as plagiarism, and will be reported to the Office of Academic Integrity.

Academic Integrity

The University of Southern California is foremost a learning community committed to fostering successful scholars and researchers dedicated to the pursuit of knowledge and the transmission of ideas. Academic misconduct is in contrast to the university's mission to educate students through a broad array of first-rank academic, professional, and extracurricular programs and includes any act of dishonesty in the submission of academic work (either in draft or final form).

This course will follow the expectations for academic integrity as stated in the <u>USC Student Handbook</u>. All students are expected to submit assignments that are original work and prepared specifically for the course/section in this academic term. You may not submit work written by others or "recycle" work prepared for other courses without obtaining written permission from the instructor(s). Students suspected of engaging in academic misconduct will be reported to the Office of Academic Integrity.

Other violations of academic misconduct include, but are not limited to, cheating, plagiarism, fabrication (e.g., falsifying data), knowingly assisting others in acts of academic dishonesty, and any act that gains or is intended to gain an unfair academic advantage.

The impact of academic dishonesty is far-reaching and is considered a serious offense against the university and could result in outcomes such as failure on the assignment, failure in the course, suspension, or even expulsion from the university.

For more information about academic integrity see the <u>student handbook</u> or the <u>Office of Academic Integrity's website</u>, and university policies on <u>Research and Scholarship Misconduct</u>.

Students and Disability Accommodations

USC welcomes students with disabilities into all of the University's educational programs. The Office of Student Accessibility Services (OSAS) is responsible for the determination of appropriate accommodations for students who encounter disability-related barriers. Once a student has completed the OSAS process (registration, initial appointment, and submitted documentation) and accommodations are determined to be reasonable and appropriate, a Letter of Accommodation (LOA) will be available to generate for each course. The LOA must be given to each course instructor by the student and followed up with a discussion. This should be done as early in the semester as possible as accommodations are not retroactive. More information can be found at osas.usc.edu. You may contact OSAS at (213) 740-0776 or via email at osas.frontdesk@usc.edu.

Support Systems

Counseling and Mental Health - (213) 740-9355 - 24/7 on call

Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

988 Suicide and Crisis Lifeline - 988 for both calls and text messages – 24/7 on call
The 988 Suicide and Crisis Lifeline (formerly known as the National Suicide Prevention Lifeline)
provides free and confidential emotional support to people in suicidal crisis or emotional distress
24 hours a day, 7 days a week, across the United States. The Lifeline is comprised of a national
network of over 200 local crisis centers, combining custom local care and resources with

national standards and best practices. The new, shorter phone number makes it easier for people to remember and access mental health crisis services (though the previous 1 (800) 273-8255 number will continue to function indefinitely) and represents a continued commitment to those in crisis.

Relationship and Sexual Violence Prevention Services (RSVP) - (213) 740-9355(WELL) - 24/7 on call

Free and confidential therapy services, workshops, and training for situations related to genderand power-based harm (including sexual assault, intimate partner violence, and stalking).

Office for Equity, Equal Opportunity, and Title IX (EEO-TIX) - (213) 740-5086 Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants.

<u>Reporting Incidents of Bias or Harassment</u> - (213) 740-5086 or (213) 821-8298 Avenue to report incidents of bias, hate crimes, and microaggressions to the Office for Equity, Equal Opportunity, and Title for appropriate investigation, supportive measures, and response.

The Office of Student Accessibility Services (OSAS) - (213) 740-0776

OSAS ensures equal access for students with disabilities through providing academic accommodations and auxiliary aids in accordance with federal laws and university policy.

USC Campus Support and Intervention - (213) 740-0411

Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity, Equity and Inclusion - (213) 740-2101

Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

<u>USC Emergency</u> - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

<u>USC Department of Public Safety</u> - UPC: (213) 740-6000, HSC: (323) 442-1200 – 24/7 on call Non-emergency assistance or information.

Office of the Ombuds - (213) 821-9556 (UPC) / (323-442-0382 (HSC)

A safe and confidential place to share your USC-related issues with a University Ombuds who will work with you to explore options or paths to manage your concern.

Occupational Therapy Faculty Practice - (323) 442-2850 or otfp@med.usc.edu
Confidential Lifestyle Redesign services for USC students to support health promoting habits and routines that enhance quality of life and academic performance.