CHE 305: Numerical and Statistical Analysis for Chemical Engineers
Fall 2022

Note: All times are in Pacific Time; PDT prior to November 6 and PST after November 6

Lectures
Mondays and Wednesdays, 10:00-11:50 AM, SOS B2

Instructor
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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 in-person 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
Blackboard help for students
Software available to USC Campus

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.

As of Fall 2022, USC Viterbi School of Engineering is not offering online support for this course. Therefore, all students are expected to attend lectures in-person. Students who miss class due to COVID-19 isolation will be granted make-up accommodations as per university health policy.

Lecture Schedule

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

Week 1: Introduction to numerical and statistical methods (Ch. 1)
Week 2: Introduction to programming in MATLAB (Appendix A)
Week 3: Introduction to linear algebra. Systems of linear equations. (Ch. 2.1-2.4)
Week 4: LU factorization. Matrix Inverse. (Ch. 2.5-2.7)
Week 5: Iterative methods. Linear regression. (Ch. 2.8-2.10)
Week 6: Polynomial regression. General linear least squares. (Ch. 2.11-2.13)
Week 7: Splines and piecewise interpolation.
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. Error propagation. 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: Multiple hypothesis testing and false discovery rate correction.

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. I generally do not assign "minus" grades (i.e., A-, B-). However, this may change if a curve is introduced.

A	B+	B	C+	C	D	F
$\geq$ 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 (e.g., optimization of an isothermal batch reactor) 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, zip file***. Zip files may be made using WinZip or 7-Zip on a PC or by right clicking and using "Compress Items" on a Mac. Programming project reports will only be accepted through Blackboard.

Assignments e-mailed to the TA or the instructor will not be accepted. Project submissions must contain 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

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 2 points. The lowest of the 6 scores will be dropped and only 5 quiz scores will count towards your final grade. The scoring for quizzes is provided below. Partial credit *may* be given where appropriate.

- 0 points: No evidence that numerical or programming concepts were understood.
- 1 point: Some evidence of the fundament concepts. Code may still have serious flaws.
- 2 points: Significant understanding of the important concepts. No penalty for incorrect answers if the fundamental concepts are demonstrated.

Quizzes cannot be rescheduled unless there are genuine extenuating circumstances.

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). All exams (in-person or take home) will be closed book and no access to previous assignment solutions is permitted. However, students are allowed one 8.5" x 11" sheet of notes for the exam. 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 30 is the last day of lecture.

Holidays:
Monday September 5: No class, Labor Day
Wednesday November 23: No class, Thanksgiving Break

Quizzes:
Wednesday September 7: Quiz 1
Wednesday September 21: Quiz 2
Wednesday October 19: Quiz 3
Wednesday November 2: Quiz 4
Wednesday November 16: Quiz 5
Wednesday November 30: Quiz 6

Project Due Dates (by 11:59 PM):
Wednesday September 14: Project 1
Wednesday September 28: Project 2
Wednesday October 26: Project 3
Wednesday November 9: Project 4
Wednesday November 30: Project 5

Exams:
Wednesday October 5: Midterm Exam
Monday December 12: 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 quizzes 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 Student Judicial Affairs and Community Standards (SJACS).

Academic Conduct
Plagiarism—presenting someone else's ideas as your own, either verbatim or recast in your own words—is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in SCampus in Section 11, Behavior Violating University Standards:
https://scampus.usc.edu/1100-behavior-violating-university-standards-and-appropriate-sanctions/

Other forms of academic dishonesty are equally unacceptable. See additional information and university policies on scientific misconduct:
http://policy.usc.edu/scientific-misconduct. Discrimination, sexual assault, and harassment are not tolerated by the university. You are encouraged to report any incidents to the Office of Equality and Diversity (http://equity.usc.edu) or to the Department of Public Safety:
http://adminopsnet.usc.edu/department/department-public-safety/online-forms/contact-us
This is important for the safety of the whole USC community. Another member of the university community—such as a friend, classmate, advisor, or faculty member—can help initiate the report, or can initiate the report on behalf of another person. The Center for Women and Men:

http://www.usc.edu/student-affairs/cwm provides 24/7 confidential support, and the sexual assault resource center webpage (https://sarc.usc.edu) describes reporting options and other resources.

Support Systems
A number of USC's schools provide support for students who need help with scholarly writing. Check with your advisor or program staff to find out more. Students whose primary language is not English should check with the American Language Institute (http://dornsife.usc.edu/ali), which sponsors courses and workshops specifically for international graduate students. The Office of Disability Services and Programs:
http://sait.usc.edu/academicsupport/centerprograms/dsp/home_index.html provides certification for students with disabilities and helps arrange the relevant accommodations. If an officially declared emergency makes travel to campus infeasible, USC Emergency Information (http://emergency.usc.edu) will provide safety and other updates, including ways in which instruction will be continued by means of Blackboard, teleconferencing, and other technology.