COM SCI 111. Introduction to Computational Science

Winter 2021

Course information, requirements, grading, and logistics

Description

Introduction to the numerical algorithms that form the foundations of data science, machine learning, and computational science and engineering. Matrix computation, linear equation systems, eigenvalue and singular value decompositions, numerical optimization. The informed use of mathematical software environments and libraries, such as Python/NumPy/SciPy.

Topics

Week 1	Tuesday	Introduction.
	Thursday	Linear systems of equations. Solving the temperature problem.
Week 2	Tuesday	Interesting matrices. Matrix manipulation in NumPy.
	Thursday	Permutations and permutation matrices. Building the temperature matrix.
Week 3	Tuesday	Introduction to matrix factorizations. LU factorization without pivoting.
	Thursday	LU factorization with partial pivoting. Vector norms, errors, and residuals.
Week 4	Tuesday	Iterative methods: Jacobi and Conjugate Gradient.
	Thursday	Matrix rank, norm, and condition number. Symmetric positive definite matrices.
Week 5	Tuesday	Orthogonality: orthogonal vectors and matrices. Introduction to QR factorization.
	Thursday	Data fitting and least squares using QR factorization.
Week 6	Tuesday	Introduction to singular value decomposition.
	Thursday	SVD theorems. Low-rank approximation of a matrix. SVD data compression.
Week 7	Tuesday	Eigendecomposition. Symmetric matrices: positive definiteness and positive semi-definiteness.
	Thursday	Graph Laplacian and Laplacian quadratic form.
Week 8	Tuesday	Graph connectivity and graph drawing.
	Thursday	Covariance of data sets. Introduction to Principal Component Analysis.
Week 9	Tuesday	Eigenfaces.
	Thursday	Floating-point representation.
Week 10	Tuesday	Ordinary differential equations and mathematical modeling.
	Thursday	Higher-dimensional differential equations, forward Euler method, and multiple-slope methods.

Grading

There will be approximately 9 homework assignments. The two lowest homework grades will be dropped, and the remaining ones will count **50%** of your course grade.

There will be approximately 9 weekly quizzes. Your two lowest quiz grades will be dropped, and the remaining ones will count **50%** of your course grade.

There will be **no midterm or final exam** in the course. The last homework assignment and quiz may be due on the scheduled final exam date (Tuesday, March 16, 8 – 11am).

Homework Policy

There will be a homework assignment every week, assigned on Monday and due Sunday before midnight.

You may work on the homework by yourself, or you may work with exactly one other person. (It's optional to work with another person.) **If you work with another person, only a single submission must be made to GradeScope** (and you must tell GradeScope who the other person is when you submit your paper). In addition, please make sure that the name and perm number of both members appear in your report. You may not discuss the homework with anyone except your (optional) partner. You may change partners between homework assignments, but you may only have one partner on any single homework assignment.

Homework is due on Sundays no later than 11:59 pm. You must turn in your homework online, in **GradeScope**, as a single PDF file. When you turn in your PDF, you must tell GradeScope which pages of your document contain each individual homework problem.

No late homework will be accepted under any circumstances, but your two lowest homework grades will be dropped. Requests for regrades must be submitted through GradeScope. The statute of limitations for regrades is one week; that is, any requests for regrades must be made no later than one week after the homework grades were made available in GradeScope. The last couple of assignments in the course will have an earlier deadline for regrade requests, which will be announced on **Piazza**.

Important

When a homework problem requires writing some Python code, you should turn in all of the following: (Watch the Piazza page for details for each particular homework assignment).

- A description in English of what you did and how. Try to be brief but clear. If we can't understand what you did, you will lose points; we won't regrade homework that was not explained well. You may provide such description in your comments or doc string within your source code.
- A listing of the Python code you wrote (can be in a screenshot from Jupyter).

- Your output from testing and running your Python code (can be in a screenshot from Jupyter).
- Any figures or plots you produced (can be in a screenshot from Jupyter).
- You will write up your homework using **LaTeX**, which is the standard markup language for mathematical documents and is good to know for any future math or CS writing you may do. To give you some examples of LaTeX, you will get both the .pdf file and the .tex file (markup source file) for every homework assignment.

Quiz Policy

There will be a short quiz every week, covering the course material from the previous week. The quiz will be **available on GradeScope at 9:30AM on Monday** and must be completed in one sitting, within **one-hour limit**, **no later than 9:30AM on Tuesday**, 24 hours later. You may not discuss the quiz questions with anyone else, or give answers to quiz questions to anyone else, or post answers anywhere.

There will be **no quiz makeups**, but your two lowest quiz grades will be dropped. Requests for regrades must be submitted through GradeScope. The statute of limitations for regrades is one week; that is, any requests for regrades must be made no later than one week after the quiz grades were made available in GradeScope. The last quiz in the course will have an earlier deadline for regrade requests, which will be announced on Piazza.

Exam Policy

There will be **no exams** in the course.

Software

We will be using Python (version 3.5 or higher) for programming in this course, leaning heavily on the following three packages:

- numpy: Numerical computing with arrays and matrices,
- scipy: More advanced numerical computing, including sparse matrices,
- matplotlib: Plotting and visualization.

We will use a handful of demo routines in Python that we will share in the package `cs111/`. Add the container of this directory to your `PYTHONPATH`. Then you will be able to import all the class software with `import cs111` and then call the routines as, for example:

```
x = cs111.LUsolve( A, b ).
```

We will use Jupyter notebooks to run Python interactively, in a web browser, both for demos in class and for your programming assignments. We strongly recommend that you set up your own laptop or computer to run Jupyter and Python 3 (and NumPy, SciPy, and Matplotlib). The easy way to do this is to download Anaconda, which will install everything you need. The TAs will demo the setup process in the first section.

It's also possible to run Python in a Jupyter notebook in a web browser at CSIL. You can go that route if it works better for you, but it's much easier to run everything on your own computer.

Previous versions of this course used MATLAB, which is a proprietary interactive numerical software package that is widely used in engineering. (UCSB has a campus wide license that you can take advantage of if you need it.) NumPy is designed to look a lot like MATLAB. They both use arrays and matrices as their main data structures; the advantage of NumPy is that you also have all of Python available. If you already know MATLAB, here is a cheat sheet for translating MATLAB into numpy. The Matplotlib library that we will use for plotting also has a lot of similarity to MATLAB's plotting routines.

Textbooks and Other Learning Materials

You do not have to buy a textbook for this course. I will assign readings from various online sources, including Numerical Computing with MATLAB by Cleve Moler (chapters are online at: https://www.mathworks.com/moler/chapters.html). This textbook uses MATLAB rather than Python, but it's still a good reference for several of the topics we will study. Handouts and readings will be announced on Piazza and posted on the GauchoSpace site.

Professor Gil Strang of MIT has videotaped his terrific lectures on linear algebra at https://ocw.mit.edu/courses/mathematics/18-06-linear-algebra-spring-2010/video-lectures/. I recommend watching the first few lectures, which are a great way to review the background for the first half of this course.

Zoom

This class will NOT meet face-to-face for either lecture or section during the Winter quarter. All of our lectures and discussion sessions will be recorded. We will then post them in GauchoSpace alongside any didactical material for your convenience. We recommend, however, that you attend the live sessions whenever possible so that you can make questions and get clarifications at the moment. Having said that, attendance will not count towards your final grade.

Last, we plan to hold live lectures on Tuesdays, and prerecorded short subject videos for Thursdays. The short subject videos will be available on GauchoSpace for you to watch them on your own time.