Applied Math 111: Scientific Computing

Spring 2017

Instructor: Thomas Fai (tfai@seas.harvard.edu)

Time: Tuesday and Thursday 1-2:30pm

Location: 60 Oxford St., Rm. 330

Office Hours: Tuesday 2:30-3pm Wednesday 1-2:30pm, Pierce Hall 314

Teaching Fellow: Taira Miyatake (tmiyatake@g.harvard.edu)

Introduction

Have you ever paused to look at the Mark I, the antique computer with all the funny knobs, on your way through the Science Center? It's well worth your attention. Besides being a direct predecessor to the laptops to smartphones of today, Howard Aiken and Admiral Grace Hopper led a team of researchers during World War II to use the Mark I to perform scientific computations related to the war effort. It's easy to lose sight of how far we've come since the Mark I, but in this course we'll strive to gain understanding and appreciation of computing by getting inside of the black boxes that surround us. Starting from seemingly modest questions such as how computers store numbers and perform arithmetic, we'll progress to deep issues of how algorithms you're already familiar with, while mathematically correct, may be horribly ineffective for practical purposes. We'll discuss efficient algorithms for solving problems that would be impossible to do by pencil and paper, paying particular attention to applications in the natural sciences, e.g. physics, chemistry, and biology.

Prerequisites

Applied Mathematics 21a and 21b, or Mathematics 21a and 21b, or permission of instructor.

Knowledge of a programming language is useful, but by no means required, and taking this course would be an excellent way to gain profiency in Matlab or another scientific computing environment. Students without such knowledge are encouraged to take advantage of the existing resources, including Matlab introductions in section, university-wide Matlab bootcamps, and online tutorials.

In particular, we strongly encourage students to the Matlab bootcamp organized by the Physics and Chemistry departments, which assumes no prior knowledge of Matlab and involves four 2-hr sessions on the evenings of Mon. 1/30, Weds. 2/1, Fri. 2/3, and Mon. 2/6. This bootcamp is open to all Harvard students, and you can sign up at the following website: `https://wiki.harvard.edu/confluence/display/fasmatlab`.

Concrete Objectives

1. Learn standard computational techniques to simulate models and analyze data
2. Avoid common pitfalls in scientific computing such as error accumulation, ill-conditioning, and instability
3. Apply computation in order to solve real-world problems
4. Implement numerical algorithms in Matlab or a similar environment

Content

The course will serve as an introduction to numerical methods for linear algebra, ordinary differential equations (ODE), and optimization. More advanced topics such as Monte Carlo methods and numerical methods for partial differential equations (PDE) will be discussed as time allows. A more detailed list of topics is below:

1. Fundamentals
   (a) Floating point arithmetic
   (b) Condition number
   (c) Stability and accuracy
2. Numerical methods for linear algebra
   (a) Linear systems without the inverse
   (b) Least squares
   (c) Singular Value Decomposition
   (d) Eigenvalue problems
3. Numerical methods for ODE
   (a) Steady-state problems and root finding
   (b) Quadrature and interpolation
   (c) Euler and Runge-Kutta methods
4. Optimization
   (a) Newton's method
   (b) Steepest descent
   (c) Linear programming
5. Advanced topics
   (a) Monte Carlo methods
   (b) Hyperbolic PDE
   (c) Fast Fourier Transform

Course Text

There are no required textbooks, but lectures will usually follow one of the following references, which can be found online or on reserve at the Gordon McKay library:

1. Numerical computing with Matlab by C. Moler, available for free download at `http://www.mathworks.com/moler/`
2. Scientific Computing: An Introductory Survey, M.T. Heath (see also the associated notes and modules at `http://web.engr.illinois.edu/~heath/scicomp/notes/`).
3. Numerical linear algebra, Trefethen, L.N. and D. Bau
4. Introduction to Scientific Computing, C. Van Loan
5. Nonlinear Dynamics and Chaos, S. Strogatz

Course Work and Grading

- Weekly homework sets: **30**% of total grade.
- Participation: **10**% of total grade.
- In-class midterm: **30**% of total grade.
- Final project: **30**% of total grade.

Participation

Attendance is expected at all class sessions, with phones and laptops stored unless they're being used for in-class worksheets. Students are encouraged to take notes in class. Many class sessions will include short interactive workshops in which students will work in groups on computing problems related to lecture. These problems will be checked for completion and will count toward the participation portion of the grade.

Section

The Teaching Fellows will hold weekly sections. The sections will cover background material, including Matlab introductions and linear algebra refreshers, and will reinforce the material covered in lecture.

Homework

You are required to hand in your problem sets electronically and to submit a paper copy in class. Please include your writeup and all relevant programs in a folder and put it into a zip or tar file to submit on the course website. Give yourself plenty of time for submitting the homework online. Homeworks turned in late will be marked 50% off (except in cases of documented illness or other emergencies). There will be a 10 minute grace period during which homeworks will still be counted as on time. Each student will be given two "joker points," which can be used to extend homework deadlines by one day each. The teaching staff must be notified when joker points are being used.

Midterm

There will be an in-class midterm covering the content of approximately the first half of the course. The midterm will take place on March 7th, the Tuesday of the week before Spring Break.

Final project

Instead of a final exam, there will be a final project in which you will use the tools learned in class. The project will involve developing a computer program to address a problem of your choice and writing a report that discusses both the mathematical methodology used and the new insights gained. You will be encouraged to work together in pairs and to come up with project ideas based on your interests, with feedback from the teaching staff.

Academic Integrity

Students are encouraged to work together on the final project and homeworks. However, homeworks, including relevant code, will be graded individually and are expected to reflect students' own thoughts and work.

Accommodations for students with disabilities

Students needing academic adjustments or accommodations because of a documented disability must present their Faculty Letter from the Accessible Education Office (AEO) and speak with the professor by the end of the second week of the term. Failure to do so may result in the Course Head's inability to respond in a timely manner. All discussions will remain confidential, although Faculty are invited to contact AEO to discuss appropriate implementation.

Detailed schedule

Day	**Content**	**Reference**
1/24	• Course introduction	
1/26	• Floating point numbers and types of error	Heath, pp.10-16
1/31	• Linear algebra review and condition number Problem Set 1 assigned	Heath, pp.56-62
2/2	• Gaussian elimination with partial pivoting	Moler, Ch. 2 pp. 2-8
2/7	• Gaussian elimination continued Problem Set 2 assigned	
2/9	• QR factorization and least squares	T & B, pp. 77-84

2/14	• QR continued Problem Set 3 assigned	
2/16	• Polynomial interpolation	Heath, pp. 309-330
2/21	• Eigenvectors and eigenvalues Problem Set 4 assigned	T & B, pp. 179-189
2/23	• Singular Value Decomposition (SVD) and the pseudoinverse	T & B, pp. 25-36
2/27	• SVD continued Practice problems posted for midterm	
3/2	• Midterm review	
3/7	• In-class midterm	
3/9	• Finite differences for boundary value problems	Heath 342-356
3/14 & 3/16	Spring Break!	
3/21	• Nonlinear dynamics Problem Set 5 assigned	Strogatz 15-28, 123-144
3/23	• Rayleigh quotient and QR eigenvalue algorithm	T & B, pp. 201-206
3/28	• Quadrature rules Problem Set 6 assigned (including project proposals)	Heath pp. 422-432
3/30	• Euler and Runge-Kutta methods	Heath, pp. 382-406
4/4	• Initial value problems ctd. Problem Set 7 assigned	
4/6	• Root-finding and Newton's method	Moler, Ch. 4 pp. 1-7
4/11	• Optimization Problem Set 8 assigned (including project warm-ups)	Heath, pp. 270-281
4/13	• Transport equation and characteristics	Heath, pp. 447-462
4/18	• Wave equation and the discrete Fourier transform Problem Set 9 assigned	Heath, pp. 495-505
4/20	• Monte Carlo methods	Heath, pp. 511-516
4/25	• Tentative work session for projects	