Applied Mathematics 205

Advanced Scientific Computing: Numerical Methods

Lecturer: Dr. David Knezevic

Logistics

Lectures: Tuesday, Thursday 10-11:30am 60 Oxford Street, Room 330

My email: dknezevic@seas.harvard.edu

Syllabus, lecture slides, assignments are on the website http://iacs-courses.seas.harvard.edu/courses/am205/

Logistics

Some lecture material will be on the whiteboard, and won't be on the website

Use the AM205 iSite dropbox for assignment submission http://isites.harvard.edu/icb/icb.do?keyword=k97747

Use Piazza for questions and discussion (see AM205 website for link to Piazza) $% \left(\frac{1}{2}\right) =0$

Logistics

My office: Cruft 402

Office hours: Tuesday 11:30am - 1pm, Cruft 403

TFs: Martin Blood-Forsythe, Alexander Robel (Sections and office hours for TFs will be coordinated soon)

Prerequisites

Prerequisites:

- Calculus
- Linear algebra
- Some programming experience

Programming Languages: Matlab

Matlab will be the "official programming language" for AM205. Why Matlab?

- Widely used, very convenient
- Interpreted language, no need for tedious compilation
- Matlab = "Matrix Laboratory," linear algebra is fundamental in scientific computing
- Efficient and powerful enough for a wide range of real-world computational challenges

Everyone should have access to Matlab, including Optimization Toolbox (free download from Harvard) Programming Languages: Other Languages

There are many other languages that are widely used for scientific computing

Other interpreted languages: Python, Julia, R, octave

Compiled languages: Fortran, C/C++

If you wish, you may use Python or Julia in order to complete your homework assignments

But be aware that if you want comprehensive programming support from me or the TFs, then you should use Matlab

Programming Languages: Assignment 0

Asssignment 0 on website, do these problems over the next week

Assignment 0 provides some problems to indicate the expected level of programming familiarity for the outset of the course

Asssignment 0 is not assessed, it should either:

- Confirm that you are already sufficiently familiar with Matlab (or Python, Julia), or
- Indicate that you need to get some programming assistance

Also, contact me or TFs regarding Matlab/programming questions (Piazza is useful for these types of questions)

Syllabus

Unit 0: Overview of Scientific Computing

Unit I: Data Fitting

Chapter I.1: Motivation Chapter I.2: Polynomial interpolation Chapter I.3: Linear least squares fitting Chapter I.4: Nonlinear least squares

Unit II: Numerical Linear Algebra

Chapter II.1: Motivation Chapter II.2: LU and Cholesky factorizations Chapter II.3: QR factorization, SVD

Unit III: Numerical Calculus and Differential Equations

Chapter III.1: Motivation Chapter III.2: Numerical differentiation, numerical integration Chapter III.3: ODE initial value problems Chapter III.4: Boundary value problems and PDEs

Syllabus

Unit IV: Nonlinear Equations and Optimization

Chapter IV.1: Motivation

Chapter IV.2: Root finding

Chapter IV.3: Conditions for optimality

Chapter IV.4: Survey of optimization methods

Unit V: Eigenvalue Problems

Chapter V.1: Motivation

Chapter V.2: Fundamentals

Chapter V.3: Algorithms for eigenvalue problems

Chapter V.4: Krylov subspace methods

Assessment: Homework Assignments

5 assessed homework assignments worth 12% each, associated with Units I–V

Homework assignments will involve both programming and theory/mathematics, submit written report and Matlab code

Late work will not be accepted, unless there are extenuating circumstances

For extenuating circumstances: Get in contact with me as early as possible, I will decide on a case-by-case basis how to proceed

Assessment: Homework Assignments

In general, use built-in Matlab functions as much as possible (no point "reinventing the wheel")

Code should be written clearly and commented thoroughly: avoid "spaghetti code"!



TFs should be able to easily run your code and reproduce your figures

Homework Assignments: Collaboration Policy

Discussion and the exchange of ideas are essential to doing academic work. For assignments in this course, you are encouraged to consult with your classmates as you work on problem sets. However, after discussion with peers, make sure that you can work through the problem sets yourself and ensure that any answers you submit for evaluation are the result of your own efforts.

In addition, you must cite any books, articles, websites, lectures, etc that have helped you with your work using appropriate citation practices. Similarly, you must list the names of students with whom you have collaborated on problem sets.

Mid-term exam, worth 10% of overall grade

Scheduled at approximately 3/4 of the way through the semester (exact date TBD)

Take home exam, 24 hours to complete

No discussion or collaboration permitted

You will receive grades and associated feedback/comments for assignments and mid-term exam via email

If you have any questions about the grade you received for any piece of work, please write up your questions in an email to me

I will then proceed as appropriate

Assessment: Final Project

Goal of this course is to get you to be a responsible, productive user of numerical algorithms for real-world applications

Best way to demonstrate this is in your final project, worth 30%, to be completed in a group of two or three students

- Use concepts/methods related to the course to solve a problem of interest to your group
- TFs will be available to discuss your choice of topic and your approach
- Project due at end of semester (exact date TBD), submit report and associated code

Text books

We will follow "Scientific Computing: An Introductory Survey," by M. T. Heath most closely



Text books Other books:



... And there are of course many other very good Scientific Computing/Numerical Analysis books...