Numerical Methods I, Fall 2010

Logistics

Course webpage
`http://cims.nyu.edu/~donev/Teaching/NMI-Fall2010`
including links to textbook and software, assignments, and lecture slides

Registration 3pts per semester, G63.2010.001 (math) or G22.2420-001 (computer science)

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Lectures: 5:10 - 7 pm Thursdays, 101 Warren Weaver Hall (Courant Institute)

Office Hours: 3 - 5 pm Tuesdays to be discussed on first class, or by appointment

Communication There is a message board on the course Blackboard page that will be used for messages related to the assignments and any scheduling changes. Blackboard will also be used to post grades (for privacy) and you can use it to submit homeworks (or email me).

Content

This course is part of a two-course series meant to introduce Ph.D. students in mathematics to the fundamentals of numerical mathematics (but any Ph.D. student seriously interested in applied mathematics should take it). It will be more technical (theoretical) than the Scientific Computing course, which is meant for masters students and covers similar material as this two-course series but in less detail. This course will not cover differential equations, which form the core of the second part of this series, Numerical Methods II.

Textbooks

Required (primary)
Numerical Mathematics by Alfio Quarteroni, Riccardo Sacco & Fausto Saleri, Springer, ***any*** *edition*. The first edition is available as an e-book through the NYU library and a paper copy is on 2h reserve in the Courant Library.

Optional (secondary)
Scientific Computing with MATLAB and Octave, Alfio M. Quarteroni & Fausto Saleri, Springer, ***any*** *edition*. The second edition is available in PDF form through the library, and a paper copy is available on 2h reserve in the Courant Library.

Additional Some suggestions are on the course webpage, and of course lots of free online materials.

Prerequisites

A good background in linear algebra, and experience with writing computer programs (in Matlab, Python, Fortran, C, C++, or other language). Prior knowledge of Matlab is not required, but it will be used as the main language for the course. If you have experience with compiled languages (Fortran, C, C++), Matlab will be easy to learn and use, and comes with a great help facility.

You will not be required to learn and use a compiled language, especially if you are relatively new to computing, but I will strongly encourage you to and assist you in the learning process (I am a Fortran expert but will do my best to help you with other languages as well).

Assignments and Grading

There will be regular assignments and a final project. The assignments will be mostly computational but some will be theoretical problems. The final project will consist of your own independent research on a topic that is related to the class material and that you choose in discussion with the instructor. A final report will be due at the end of finals week. The final "exam" will consist of presentations of your final project to the class, and will be scheduled in consultation with all of the participants.

Computing

Computing on your own will form an essential part of the learning process and you will be exposed to Linux, Matlab, compiled languages, LaTex, and other tools commonly used by computational scientists. The Courant Institute has computer labs with Linux workstations that have Matlab (matlab), Maple (xmaple), Mathematica (mathematica), the GNU (gcc, g++, gfortran), Intel and Pathscale C/C++/Fortran compiler suites, and other useful software installed.

Tentative Schedule

This is only a tentative agenda for the lectures. I left two classes near the end of the semester open, but adjustments will be made as we go along, partly depending on the interests of the enrolled students and the homework reports.

Recommended preparation (before first class!): Read chapter I of the textbook on your own and make sure you can follow it. Also start playing with MATLAB.

- Sept 9th: Numerical Computing: Well posedeness, numerical conditioning, stability, floating point calculations (IEEE, roundoff, truncation errors), scientific software (MATLAB, compiled languages, GPUs, etc).
- Sept 16th: Direct methods for linear systems: Gaussian elimination, LU, Cholesky factorization, pivoting, dense and banded systems.
- Sept 23rd: Brief mention of iterative methods. Importance of definiteness, conditioning, symmetry, and sparsity. Under-determined and over-determined systems. Sparse factorizations and reordering.
- Sept 30th: Dense eigenvalue problems: diagonalization, and QR and SVD decompositions.
- Oct 7th: Iterative methods for eigenvalues: power method, spectral radius and convergence of iterative schemes. Applications of eigenvalue methods such as principal component analysis.
- Oct 14th: Nonlinear equations: One dimensional root finding (bisection, secant), fixed-point iteration, Newton's method, safeguarded Newton, Aitken acceleration, higher dimensions.
- Oct 21st: Unconstrained optimization: steepest descent, conjugate-gradient, Quasi-Newton methods. Brief mention of constrained optimization.
- Oct 28th: Interpolation: One dimensional polynomial interpolation (Newton, Lagrange), extensions to two and three dimensions. Splines (cubic and B-splines).
- Nov 4th: Orthogonal polynomials: Interpolation (Chebyshev, Legendre, Gauss), approximation. Least squares approximation.
- Nov 11th: Spectral approximation and accuracy. Orthogonal trigonometric polynomials and Discrete Fourier Transforms (DFT).
- Nov 18th: Fast Fourier transforms (FFT) and wavelets. Convolution. Filtering/smoothing. Numerical differentiation via finite differences and spectral methods.
- Nov 25th: No class due to Thanksgiving holiday
- Dec 2nd: Numerical integration: One-dimensional quadrature (midpoint, trapezoidal, Simpson, Newton-Cotes, Hermite methods, etc.), Richardson extrapolation, automatic integration, extensions to two and three dimensions and the curse of dimensionality.
- Dec 9th: Monte Carlo Methods: Pseudo-random numbers (uniform, normal, and other distributions), numerical integration in high dimensions, sampling variance, and variance reduction.
- Dec 16th, 21st and 23rd: Student presentations of final research project. Research report due Dec. 23rd.