

Math 224: Scientific Computing I

A graduate course in numerical analysis

Fall 2004, MWF 10:20-11:10 pm, Room 120 Physics Building

<http://www.math.duke.edu/~witelski/224>

num-er-i-cal a-nal-y-sis: *noun* **1.** the use of numerical methods to compute results for mathematical problems (*see* scientific computing, computational physics), **2.** the use of analysis to formulate and study the accuracy of methods of numerical computations (*see* mathematics of computation, error analysis, discretization of continuous problems).

This course will develop the theoretical basis and computational techniques for: (*i*) finding roots of nonlinear functions (bisection, linear iterative methods, Newton's method) (*ii*) numerical linear algebra (direct and iterative solutions for large matrix-vector systems, solutions of eigenvalue problems), and (*iii*) the solution of nonlinear systems (Newton's method). Error analysis and formulation of convergent mathematical schemes will be used to derive stable, reliable, efficient, and accurate numerical methods for large classes of problems.

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Textbooks: *An Introduction to Numerical Analysis*, 2nd edition, by K. E. Atkinson (Chapters 1, 2, 7-9), *Scientific Computing* (Online notes) by John Trangenstein, 2002 (Chapters 1-8)

Homework: Weekly problem sets will include analysis and computing. Written hard-copies and electronically submitted codes will be required. Late assignments will be penalized.

You are encouraged to discuss the homework problems with your classmates, but your final submission must be entirely your own independent work.¹

Office hours: TBA

Computing: Accounts for the course will be provided on the `math.duke.edu` UNIX network

Recommended²: Programming language: C/C++

Symbolic algebra program: `xmaple`

Plotting programs: `gnuplot` or `xmgr/grace`

Document preparation: `LATEX`

Operating system: LINUX/UNIX w/X11-windows

Reference books: *Numerical Linear Algebra* by L. N. Trefethen and D. Bau

Matrix computations by G. H. Golub and C. F. Van Loan

Solving Nonlinear Equations with Newton's Method by C.T. Kelley

Numerical Recipes in C, 2nd edition, by Press et al

Numerical Mathematics by Quarteroni, Sacco, and Saleri, 2000 (Chapters 1-7)

(on reserve in VESIC)

¹The Duke Community Standard will be assumed in full effect throughout this course "I have adhered to the Duke Community Standard in completing this assignment."

²`matlab` is **NOT** an acceptable alternative programming environment

Course Outline

- **Programming for scientific applications** Chapter 1
 - Modular Programming and Data Structures
 - Analysis of floating point arithmetic and round-off errors
 - Evaluating accuracy and efficiency of programs
 - Written and graphical presentation of scientific results

 - **Finding roots of nonlinear functions** Chapter 2
 - Iterative Methods for scalar problems**
 - The bisection method 2.1
 - Fixed point theorems and Convergence results 2.5
 - Newton's method 2.2-3
 - Roots of polynomials 2.9
 - Additional topics

 - **Numerical linear algebra** Chapters 7-9
 - A brief review of matrix analysis** Chapter 7
 - Linear systems
 - Matrix and vector norms
 - Vector spaces, eigenvalues, and SVD
 - Solving linear systems**
 - Direct methods** Chapter 8
 - Gaussian elimination 8.1
 - Matrix factorizations
 - Sparse matrices
 - Iterative methods**
 - Convergence theorems 8.6
 - Linear iterative methods 8.4
 - Conjugate gradient methods 8.7
 - Subspace iteration methods 8.9
 - Eigenvalue problems** Chapter 9
 - The inverse power method 9.2,6
 - QR factorization 9.5
 - The SVD decomposition

 - **Solving nonlinear systems** 2.10
 - Fixed point theorems and Convergence results
 - Linear iterative methods
 - Newton's method for systems of equations 2.11
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