CSc 301: Numerical Issues in Scientific Programming

Prof. Irina Gladkova
Office: NAC 8/212
Hours: Th 10:00–11:00 am
Phone: (212) 650-6135
e-mail: gladkova@cs.ccny.cuny.edu

Fall Semester, 2012

Course Description:

Numerical issues: roundoff error, truncation error, overflow and underflow errors. Numerical integration; solution of simultaneous equations; curve fitting. A thorough introduction to scientific programming, using a modern version of the Fortran or Matlab language. Written reports and oral presentation of projects.

Prerequisite(s):
Calculus (Math 20300), Linear algebra (Math 34600), Probability (CSc 21700), Algorithms (CSc 22000).

Required text:

Course objectives:

Learn about the effects of round-off, truncation, overflow and underflow errors on numerical computations;

Learn how to select/construct an appropriate algorithm/method for given problem;

Learn to estimate the magnitude of an error, determine an appropriate step size or the number of iterations required;

Learn to provide for adequate checks on the accuracy, and make allowance for corrective action in cases of non-convergence.

Topics covered:

Description of Matlab - Examples, error, condition number, random variables
Polynomial interpolation, Piecewise Polynomial Interpolation

Numerical Integration

Matrix Computations, Linear Systems, QR and Cholesky Factorization

Nonlinear Equations and Optimization.

**Homework:**
There will be substantial homework assignments aimed at reinforcing the material covered in class.

**Homework rules:**

- Never hand programs that do something different than what is asked in the homework
- You are welcome to discuss and work in groups, but the final submission of your homework has to be written by you. Do not copy assignment from someone else
- There is no late submission

**Grades:**
based on homework assignments (30%), midterm (30%) and final (40%).

**Topics (Chapters/Sections in the book):**

- Chapter 1. Power Tools of the Trade
  1.1 Vectors and Plotting
  1.2 More Vectors, More Plotting, and Now Matrices
  1.3 Building Exploratory Environments
  1.4 Error
  1.5 Designing Functions
  1.6 Structure Arrays and Cell Arrays
  1.7 More Refined Graphics
- Chapter 2. Polynomial Interpolation
  2.1 The Vandermonde Approach
  2.2 The Newton Representation
  2.3 Properties
  2.4 Special Topics
- Chapter 3. Piecewise Polynomial Interpolation
3.1 Piecewise Linear Interpolation
3.2 Piecewise Cubic Hermite Interpolation
3.3 Cubic Splines

• Chapter 4. Numerical Integration
  4.1 The Newton-Cotes Rules
  4.2 Composite Rules
  4.3 Adaptive Quadrature

• Chapter 5. Matrix Computations
  5.1 Setting Up Matrix Problems
  5.2 Matrix Operations
  5.3 Once Again, Setting Up Matrix Problems
  5.4 Recursive Matrix Operations

• Chapter 6. Linear Systems
  6.1 Triangular Problems
  6.2 Banded Problems
  6.3 Full Problems
  6.4 Analysis

• Chapter 7. The QR and Cholesky Factorizations
  7.1 Least Squares Fitting
  7.2 The QR factorization
  7.3 The Cholesky Factorization

• Chapter 8. Nonlinear Equations and Optimization
  8.1 Finding Roots
  8.2 Minimizing a Function of One Variable

• Chapter 9. The Initial Value Problem
  9.1 Basic Concepts
  9.2 The Runge-Kutta Methods