

# CSc 301: Numerical Issues in Scientific Programming

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Office: NAC 8/212  
Hours: Tu/Th 10:00–11:00 am

## **Course Description:**

Numerical issues: roundoff error, truncation error, overflow and underflow errors. Numerical differentiation and integration; solution of simultaneous equations; Approximation, curve fitting. A thorough introduction to scientific programming, using a modern version of the Python 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:**

Introduction to Scientific Computing: A Matrix-Vector approach using Matlab, Charles F. Van Loan, Prentice Hall, 2000.

## **Grades:**

homework assignments (30%), midterm (30%) and final (40%).

## **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 variable
- Polynomial interpolation, Piecewise Polynomial Interpolation
- Numerical Differentiation and 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 absolutely no late submissions;

**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 Spline

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 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