CS/SE 4X03 SCIENTIFIC COMPUTATION

NED NEDIALKOV
DEPARTMENT OF COMPUTING AND SOFTWARE
MCMASTER UNIVERSITY
FALL 2021

Lectures:	Tuesday, Thursday, Friday	11:30 - 12:20	Virtual Classroom
Tutorials:	Monday	10:30 - 11:20	ABB 271
	Wednesday	10:30 - 11:20	ETB 238
	Thursday	1:30 - 2:20	ETB 235
	Friday	3:30 - 4:20	ETB 235
Office hours:	Tuesday	5:30 - 6:30	Virtual

Instructor

Ned Nedialkov nedialk@mcmaster.ca

Teaching assistants

Dylan Bassi	bassidj@mcmaster.ca
Shahrooz Derakhshan	derakhsb@mcmaster.ca
Fernando Martinez Garcia	martinef@mcmaster.ca
Chevulana Daman	damanc@mcmaster.ca

1. Introduction

This is an introductory course to scientific computing. We will study floating-point issues in numerical computing and various numerical algorithms. We will learn about numerical differentiation and integration, solving linear systems, computing eigenvalues, least-squares problems, and numerical methods for ordinary differential equations. This course also gives a brief introduction to deep learning. We will study error analysis, convergence, and stability of numerical algorithms. We will use Matlab as a programming language and environment.

2. Learning objectives

Postcondition A *learning objective* for a course is something the student is expected to know and understand or to be able to do by the end of the course. The learning objectives for this course are given below. Taken together, this set of learning objectives constitute the *postcondition* of the course.

1. Students should know and understand
   - (a) issues in floating-point (FP) computations, overflow, cancellations, roundoff errors
   - (b) truncation errors
   - (c) solving linear systems
   - (d) linear least squares
   - (e) solving non-linear equations
   - (f) interpolation

    (g) numerical integration
    (h) stability of methods for initial-value problems in ordinary differential equations

2. Students should be able to
    (a) perform roundoff error analysis
    (b) derive error bounds
    (c) interpret numerical results
    (d) perform simple complexity analysis
    (e) analyze convergence
    (f) analyze stability
    (g) write Matlab programs implementing numerical methods

Precondition The *precondition* of the course is the set of university-level learning objectives that the student is expected to have achieved before the start of the course.

The precondition includes knowledge of calculus and linear algebra

3. Materials

- Required: Ward Cheney and David Kinkaid. Numerical Mathematics and Computing
- Optional: Student Solution Manual
- You are not requited to purchase a Matlab's license. You can access Matlab on mills.mcmaster.ca.
- McMaster standard calculator will be needed for the midterm and the final.

4. Topics

- Floating-point arithmetic
- Interpolation and numerical differentiation
- Numerical integration
- Solving systems of linear equations
- Computing eigenvalues
- Least squares
- Solving nonlinear equations
- Introduction to machine learning
- Methods for initial value problems for ordinary differential equations

5. Reading and suggested exercises

These may be updated as we progress with the course.
§X: Y means Section X should be studied and exercise Y is suggested
The corresponding numbers from the 6th edition are given in $(\cdots)$.

- Chapter 1
    - §1.1: 8, 10 (§1.1: 8, 10)
    - §1.2: 8, 9, 23, 30, 41 (§1.2: 8, 9, 23, 30, 41)
    - §1.3: 13, 14, 18, 22, 24, 45 (§2.1: 13, 14, 18, 24, 45)
    - §1.4: 8, 11, 13, 14, 24, 26, 29 (§2.2: 8, 11, 14, 24, 26, 29)
      Note: you can skip the theorem on loss of precision
- Chapter 2
    - §2.1: 1, 2, 7a (§7.1: 1, 2, 7a)

  - §2.2: 1, 8, 9, 23 (§7.2: 1, 8, 9, 23)
- Chapter 8
  - §8.1, pp. 358–365, 371–373: 2, 4, 11, 15, 18, 23 (§8.1, pp. 293–302, 306–307: 2, 4, 11, 15, 18, 23)
- Chapter 4
  - §4.1, pp. 153–168: 1, 9, 12, 18, 40 (§4.1, pp. 124–141: 1, 9, 12, 18, 40)
  - §4.2: 5, 9, 10, 15 (§4.2: 5, 9, 10, 15)
- Chapter 5
  - §5.1, up to p. 210: 1, 6, 7, 8, 11 (§5.2, up to p. 196: 2, 4, 5, 7, 19)
  - §5.3: 1, 2, 4 (§6.1: 1, 2, 4)
- Chapter 9
  - §9.1: 3, 5, 13, 25 (§12.1: 3, 5, 13, 25)
- Chapter 3
  - §3.2: 1, 3, 13, 14, 23 (§3.2: 1, 3, 13, 14, 23)
  - §3.1: 8, 12, 13 (§3.1: 8, 12, 13)
  - §3.3: 2, 3 (§3.3: 2, 3)
- Chapter 8
- Chapter 7

6. Grading scheme

These are tentative dates and may change depending on how we progress with the material.

Assignment 1	10%	21 September – 1 October
Assignment 2	10%	1 October – 21 October
Midterm	15%	29 October, during class
Assignment 3	10%	2 November – 16 November
Assignment 4	10%	16 November – 30 November
Final exam	45%	

The assignments will include writing Matlab programs and pencil-and-paper questions.

7. Course Policy

Lectures

- Lectures will be live, online, and recorded.
- All the course material will be posted on Teams.

Tutorials

- One of the tutorials will be recorded.

Assignments

- Late work will not be graded without an MSAF.

Missed work

- The MSAF accommodation for a missed assignment is a three calendar day extension from the original assignment deadline.
- The MSAF accommodation for a missed midterm is to roll the weight of the midterm into the weight of the final examination.

Remarking

- Requests for remarking of an assignment or a test must be made within one week after the marked assignment/test is returned.
- Requests that are later than a week will not be accommodated.

Changes

- The instructor reserves the right to modify elements of this course and will notify students accordingly.

8. Resources

- Get Started with MATLAB
- Floating Points
- D. Goldberg. What Every Computer Scientist Should Know About Floating-Point Arithmetic

9. Faculty Notices

"The Faculty of Engineering is concerned with ensuring an environment that is free of all discrimination. If there is a problem, individuals are reminded that they should contact the Department Chair, the Sexual Harassment Officer or the Human Rights Consultant, as the problem occurs."