CAS 708/CSE 700 SCIENTIFIC COMPUTATION

DEPARTMENT OF COMPUTING AND SOFTWARE MCMASTER UNIVERSITY FALL 2018

1. INTRODUCTION

This course is a graduate level introduction to scientific computing. Essential prerequisite is a strong background in linear algebra and calculus. Some background in numerical methods is assumed. Basic methods (e.g. Gauss elimination, polynomial interpolation), typically covered in an undergraduate course, will not be covered in detail. We will be using Matlab in this course. Knowledge of C/C++ is desirable.

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2. Topics

- 1. Scientific computing, numerical algorithms, errors in numerical computing
- 2. Floating-point arithmetic, roundoff error analysis
- 3. Linear systems; direct and iterative methods
- 4. Linear least squares; normal equations, orthogonal transformations, QR
- 5. Eigenvalues and singular values
- 6. Nonlinear systems
- 7. Piecewise polynomial interpolation
- 8. Numerical differentiation
- 9. Numerical integration
- 10. Initial value problems in ordinary differential equations

3. Required text

Uri Ascher and Chen Greif, A First Course in Numerical Methods http://www.siam.org/books/cs07/

4. LEARNING OBJECTIVES

The students in this course should learn

- issues in floating-point computations and roundoff error analysis
- fundamental numerical algorithms
- techniques for analyzing numerical algorithms

and should be able to

- analyze numerical algorithms
- implement numerical algorithms efficiently
- interpret numerical results
- choose the appropriate numerical method for a particular problem

5. Grading scheme

Four assignments 60% and final exam 40%.

10%	27 Sep - 9 Oct
10%	9 Oct - 25 Oct
15%	30 Oct – 12 Nov
20%	15 Nov – 29 Nov
45%	
	$10\% \\ 10\% \\ 15\% \\ 20\% \\ 45\%$

6. References

W. Cheney and D. Kincaid. Numerical Mathematics and Computing. Brooks/Cole.

- G. Dahlquist and A. Björck. Numerical Methods in Scientific Computing. SIAM, 2008.
- M. Heath. Scientific Computing. McGraw-Hill 2002

N. Higham. Accuracy and Stability of Numerical Algorithms. SIAM.

G. W. Steward. Afternotes on Numerical Analysis. SIAM, 1996.

C. van Loan. Introduction to Scientific Computing. A Matrix-Vector Approach using MATLAB, Prentice-Hall, 2000.

T. Kelly Iterative Methods for Linear and Nonlinear Equations

D. Goldberg. What Every Computer Scientist Should Know About Floating-Point Arithmetic. HTML http://docs.oracle.com/cd/E19957-01/806-3568/ncg_goldberg.html PDF http://www.validlab.com/goldberg/paper.pdf

7. Resources

- Lecture slides by U. Ascher and C. Greif http://www.cs.ubc.ca/~ascher/ag_teach.html
- In addition to Matlab, you may consider using Octave http://www.octave.org.
- You may find this Matlab Primer https://www.mathworks.com/help/pdf_doc/matlab/getstart.pdf helpful.
- Short introduction to floating-point numbers by Clever Moler https://www.mathworks. com/company/newsletters/news_notes/pdf/Fall96Cleve.pdf

8. Course Policy

Assignments

- The assignments will be due at the beginning of the lectures.
- A late assignment will receive 10% penalty per day.
- You are allowed to discuss the problems from the assignments. However, you MUST SUBMIT YOUR OWN WORK.

Changes

• The instructor reserves the right to modify elements of this course and will notify students accordingly (in class and post any changes to the course website).

9. Academic Dishonesty

You are expected to exhibit honesty and use ethical behaviour in all aspects of the learning process. Academic credentials you earn are rooted in principles of honesty and academic integrity.

Academic dishonesty is to knowingly act or fail to act in a way that results or could result in unearned academic credit or advantage. This behaviour can result in serious consequences, e.g. the grade of zero on an assignment, loss of credit with a notation on the transcript (notation reads: 'Grade of F assigned for academic dishonesty'), and/or suspension or expulsion from the university.

It is your responsibility to understand what constitutes academic dishonesty. For information on the various types of academic dishonesty please refer to the Academic Integrity Policy, located at http://www.mcmaster.ca/academicintegrity

The following illustrates only three forms of academic dishonesty:

- 1. Plagiarism, e.g. the submission of work that is not one's own or for which other credit has been obtained.
- 2. Improper collaboration in group work.
- 3. Copying or using unauthorized aids in tests and examinations.

10. Academic Accommodation of Students with Disabilities

Students who require academic accommodation must contact Student Accessibility Services (SAS) to make arrangements with a Program Coordinator. Academic accommodations must be arranged for each term of study. Student Accessibility Services can be contacted by phone 905-525-9140, ext. 2865 or e-mail sas@mcmaster.ca. For further information, consult McMaster Universitys Policy for Academic Accommodation of Students with Disabilities.

11. 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."