TANA21/22 Introduction to Scientific Computing

Prerequisites

Linear algebra topics, solving linear systems of equations, differential and integral calculus, multivariable calculus, ordinary differential equations, basic computer programming.

Overview

The goal of this course is to introduce fundamental tools and concepts for solving mathematical problems with a computer. Such numerical computations allow us to solve problems we otherwise could not with pen-and-paper. However, there are many considerations we must make when using a computer to solve mathematical problems. Scientific computing is not simply a matter of translating formulas from the page to a machine. Though incredibly powerful, computers lack the intuition of their human users. This course aims to teach not only how a computer can solve a mathematical problem, but also how to *interpret* the results and understand when the numerical computation is reliable and accurate (and when it is not). Apart from theoretical discussions, the course also includes the development of practical coding and implementation skills in the software tool Matlab.

It turns out to do this we have to start from the beginning. This course revisits basic mathematical operations, like subtraction, to more advanced topics, like integration, and "reconstructs" our mathematical knowledge for use on a computer. In doing so, this course lays the groundwork for a student's scientific computing knowledge. Broadly, topics covered in this course include, but are not limited to,

- Finite precision, representing and manipulating numbers on a machine.

- Solving nonlinear equations.

- Solving linear systems of equations (Linear algebra).

- Approximating functions with interpolation.

- Approximating derivatives and integrals.

- Approximating the solution of ordinary differential equations (ODEs).

Teacher information

Lecturer

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Group leaders

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Course website

Information to the course participants will be continuously updated to the course site on LISAM. The website also includes lecture notes, lecture slides, written exercises, computer lab exercises and old exams.

Overview information is available at http://liu.se/studieinfo/kurs/tana21/ht-2020

Course literature

The lecture notes, slides, and exercises are self-contained to present and discuss the topics covered in this course. The literature is recommended for reference and additional examples to enhance understanding.

The content of this course is primary derived from the book

> *Numeriska beräkningar – analys och illustrationer med MATLAB* by Lars Eldén and Linde Wittneyer-Koch

Supplementary material and topics are taken from:

> *Scientific Computing: An Introductory Survey* by Michael T. Heath

There are free online resources available for learning MATLAB:

> *Numerical Computing with MATLAB* (http://www.mathworks.com/moler/index_ncm.html) by Cleve Moler

Note, you will need to register with MathWorks to download this text.

Course requirements

The topics and course content are defined in the next section. The student will need to demonstrate knowledge and understanding in the topics during the examination. Keep in mind that the topics build upon one another. So, some topics may not be explicitly tested, but their importance as background knowledge is implicitly included when testing more complex tasks.

Lecture plan

We give a (rough) schedule for the topics covered in this course. The recommended reading that accompanies each lecture come from the books listed above by Eldén and Wittmeyer-Koch (EWK) as well as Michael Heath (M).

Lecture	Topic(s)	Recommended reading
Fö 1	Introduction, sources of error, and finite precision	Chap. 2.1 - 2.6 (EWK)
Fö 2	Solving nonlinear equations of a single variable and fixed point iteration	Chap. 4.1 - 4.5 (EWK)
Fö 3	Matrix and vector norms, conditioning, Gauss-Jordon elimination, and operation counting	Chap. 8.2, 8.3, 8.9, 8.10 - 8.12 (EWK)
Fö 4	LU factorization, pivoting, and iterative methods for systems (Jacobi and Gauss-Seidel)	Chap. 8.2 - 8.8 (EWK) Chap. 2.4 - 2.6 (M)
Fö 5	Linear least squares and QR factorization. Introduction to interpolation	Chap. 8.13, 8.14 (EWK) Chap. 7.1, 7.2 (M)
Fö 6	Interpolation techniques	Chap. 5.1 - 5.4, 5.6 - 5.10 (EWK) Chap. 7.3, 7.4 (M)
Fö 7	Orthogonal polynomials, function approximation, and approximation of derivatives	Chap. 9.1, 9.2, 9.5 - 9.7, Chap. 6.1 - 6.4 (EWK)
Fö 8	Numerical integration (quadrature) techniques	Chap. 7.1 - 7.6 (EWK) Chap. 8.1 - 8.3 (M)
Fö 9	Ordinary differential equations, explicit vs. implicit methods, truncation error analysis, stability	Chap. 10.1 - 10.3, 10.5, 10.7 (EWK)
Fö 10	Runge-Kutta methods for initial value problems, outlook to numerics for partial differential equations	Chap. 10.4, 10.6, 10.7 (EWK) Chap. 11.1, 11.2 (M)

Course breakdown

The core of the course is divided into ten lectures, seven exercise sessions, and four computer labs. Additionally, there is a project component of the course; details of which can be found in the Project folder in the Course Documents on Lisam.

Examination

For this course it consists of two independent components:

Exam: The written exam will be held from **14:00 - 18:00 on Thursday October 29**. A student is allowed to bring an A4 sheet of paper (doubled-sided) that contain *handwritten* notes or formulas. Note that copied sheets are not allowed. A calculator is also allowed. Previous exams can be found at the Lisam course site.

Computer labs and Project/Seminar: The course includes four compulsory computer tasks as well as a project task. All of these elements should be completed in a group of (at most) two students. The student groups can discuss the lab tasks as well as the project

components. However, it is incumbent upon the student group to ensure that answers are not plagerized and numerical code is your own. The information for the computer lab tasks is available in the Course documents of the LISAM site.

Near the end of the course, the results of the project for each group will be written in a report and cross-presented in a small oral presentation between two groups. After these presentations and discussions, the write-up of the project can be adjusted (if necessary) before it is submitted for grading. Complete details on the project requirements and tasks are available on LISAM.