Applied Mathematics 205
Advanced Scientific Computing: Numerical Methods

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Course Description

Scientific computing has become an indispensable tool in many branches of research, and is vitally important for studying a wide range of physical and social phenomena. In this course we will examine the mathematical foundations of well-established numerical algorithms and explore their use through practical examples drawn from a range of scientific and engineering disciplines.

There will be an emphasis on mathematical theory and numerical analysis to ensure that students understand the concepts that underpin each algorithm that we consider. There will also be a significant programming component in the course. Students will be expected to implement a range of numerical methods in homework assignments to get hands-on experience with modern scientific computing. In-class demos will be performed with Python, and the homework assignments can be completed in any programming language of the student's choice.

Learning objectives

After taking this course, students should be able to:

- Apply standard techniques to analyze key properties of numerical algorithms, such as stability and convergence.
- Understand and analyze common pitfalls in numerical computing such as ill-conditioning and instability.
- Perform data analysis efficiently and accurately using data fitting methods.

- Derive and analyze numerical methods for ODEs and PDEs.
- Perform optimization using well-established algorithms.
- Implement a range of numerical algorithms efficiently in a modern scientific computing programming language.

Prerequisites

The course material will assume some familiarity with linear algebra and calculus. The third topic will assume some basic knowledge of partial differential equations.

Intended Audience

This course is aimed at students who will employ numerical algorithms in their research. This generally includes students from a wide range of disciplines including life sciences, physical sciences, the humanities, engineering and applied mathematics.

Course Content

The course content will be divided into five main topics:

1. **Data Fitting**
   (a) Polynomial interpolation
   (b) Linear least squares fitting
   (c) Nonlinear least squares
2. **Numerical Linear Algebra**
   (a) LU and Cholesky factorizations
   (b) QR factorization, singular value decomposition
3. **Numerical Calculus and Differential Equations**
   (a) Numerical differentiation, numerical integration
   (b) ODEs, forward/backward Euler, Runge–Kutta schemes
   (c) Lax equivalence theorem, stability regions for ODE solvers
   (d) Boundary value problems, PDEs, finite difference method
4. **Nonlinear Equations and Optimization**
   (a) Root finding, univariate and multivariate cases

   (b) Necessary conditions for optimality
   (c) Survey of optimization algorithms

5. **Eigenvalue problems**
   (a) QR algorithm
   (b) Power method, inverse iteration
   (c) Lanczos algorithm, Arnoldi algorithm

The material covered will be similar to that of previous years lectured by Prof. Chris Rycroft, Dr. David Knezevic, and Prof. Efthimios Kaxiras.

Assessment

The course will be graded in the following way:

Homework (five assignments) :	60%
Take-home midterm exam:	10%
Final project:	30%

Homework assignments: collaboration policy

Discussion and the exchange of ideas are essential to doing academic work. For assignments in this course, you are encouraged to consult with your classmates as you work on problem sets. However, after discussion with peers, make sure that you can work through the problem sets yourself and ensure that any answers you submit for evaluation are written *in your own words*.

In addition, you must cite any books, articles, websites, lectures, *etc.* that have helped you with your work using appropriate citation practices. Similarly, you must list the names of students with whom you have collaborated on problem sets. Using homework solutions from previous years is forbidden.

Final project

In general, the project will be completed in groups of two or three students. One-student projects will also be allowed with permission of the instructor. Groups with four or more students will be allowed with permission of the instructor and a statement about how the work will be divided.

- Each group will propose a project topic drawn from an application area of interest. The project should make use of concepts covered in the course.

- The project should be roughly equivalent in scope to a section of a published research article.
- You will be required to write software to solve your problem, and to submit a report that includes a mathematical discussion of your methodology in relation to the theory covered in the course.
- Projects will be assessed based on a written report, and the quality and correctness of software. Code should be well-documented and should be organized so that figures submitted in the report can be easily reproduced by the graders.
- Further guidance on project topics can be obtained by scheduling a meeting with one of the teaching staff during the latter part of the semester.

References

The course will not have a required textbook. However, the most relevant book is *Scientific Computing: An Introductory Survey* by Michael T. Heath, which covers many of the course topics in a similar level of detail. The books listed below may also be useful.

- A. Greenbaum and T. P. Chartier. *Numerical Methods: Design, Analysis and Computer Implementation of Algorithms.* Princeton University Press, 2012.
- C. Moler. Numerical Computing with MATLAB. SIAM, 2004.
- L. N. Trefethen and D. Bau. *Numerical Linear Algebra*. SIAM, 1997.
- W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery. *Numerical Recipes: The Art of Scientific Computing.* Cambridge University Press, 2007.
- L. R. Scott. *Numerical Analysis.* Princeton University Press, 2011.
- E. Suli, D. F. Mayers. *An Introduction to Numerical Analysis.* Cambridge University Press, 2003.
- J. Demmel. *Applied Numerical Linear Algebra*. SIAM, 1997.