MATH0033: Numerical Methods

David Hewett

2022-2023

Contents

1 Introduction **4**

1.1 Course outline . . . 5

1.2 Suggested reading . . . 6

1.3 Assessment . . . 6

2 Fundamental concepts **7**

2.1 Norms . . . 7

2.2 Errors and convergence . . . 9

2.3 Asymptotic notation . . . 10

2.4 The mean value theorem and Taylor expansions . . . 11

3 Nonlinear equations **12**

3.1 Examples and motivation . . . 13

3.2 Bisection method . . . 14

3.3 Fixed point methods . . . 16

3.4 Newton's method . . . 22

3.5 The secant method . . . 25

3.6 The chord method . . . 25

3.7 Systems of nonlinear equations . . . 27

3.7.1 Simultaneous iteration . . . 27

3.7.2 Newton's method for systems . . . 30

3.8 Stopping criteria 33

4 Linear systems **36**

4.1 Introduction 36

4.1.1 Example and motivation 37

4.2 Matrix norms 39

4.3 Eigenvalues and spectrum of a matrix 40

4.4 Spectral radius and condition number 42

4.5 Direct solvers 45

4.6 Iterative methods for linear systems 49

4.7 Basic stationary method and preconditioning 51

4.8 Stationary Richardson method 52

4.9 The Jacobi method and the Gauss-Seidel method 53

4.10 Non-stationary methods 55

4.10.1 The gradient method 56

4.10.2 The conjugate gradient method 59

4.11 Stopping criteria for iterative methods 67

4.12 Computational cost 68

5 Ordinary differential equations **74**

5.1 Example and motivation 74

5.2 Initial value problems 75

5.3 Numerical discretization 77

5.4 Discretizations from quadrature 79

5.5 One-step methods 80

5.5.1 Truncation error 81

5.5.2 Zero stability 83

5.5.3 Convergence 85

5.5.4 Absolute stability 86
5.6 Runge-Kutta methods 92
5.7 Systems of ordinary differential equations 97
5.8 Applications 98
5.9 Boundary value problems 101
5.9.1 Finite difference approximation 101

Chapter 1

Introduction

Many phenomena in engineering and the physical and biological sciences can be described using mathematical models. Frequently the resulting models cannot be solved analytically, in which case a common approach is to use a *numerical* or *computational* method to find an approximate solution. A *numerical method* is an *algorithm* that produces an approximate solution to a problem. Ideally, a numerical method should be able to achieve a required accuracy provided that sufficient time and computational resources are made available. *Numerical analysis* is the area of mathematics concerned with the design and analysis of numerical methods.

Numerical methods have existed for thousands years (for instance for calculating approximate values of various irrational numbers), and many of the greatest scientists, such as Isaac Newton, devised and used numerical methods in their works. Today, modern computing capabilities have lead to numerical methods becoming ubiquitous in mathematics, technology, science and engineering.

The aim of this course is to introduce the basic ideas underpinning numerical analysis, study a series of numerical methods to solve different problems, and carry out a rigorous mathematical analysis of their accuracy and stability. Such analysis is important to ensure that the methods accurately capture the desired solution. Failure to apply computational algorithms correctly can be costly, as is illustrated here:

`https://www-users.cse.umn.edu/~arnold/disasters/disasters.html`

The overarching theme of the course is the solution of large-scale differential equations. Such problems require the solution of several subproblems and in this course we introduce numerical methods for the most important building blocks:

- solution methods for nonlinear equations and systems;
- solution methods for large linear systems;

- solution methods for ordinary differential equations.

For each method we typically ask two questions:

1. Under what circumstances is the numerical solution a good approximation of the true solution?
2. How does the approximation improve if we are able to devote more computational resources to its calculation?

To answer these questions we will draw on standard tools from analysis including the mean value theorem, Taylor's theorem and the contraction mapping theorem.

The course assumes only knowledge of basic analysis and linear algebra. However, familiarity with the basic notions of numerical analysis, as covered for example in MATH0058 (formerly MATH7601), is of course helpful (but not indispensable), namely:

- interpolation of functions
- numerical integration
- direct solution of linear systems by factorization

Some basic knowledge of programming will also be required.

1.1 Course outline

These lecture notes consist of five chapters:

1. Introduction
2. Fundamental concepts
3. Nonlinear equations
4. Linear systems
5. Ordinary differential equations - initial and boundary value problems

1.2 Suggested reading

The suggested textbooks for the course are:

- Süli, Endre; Mayers, David F. *An Introduction to Numerical Analysis.* Cambridge University Press, Cambridge, 2003. x+433 pp. ISBN: 0-521-81026-4, 0-521-00794-1

which covers the material on nonlinear equations and ODEs, and

- Quarteroni, Alfio; Sacco, Riccardo; Saleri, Fausto. *Numerical Mathematics.* Second edition. Springer, 2007. xviii + 657 pp. ISBN: 3-540-34658-9, 978-3-540-34658-6

which covers the material on linear systems.

The computational exercises and examples use the Matlab programming language. Many basic online tutorials are available, but the following textbook may also be helpful:

- Driscoll, Tobin A. *Learning MATLAB.* SIAM, 2009.
  110 pp. ISBN: 0-898-71683-7, 978-0-898-71683-2

1.3 Assessment

The assessment will consist of:

- Homework (20%)

  For each of chapters 3-5, there will be a set of theoretical exercises and a set of computational exercises, a subset of which are to be handed in and assessed.

  The theoretical and the computational exercises carry equal weight (10% each in total).

- Unseen exam (80%)