An Introduction to Numerical Analysis

Endre Süli and David F. Mayers

University of Oxford



> PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS The Edinburgh Building, Cambridge CB2 2RU, UK 40 West 20th Street, New York, NY 10011-4211, USA 477 Williamstown Road, Port Melbourne, VIC 3207, Australia Ruiz de Alarcón 13, 28014 Madrid, Spain Dock House, The Waterfront, Cape Town 8001, South Africa

http://www.cambridge.org

© Cambridge University Press, 2003

This book is in copyright. Subject to statutory exception and to the provisions of relevant collective licensing agreements, no reproduction of any part may take place without the written permission of Cambridge University Press.

First published 2003

Printed in the United Kingdom at the University Press, Cambridge

Typeface CMR 10/13 pt System $IAT_EX 2_{\varepsilon}$ [TB]

A catalogue record for this book is available from the British Library

Library of Congress Cataloguing in Publication data

ISBN 0 521 81026 4 hardback ISBN 0 521 00794 1 paperback

Contents

Preface		page vii
1	Solution of equations by iteration	1
1.1	Introduction	1
1.2	Simple iteration	2
1.3	Iterative solution of equations	17
1.4	Relaxation and Newton's method	19
1.5	The secant method	25
1.6	The bisection method	28
1.7	Global behaviour	29
1.8	Notes	32
	Exercises	35
2	Solution of systems of linear equations	39
2.1	Introduction	39
2.2	Gaussian elimination	44
2.3	LU factorisation	48
2.4	Pivoting	52
2.5	Solution of systems of equations	55
2.6	Computational work	56
2.7	Norms and condition numbers	58
2.8	Hilbert matrix	72
2.9	Least squares method	74
2.10	Notes	79
	Exercises	82
3	Special matrices	87
3.1	Introduction	87
3.2	Symmetric positive definite matrices	87
3.3	Tridiagonal and band matrices	93

iv	Contents	
3.4	Monotone matrices	98
3.5	Notes	101
	Exercises	102
4	Simultaneous nonlinear equations	104
4.1	Introduction	104
4.2	Simultaneous iteration	106
4.3	Relaxation and Newton's method	116
4.4	Global convergence	123
4.5	Notes	124
	Exercises	126
5	Eigenvalues and eigenvectors of a symmetric matrix	133
5.1	Introduction	133
5.2	The characteristic polynomial	137
5.3	Jacobi's method	137
5.4	The Gerschgorin theorems	145
5.5	Householder's method	150
5.6	Eigenvalues of a tridiagonal matrix	156
5.7	The QR algorithm	162
5.7.1	The QR factorisation revisited	162
5.7.2	The definition of the QR algorithm	164
5.8	Inverse iteration for the eigenvectors	166
5.9	The Rayleigh quotient	170
5.10	Perturbation analysis	172
5.11	Notes	174
	Exercises	175
6	Polynomial interpolation	179
6.1	Introduction	179
6.2	Lagrange interpolation	180
6.3	Convergence	185
6.4	Hermite interpolation	187
6.5	Differentiation	191
6.6	Notes	194
	Exercises	195
7	Numerical integration $-I$	200
7.1	Introduction	200
7.2	Newton–Cotes formulae	201
7.3	Error estimates	204
7.4	The Runge phenomenon revisited	208
7.5	Composite formulae	209

Cambridge University Press
0521810264 - An Introduction to Numerical Analysis
Endre Suli and David F. Mayers
Frontmatter
Moreinformation

	Contents	v
7.6	The Euler–Maclaurin expansion	211
7.7	Extrapolation methods	215
7.8	Notes	219
	Exercises	220
8	Polynomial approximation in the ∞ -norm	224
8.1	Introduction	224
8.2	Normed linear spaces	224
8.3	Best approximation in the ∞ -norm	228
8.4	Chebyshev polynomials	241
8.5	Interpolation	244
8.6	Notes	247
	Exercises	248
9	Approximation in the 2-norm	252
9.1	Introduction	252
9.2	Inner product spaces	253
9.3	Best approximation in the 2-norm	256
9.4	Orthogonal polynomials	259
9.5	Comparisons	270
9.6	Notes	272
	Exercises	273
10	Numerical integration – II	277
10.1	Introduction	277
10.2	Construction of Gauss quadrature rules	277
10.3	Direct construction	280
10.4	Error estimation for Gauss quadrature	282
10.5	Composite Gauss formulae	285
10.6	Radau and Lobatto quadrature	287
10.7	Note	288
	Exercises	288
11	Piecewise polynomial approximation	292
11.1	Introduction	292
11.2	Linear interpolating splines	293
11.3	Basis functions for the linear spline	297
11.4	Cubic splines	298
11.5	Hermite cubic splines	300
11.6	Basis functions for cubic splines	302
11.7	Notes	306
	Exercises	307

vi	Contents	
12	Initial value problems for ODEs	310
12.1	Introduction	310
12.2	One-step methods	317
12.3	Consistency and convergence	321
12.4	An implicit one-step method	324
12.5	Runge–Kutta methods	325
12.6	Linear multistep methods	329
12.7	Zero-stability	331
12.8	Consistency	337
12.9	Dahlquist's theorems	340
12.10	Systems of equations	341
12.11	Stiff systems	343
12.12	Implicit Runge–Kutta methods	349
12.13	Notes	353
	Exercises	355
13	Boundary value problems for ODEs	361
13.1	Introduction	361
13.2	A model problem	361
13.3	Error analysis	364
13.4	Boundary conditions involving a derivative	367
13.5	The general self-adjoint problem	370
13.6	The Sturm–Liouville eigenvalue problem	373
13.7	The shooting method	375
13.8	Notes	380
	Exercises	381
14	The finite element method	385
14.1	Introduction: the model problem	385
14.2	Rayleigh–Ritz and Galerkin principles	388
14.3	Formulation of the finite element method	391
14.4	Error analysis of the finite element method	397
14.5	A posteriori error analysis by duality	403
14.6	Notes	412
	Exercises	414
Appe	endix A An overview of results from real analysis	419
Appe	endix B WWW-resources	423
Bibliography		424
Index		429

Preface

This book has grown out of printed notes which accompanied lectures given by ourselves and our colleagues over many years to undergraduate mathematicians at Oxford. During those years the contents and the arrangement of the lectures have changed substantially, and this book has a wider scope than is currently taught. It contains mathematics which, in an ideal world, would be part of the equipment of any welleducated mathematician.

Numerical analysis is the branch of mathematics concerned with the theoretical foundations of numerical algorithms for the solution of problems arising in scientific applications. The subject addresses a variety of questions ranging from the approximation of functions and integrals to the approximate solution of algebraic, transcendental, differential and integral equations, with particular emphasis on the stability, accuracy, efficiency and reliability of numerical algorithms. The purpose of this book is to provide an elementary introduction into this active and exciting field, and is aimed at students in the second year of a university mathematics course.

The book addresses a wide range of numerical problems in algebra and analysis. Chapter 2 deals with the solution of systems of linear equations, a process which can be completed in a finite number of arithmetical operations. In the rest of the book the solution of a problem is sought as the limit of an infinite sequence; in that sense the output of the numerical algorithm is an 'approximate' solution. This need not, however, mean any relaxation of the usual standards of rigorous analysis. The idea of convergence of a sequence of real numbers (x_n) to a real number ξ is very familiar: given any positive value of ε there exists a positive integer N_0 such that $|x_n - \xi| < \varepsilon$ for all n such that $n > N_0$. In such a situation one can obtain as accurate an approximation to ξ as

viii

Preface

required by calculating sufficiently many members of the sequence, or just one member, sufficiently far along. A 'pure mathematician' would prefer the exact answer, ξ , but the sorts of guaranteed accurate approximations which will be discussed here are entirely satisfactory in real-life applications.

Numerical analysis brings two new ideas to the usual discussion of convergence of sequences. First, we need, not just the existence of N_0 , but a good estimate of how large it is; and it may be too large for practical calculations. Second, rather than being asked for the limit of a given sequence, we are usually given the existence of the limit ξ (or its approximate location on the real line) and then have to construct a sequence which converges to it. If the rate of convergence is slow, so that the value of N_0 is large, we must then try to construct a better sequence, one that converges to ξ more rapidly. These ideas have direct applications in the solution of a single nonlinear equation in Chapter 1, the solution of systems of nonlinear equations in Chapter 4 and the calculation of the eigenvalues and eigenvectors of a matrix in Chapter 5.

The next six chapters are concerned with polynomial approximation, and show how, in various ways, we can construct a polynomial which approximates, as accurately as required, a given continuous function. These ideas have an obvious application in the evaluation of integrals, where we calculate the integral of the approximating polynomial instead of the integral of the given function.

Finally, Chapters 12 to 14 deal with the numerical solution of ordinary differential equations, with Chapter 14 presenting the fundamentals of the finite element method. The results of Chapter 14 can be readily extended to linear second-order partial differential equations.

We have tried to make the coverage as complete as is consistent with remaining quite elementary. The limitations of size are most obvious in Chapter 12 on the solution of initial value problems for ordinary differential equations. This is an area where a number of excellent books are available, at least one of which is published in two weighty volumes. Chapter 12 does not describe or analyse anything approaching all the available methods, but we hope we have included some of those in most common use.

There is a selection of Exercises at the end of each chapter. All these exercises are theoretical; students are urged to apply all the methods described to some simple examples to see what happens. A few of the exercises will be found to require some heavy algebraic manipulation; these have been included because we assume that readers will have ac-

Preface

cess to some computer algebra system such as Maple or Mathematica, which then make the algebraic work almost trivial. Those involved in teaching courses based on this book may obtain copies of LATEX files containing solutions to these exercises by applying to the publisher by email (solutions@cambridge.org). Although the material presented in this book does not presuppose the reader's acquaintance with mathematical software packages, the importance of these cannot be overemphasised. In Appendix B, a brief set of pointers is provided to relevant software repositories.

Our treatment is intended to maintain a reasonably high standard of rigour, with many theorems and formal proofs. The main prerequisite is therefore some familiarity with elementary real analysis. Appendix A lists the standard theorems (labelled **Theorem A.1, A.2, ..., A7**) which are used in the book, together with proofs of one or two of them which might be less familiar. Some knowledge of basic matrix algebra is assumed. We have also used some elementary ideas from the theory of normed linear spaces in a number of places; complete definitions and examples are given. Some prior knowledge of these areas would be helpful, although not essential.

The chart below indicates how the chapters of the book are interrelated. They show, in particular, how Chapters 1 to 5 form a largely self-contained unit, as do Chapters 6 to 10.

Roadmap of the book



х

Preface

We have included some historical notes throughout the book. As well as hoping to stimulate an interest in the development of the subject, these notes show how wide a historical range even this elementary book covers. Many of the methods were developed by the great mathematicians of the seventeenth and eighteenth centuries, including Newton, Euler and Gauss, but what is usually known as Gaussian elimination for the solution of systems of linear equations was known to the Chinese two thousand years ago. At the other end of the historical scale, the analysis of the eigenvalue problem, and the numerical solution of differential equations, are much more recent, and are due to mathematicians who are still very much alive. Many of our historical notes are based on the excellent biographical database at the history of mathematics website

http://www-history.mcs.st-andrews.ac.uk/history/

We have tried to eradicate as many typographical errors from the text as possible; however, we are mindful that some may have escaped our attention. We plan to post any typos reported to us on

http://web.comlab.ox.ac.uk/oucl/work/endre.suli/index.html

We wish to express our gratitude to Professor Bill Morton for setting us off on this *tour de force*, to David Tranah at Cambridge University Press for encouraging us to persist with the project, and to the staff of the Press for not only improving the appearance of the book and eliminating a number of typographical errors, but also for correcting and improving some of our mathematics. We also wish to thank our colleagues at the Oxford University Computing Laboratory, particularly Nick Trefethen, Mike Giles and Andy Wathen, for keeping our spirits up, and to Paul Houston at the Department of Mathematics and Computer Science of the University of Leicester for his help with the final example in the book.

Above all, we are grateful to our families for their patience, support and understanding: this book is dedicated to them.

 $ES \ {\mathcal E} DFM$

Oxford, September 2002.