

Texts in Applied Mathematics 37

Editors

J.E. Marsden
L. Sirovich
S.S. Antman

Advisors

G. Iooss
P. Holmes
D. Barkley
M. Dellnitz
P. Newton

Texts in Applied Mathematics

1. *Sirovich*: Introduction to Applied Mathematics.
2. *Wiggins*: Introduction to Applied Nonlinear Dynamical Systems and Chaos.
3. *Hale/Koçak*: Dynamics and Bifurcations.
4. *Chorin/Marsden*: A Mathematical Introduction to Fluid Mechanics, Third Edition.
5. *Hubbard/West*: Differential Equations: A Dynamical Systems Approach: Ordinary Differential Equations.
6. *Sontag*: Mathematical Control Theory: Deterministic Finite Dimensional Systems Second Edition.
7. *Perko*: Differential Equations and Dynamical Systems, Third Edition.
8. *Seaborn*: Hypergeometric Functions and Their Applications.
9. *Pipkin*: A Course on Integral Equations.
10. *Hoppensteadt/Peskin*: Modeling and Simulation in Medicine and the Life Sciences, Second Edition.
11. *Braun*: Differential Equations and Their Applications, Fourth Edition.
12. *Stoer/Bulirsch*: Introduction to Numerical Analysis, Third Edition.
13. *Renardy/Rogers*: An Introduction to Partial Differential Equations.
14. *Banks*: Growth and Diffusion Phenomena: Mathematical Frameworks and Applications.
15. *Brenner/Scott*: The Mathematical Theory of Finite Element Methods, Second Edition.
16. *Van de Velde*: Concurrent Scientific Computing.
17. *Marsden/Ratiu*: Introduction to Mechanics and Symmetry, Second Edition.
18. *Hubbard/West*: Differential Equations: A Dynamical Systems Approach: Higher-Dimensional Systems.
19. *Kaplan/Glass*: Understanding Nonlinear Dynamics.
20. *Holmes*: Introduction to Perturbation Methods.
21. *Curtain/Zwart*: An Introduction to Infinite-Dimensional Linear Systems Theory.
22. *Thomas*: Numerical Partial Differential Equations: Finite Difference Methods.
23. *Taylor*: Partial Differential Equations: Basic Theory.
24. *Merkin*: Introduction to the Theory of Stability of Motion.
25. *Naber*: Topology, Geometry, and Gauge Fields: Foundations.
26. *Polderman/Willems*: Introduction to Mathematical Systems Theory: A Behavioral Approach.
27. *Reddy*: Introductory Functional Analysis: with Applications to Boundary Value Problems and Finite Elements.
28. *Gustafson/Wilcox*: Analytical and Computational Methods of Advanced Engineering Mathematics.

(continued after index)

Alfio Quarteroni Riccardo Sacco Fausto Saleri

Numerical Mathematics

Second Edition

With 135 Figures and 45 Tables

 Springer

Alfio Quarteroni
SB-IACS-CMS, EPFL
1015 Lausanne, Switzerland
and
Dipartimento di Matematica-MOX
Politecnico di Milano
Piazza Leonardo da Vinci, 32
20133 Milano, Italy
E-mail: alfio.quarteroni@epfl.ch

Riccardo Sacco
Dipartimento di Matematica
Politecnico di Milano
Piazza Leonardo da Vinci, 32
20133 Milano, Italy
E-mail: riccardo.sacco@polimi.it

Fausto Saleri
Dipartimento di Matematica-MOX
Politecnico di Milano
Piazza Leonardo da Vinci, 32
20133 Milano, Italy
E-mail: fausto.saleri@polimi.it

Series Editors

J.E. Marsden
Control and Dynamical Systems
107-81 California Institute of Technology
Pasadena, CA 91125
USA
marsden@cds.caltech.edu

S.S. Antman
Department of Mathematics
and
Institute for Physical Science
and Technology
University of Maryland
College Oark, MD 20742-4015
USA
ssa@math.umd.edu

L. Sirovich
Laboratory of Applied Mathematics
Department of Biomathematics
Mt. Sinai School of Medicine
Box 1012
New York, NY 10029-6574
USA

Mathematics Subject Classification (2000): 15-01, 34-01, 35-01, 65-01

ISBN 0939-2475
ISBN-10 3-540-34658-9 Springer Berlin Heidelberg New York
ISBN-13 978-3-540-34658-6 Springer Berlin Heidelberg New York
Library of Congress Control Number: 2006930676

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer-Verlag. Violations are liable to prosecution under the German Copyright Law.

Springer is a part of Springer Science+Business Media.

springer.com

© Springer Berlin Heidelberg 2007

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Typesetting by the Authors and Spi using Springer L^AT_EX macro package
Cover design: design & production GmbH, Heidelberg

Printed on acid-free paper SPIN: 11304951 37/2244/SPi 5 4 3 2 1 0

Preface

Numerical mathematics is the branch of mathematics that proposes, develops, analyzes and applies methods from scientific computing to several fields including analysis, linear algebra, geometry, approximation theory, functional equations, optimization and differential equations. Other disciplines such as physics, the natural and biological sciences, engineering, and economics and the financial sciences frequently give rise to problems that need scientific computing for their solutions.

As such, numerical mathematics is the crossroad of several disciplines of great relevance in modern applied sciences, and can become a crucial tool for their qualitative and quantitative analysis. This role is also emphasized by the continual development of computers and algorithms, which make it possible nowadays, using scientific computing, to tackle problems of such a large size that real-life phenomena can be simulated providing accurate responses at affordable computational cost.

The corresponding spread of numerical software represents an enrichment for the scientific community. However, the user has to make the correct choice of the method (or the algorithm) which best suits the problem at hand. As a matter of fact, no black-box methods or algorithms exist that can effectively and accurately solve all kinds of problems.

One of the purposes of this book is to provide the mathematical foundations of numerical methods, to analyze their basic theoretical properties (stability, accuracy, computational complexity), and demonstrate their performances on examples and counterexamples which outline their pros and cons. This is done using the MATLAB[®]¹ software environment. This choice satisfies the two fundamental needs of user-friendliness and wide-spread diffusion, making it available on virtually every computer.

Every chapter is supplied with examples, exercises and applications of the discussed theory to the solution of real-life problems. The reader is thus in the ideal condition for acquiring the theoretical knowledge that is required to

¹ MATLAB is a trademark of The MathWorks, Inc.

make the right choice among the numerical methodologies and make use of the related computer programs.

This book is primarily addressed to undergraduate students, with particular focus on the degree courses in Engineering, Mathematics, Physics and Computer Science. The attention which is paid to the applications and the related development of software makes it valuable also for graduate students, researchers and users of scientific computing in the most widespread professional fields.

The content of the volume is organized into four Parts and 13 chapters.

Part I comprises two chapters in which we review basic linear algebra and introduce the general concepts of consistency, stability and convergence of a numerical method as well as the basic elements of computer arithmetic.

Part II is on numerical linear algebra, and is devoted to the solution of linear systems (Chapters 3 and 4) and eigenvalues and eigenvectors computation (Chapter 5).

We continue with Part III where we face several issues about functions and their approximation. Specifically, we are interested in the solution of nonlinear equations (Chapter 6), solution of nonlinear systems and optimization problems (Chapter 7), polynomial approximation (Chapter 8) and numerical integration (Chapter 9).

Part IV, which demands a mathematical background, is concerned with approximation, integration and transforms based on orthogonal polynomials (Chapter 10), solution of initial value problems (Chapter 11), boundary value problems (Chapter 12) and initial-boundary value problems for parabolic and hyperbolic equations (Chapter 13).

Part I provides the indispensable background. Each of the remaining Parts has a size and a content that make it well suited for a semester course.

A guideline index to the use of the numerous MATLAB programs developed in the book is reported at the end of the volume. These programs are also available at the web site address:

<http://www1.mate.polimi.it/~calnum/programs.html>

For the reader's ease, any code is accompanied by a brief description of its input/output parameters.

We express our thanks to the staff at Springer-Verlag New York for their expert guidance and assistance with editorial aspects, as well as to Dr. Martin Peters from Springer-Verlag Heidelberg and Dr. Francesca Bonadei from Springer-Italia for their advice and friendly collaboration all along this project.

We gratefully thank Professors L. Gastaldi and A. Valli for their useful comments on Chapters 12 and 13.

We also wish to express our gratitude to our families for their forbearance and understanding, and dedicate this book to them.

Lausanne, Milan
January 2000

Alfio Quarteroni
Riccardo Sacco
Fausto Saleri

Preface to the Second Edition

This second edition is characterized by a thorough overall revision.

Regarding the styling of the book, we have improved the readability of pictures, tables and program headings.

Regarding the scientific contents, we have introduced several changes in the chapter on iterative methods for the solution of linear systems as well as in the chapter on polynomial approximation of functions and data.

Lausanne, Milan
September 2006

Alfio Quarteroni
Riccardo Sacco
Fausto Saleri

Contents

Part I Getting Started

| | | |
|----------|-------------------------------------------------------------------------|-----------|
| 1 | Foundations of Matrix Analysis | 3 |
| 1.1 | Vector Spaces | 3 |
| 1.2 | Matrices | 5 |
| 1.3 | Operations with Matrices | 6 |
| 1.3.1 | Inverse of a Matrix | 7 |
| 1.3.2 | Matrices and Linear Mappings | 8 |
| 1.3.3 | Operations with Block-Partitioned Matrices | 9 |
| 1.4 | Trace and Determinant of a Matrix | 10 |
| 1.5 | Rank and Kernel of a Matrix | 11 |
| 1.6 | Special Matrices | 12 |
| 1.6.1 | Block Diagonal Matrices | 12 |
| 1.6.2 | Trapezoidal and Triangular Matrices | 12 |
| 1.6.3 | Banded Matrices | 13 |
| 1.7 | Eigenvalues and Eigenvectors | 13 |
| 1.8 | Similarity Transformations | 15 |
| 1.9 | The Singular Value Decomposition (SVD) | 17 |
| 1.10 | Scalar Product and Norms in Vector Spaces | 18 |
| 1.11 | Matrix Norms | 22 |
| 1.11.1 | Relation between Norms and the Spectral Radius of a Matrix | 25 |
| 1.11.2 | Sequences and Series of Matrices | 26 |
| 1.12 | Positive Definite, Diagonally Dominant and M-matrices | 27 |
| 1.13 | Exercises | 30 |
| 2 | Principles of Numerical Mathematics | 33 |
| 2.1 | Well-posedness and Condition Number of a Problem | 33 |
| 2.2 | Stability of Numerical Methods | 37 |
| 2.2.1 | Relations between Stability and Convergence | 40 |
| 2.3 | A priori and a posteriori Analysis | 42 |

| | | |
|-------|------------------------------------------------------------------|----|
| 2.4 | Sources of Error in Computational Models | 43 |
| 2.5 | Machine Representation of Numbers | 45 |
| 2.5.1 | The Positional System | 45 |
| 2.5.2 | The Floating-point Number System..... | 46 |
| 2.5.3 | Distribution of Floating-point Numbers | 49 |
| 2.5.4 | IEC/IEEE Arithmetic | 49 |
| 2.5.5 | Rounding of a Real Number in its Machine Representation | 50 |
| 2.5.6 | Machine Floating-point Operations | 52 |
| 2.6 | Exercises | 54 |

Part II Numerical Linear Algebra

| | | |
|----------|-------------------------------------------------------------------------------|-----------|
| 3 | Direct Methods for the Solution of Linear Systems | 59 |
| 3.1 | Stability Analysis of Linear Systems | 60 |
| 3.1.1 | The Condition Number of a Matrix..... | 60 |
| 3.1.2 | Forward a priori Analysis..... | 62 |
| 3.1.3 | Backward a priori Analysis | 65 |
| 3.1.4 | A posteriori Analysis | 65 |
| 3.2 | Solution of Triangular Systems | 66 |
| 3.2.1 | Implementation of Substitution Methods | 67 |
| 3.2.2 | Rounding Error Analysis | 69 |
| 3.2.3 | Inverse of a Triangular Matrix | 70 |
| 3.3 | The Gaussian Elimination Method (GEM) and LU Factorization..... | 70 |
| 3.3.1 | GEM as a Factorization Method | 73 |
| 3.3.2 | The Effect of Rounding Errors | 78 |
| 3.3.3 | Implementation of LU Factorization | 78 |
| 3.3.4 | Compact Forms of Factorization..... | 80 |
| 3.4 | Other Types of Factorization..... | 81 |
| 3.4.1 | LDM ^T Factorization | 81 |
| 3.4.2 | Symmetric and Positive Definite Matrices: The Cholesky Factorization | 82 |
| 3.4.3 | Rectangular Matrices: The QR Factorization..... | 84 |
| 3.5 | Pivoting..... | 87 |
| 3.6 | Computing the Inverse of a Matrix | 91 |
| 3.7 | Banded Systems..... | 92 |
| 3.7.1 | Tridiagonal Matrices | 93 |
| 3.7.2 | Implementation Issues | 94 |
| 3.8 | Block Systems | 96 |
| 3.8.1 | Block LU Factorization | 97 |
| 3.8.2 | Inverse of a Block-partitioned Matrix | 97 |
| 3.8.3 | Block Tridiagonal Systems..... | 98 |
| 3.9 | Sparse Matrices | 99 |

| | | |
|----------|------------------------------------------------------------------|------------|
| 3.9.1 | The Cuthill-McKee Algorithm | 102 |
| 3.9.2 | Decomposition into Substructures | 103 |
| 3.9.3 | Nested Dissection | 105 |
| 3.10 | Accuracy of the Solution Achieved Using GEM | 106 |
| 3.11 | An Approximate Computation of $K(A)$ | 108 |
| 3.12 | Improving the Accuracy of GEM | 112 |
| 3.12.1 | Scaling | 112 |
| 3.12.2 | Iterative Refinement | 113 |
| 3.13 | Undetermined Systems | 114 |
| 3.14 | Applications | 117 |
| 3.14.1 | Nodal Analysis of a Structured Frame | 117 |
| 3.14.2 | Regularization of a Triangular Grid | 120 |
| 3.15 | Exercises | 123 |
| 4 | Iterative Methods for Solving Linear Systems | 125 |
| 4.1 | On the Convergence of Iterative Methods | 125 |
| 4.2 | Linear Iterative Methods | 128 |
| 4.2.1 | Jacobi, Gauss-Seidel and Relaxation Methods | 128 |
| 4.2.2 | Convergence Results for Jacobi and Gauss-Seidel Methods | 130 |
| 4.2.3 | Convergence Results for the Relaxation Method | 132 |
| 4.2.4 | A priori Forward Analysis | 133 |
| 4.2.5 | Block Matrices | 134 |
| 4.2.6 | Symmetric Form of the Gauss-Seidel and SOR Methods | 135 |
| 4.2.7 | Implementation Issues | 137 |
| 4.3 | Stationary and Nonstationary Iterative Methods | 138 |
| 4.3.1 | Convergence Analysis of the Richardson Method | 139 |
| 4.3.2 | Preconditioning Matrices | 141 |
| 4.3.3 | The Gradient Method | 148 |
| 4.3.4 | The Conjugate Gradient Method | 152 |
| 4.3.5 | The Preconditioned Conjugate Gradient Method | 158 |
| 4.3.6 | The Alternating-Direction Method | 160 |
| 4.4 | Methods Based on Krylov Subspace Iterations | 160 |
| 4.4.1 | The Arnoldi Method for Linear Systems | 164 |
| 4.4.2 | The GMRES Method | 167 |
| 4.4.3 | The Lanczos Method for Symmetric Systems | 168 |
| 4.5 | The Lanczos Method for Unsymmetric Systems | 170 |
| 4.6 | Stopping Criteria | 173 |
| 4.6.1 | A Stopping Test Based on the Increment | 174 |
| 4.6.2 | A Stopping Test Based on the Residual | 175 |
| 4.7 | Applications | 175 |
| 4.7.1 | Analysis of an Electric Network | 176 |
| 4.7.2 | Finite Difference Analysis of Beam Bending | 178 |
| 4.8 | Exercises | 180 |

| | | |
|----------|---------------------------------------------------------------|-----|
| 5 | Approximation of Eigenvalues and Eigenvectors | 183 |
| 5.1 | Geometrical Location of the Eigenvalues | 183 |
| 5.2 | Stability and Conditioning Analysis | 186 |
| 5.2.1 | A priori Estimates | 187 |
| 5.2.2 | A posteriori Estimates | 190 |
| 5.3 | The Power Method | 192 |
| 5.3.1 | Approximation of the Eigenvalue of Largest Module | 192 |
| 5.3.2 | Inverse Iteration | 195 |
| 5.3.3 | Implementation Issues | 196 |
| 5.4 | The QR Iteration | 199 |
| 5.5 | The Basic QR Iteration | 201 |
| 5.6 | The QR Method for Matrices in Hessenberg Form | 203 |
| 5.6.1 | Householder and Givens Transformation Matrices | 203 |
| 5.6.2 | Reducing a Matrix in Hessenberg Form | 207 |
| 5.6.3 | QR Factorization of a Matrix in Hessenberg Form | 209 |
| 5.6.4 | The Basic QR Iteration Starting from Upper Hessenberg Form | 209 |
| 5.6.5 | Implementation of Transformation Matrices | 212 |
| 5.7 | The QR Iteration with Shifting Techniques | 214 |
| 5.7.1 | The QR Method with Single Shift | 215 |
| 5.7.2 | The QR Method with Double Shift | 217 |
| 5.8 | Computing the Eigenvectors and the SVD of a Matrix | 220 |
| 5.8.1 | The Hessenberg Inverse Iteration | 220 |
| 5.8.2 | Computing the Eigenvectors from the Schur Form of a Matrix | 221 |
| 5.8.3 | Approximate Computation of the SVD of a Matrix | 222 |
| 5.9 | The Generalized Eigenvalue Problem | 223 |
| 5.9.1 | Computing the Generalized Real Schur Form | 224 |
| 5.9.2 | Generalized Real Schur Form of Symmetric-Definite Pencils | 225 |
| 5.10 | Methods for Eigenvalues of Symmetric Matrices | 226 |
| 5.10.1 | The Jacobi Method | 226 |
| 5.10.2 | The Method of Sturm Sequences | 229 |
| 5.11 | The Lanczos Method | 233 |
| 5.12 | Applications | 236 |
| 5.12.1 | Analysis of the Buckling of a Beam | 236 |
| 5.12.2 | Free Dynamic Vibration of a Bridge | 238 |
| 5.13 | Exercises | 240 |

Part III Around Functions and Functionals

| | | |
|----------|--------------------------------------------------------------------------------|-----|
| 6 | Rootfinding for Nonlinear Equations | 247 |
| 6.1 | Conditioning of a Nonlinear Equation | 248 |
| 6.2 | A Geometric Approach to Rootfinding | 250 |
| 6.2.1 | The Bisection Method | 250 |
| 6.2.2 | The Methods of Chord, Secant and Regula Falsi and Newton's Method | 253 |
| 6.2.3 | The Dekker-Brent Method | 259 |
| 6.3 | Fixed-point Iterations for Nonlinear Equations | 260 |
| 6.3.1 | Convergence Results for Some Fixed-point Methods | 263 |
| 6.4 | Zeros of Algebraic Equations | 264 |
| 6.4.1 | The Horner Method and Deflation | 265 |
| 6.4.2 | The Newton-Horner Method | 266 |
| 6.4.3 | The Muller Method | 269 |
| 6.5 | Stopping Criteria | 273 |
| 6.6 | Post-processing Techniques for Iterative Methods | 275 |
| 6.6.1 | Aitken's Acceleration | 275 |
| 6.6.2 | Techniques for Multiple Roots | 278 |
| 6.7 | Applications | 280 |
| 6.7.1 | Analysis of the State Equation for a Real Gas | 280 |
| 6.7.2 | Analysis of a Nonlinear Electrical Circuit | 281 |
| 6.8 | Exercises | 283 |
| 7 | Nonlinear Systems and Numerical Optimization | 285 |
| 7.1 | Solution of Systems of Nonlinear Equations | 286 |
| 7.1.1 | Newton's Method and Its Variants | 286 |
| 7.1.2 | Modified Newton's Methods | 288 |
| 7.1.3 | Quasi-Newton Methods | 292 |
| 7.1.4 | Secant-like Methods | 292 |
| 7.1.5 | Fixed-point Methods | 295 |
| 7.2 | Unconstrained Optimization | 298 |
| 7.2.1 | Direct Search Methods | 300 |
| 7.2.2 | Descent Methods | 305 |
| 7.2.3 | Line Search Techniques | 307 |
| 7.2.4 | Descent Methods for Quadratic Functions | 309 |
| 7.2.5 | Newton-like Methods for Function Minimization | 311 |
| 7.2.6 | Quasi-Newton Methods | 312 |
| 7.2.7 | Secant-like methods | 313 |
| 7.3 | Constrained Optimization | 315 |
| 7.3.1 | Kuhn-Tucker Necessary Conditions for Nonlinear Programming | 318 |
| 7.3.2 | The Penalty Method | 319 |

| | | |
|----------|-------------------------------------------------------------------------------------------------------|------------|
| 7.3.3 | The Method of Lagrange Multipliers | 321 |
| 7.4 | Applications | 325 |
| 7.4.1 | Solution of a Nonlinear System Arising from Semiconductor Device Simulation | 325 |
| 7.4.2 | Nonlinear Regularization of a Discretization Grid | 328 |
| 7.5 | Exercises | 330 |
| 8 | Polynomial Interpolation | 333 |
| 8.1 | Polynomial Interpolation | 333 |
| 8.1.1 | The Interpolation Error | 335 |
| 8.1.2 | Drawbacks of Polynomial Interpolation on Equally Spaced Nodes and Runge's Counterexample | 336 |
| 8.1.3 | Stability of Polynomial Interpolation | 337 |
| 8.2 | Newton Form of the Interpolating Polynomial | 339 |
| 8.2.1 | Some Properties of Newton Divided Differences | 341 |
| 8.2.2 | The Interpolation Error Using Divided Differences | 343 |
| 8.3 | Barycentric Lagrange Interpolation | 344 |
| 8.4 | Piecewise Lagrange Interpolation | 346 |
| 8.5 | Hermite-Birkoff Interpolation | 349 |
| 8.6 | Extension to the Two-Dimensional Case | 351 |
| 8.6.1 | Polynomial Interpolation | 351 |
| 8.6.2 | Piecewise Polynomial Interpolation | 352 |
| 8.7 | Approximation by Splines | 355 |
| 8.7.1 | Interpolatory Cubic Splines | 357 |
| 8.7.2 | B-splines | 361 |
| 8.8 | Splines in Parametric Form | 365 |
| 8.8.1 | Bézier Curves and Parametric B-splines | 367 |
| 8.9 | Applications | 370 |
| 8.9.1 | Finite Element Analysis of a Clamped Beam | 370 |
| 8.9.2 | Geometric Reconstruction Based on Computer Tomographies | 374 |
| 8.10 | Exercises | 375 |
| 9 | Numerical Integration | 379 |
| 9.1 | Quadrature Formulae | 379 |
| 9.2 | Interpolatory Quadratures | 381 |
| 9.2.1 | The Midpoint or Rectangle Formula | 381 |
| 9.2.2 | The Trapezoidal Formula | 383 |
| 9.2.3 | The Cavalieri-Simpson Formula | 385 |
| 9.3 | Newton-Cotes Formulae | 386 |
| 9.4 | Composite Newton-Cotes Formulae | 392 |
| 9.5 | Hermite Quadrature Formulae | 394 |
| 9.6 | Richardson Extrapolation | 396 |
| 9.6.1 | Romberg Integration | 397 |
| 9.7 | Automatic Integration | 400 |

| | | |
|--------|----------------------------------------------------------------------|-----|
| 9.7.1 | Nonadaptive Integration Algorithms | 400 |
| 9.7.2 | Adaptive Integration Algorithms | 402 |
| 9.8 | Singular Integrals | 406 |
| 9.8.1 | Integrals of Functions with Finite Jump Discontinuities | 406 |
| 9.8.2 | Integrals of Infinite Functions | 407 |
| 9.8.3 | Integrals over Unbounded Intervals | 409 |
| 9.9 | Multidimensional Numerical Integration | 411 |
| 9.9.1 | The Method of Reduction Formula | 411 |
| 9.9.2 | Two-Dimensional Composite Quadratures | 413 |
| 9.9.3 | Monte Carlo Methods for Numerical Integration | 416 |
| 9.10 | Applications | 417 |
| 9.10.1 | Computation of an Ellipsoid Surface | 417 |
| 9.10.2 | Computation of the Wind Action on a Sailboat Mast | 418 |
| 9.11 | Exercises | 421 |

Part IV Transforms, Differentiation and Problem Discretization

| | | |
|-----------|----------------------------------------------------------------------|------------|
| 10 | Orthogonal Polynomials in Approximation Theory | 425 |
| 10.1 | Approximation of Functions by Generalized Fourier Series | 425 |
| 10.1.1 | The Chebyshev Polynomials | 427 |
| 10.1.2 | The Legendre Polynomials | 428 |
| 10.2 | Gaussian Integration and Interpolation | 429 |
| 10.3 | Chebyshev Integration and Interpolation | 433 |
| 10.4 | Legendre Integration and Interpolation | 436 |
| 10.5 | Gaussian Integration over Unbounded Intervals | 438 |
| 10.6 | Programs for the Implementation of Gaussian Quadratures | 439 |
| 10.7 | Approximation of a Function in the Least-Squares Sense | 441 |
| 10.7.1 | Discrete Least-Squares Approximation | 442 |
| 10.8 | The Polynomial of Best Approximation | 443 |
| 10.9 | Fourier Trigonometric Polynomials | 445 |
| 10.9.1 | The Gibbs Phenomenon | 449 |
| 10.9.2 | The Fast Fourier Transform | 450 |
| 10.10 | Approximation of Function Derivatives | 452 |
| 10.10.1 | Classical Finite Difference Methods | 452 |
| 10.10.2 | Compact Finite Differences | 454 |
| 10.10.3 | Pseudo-Spectral Derivative | 458 |
| 10.11 | Transforms and Their Applications | 460 |
| 10.11.1 | The Fourier Transform | 460 |
| 10.11.2 | (Physical) Linear Systems and Fourier Transform | 463 |
| 10.11.3 | The Laplace Transform | 465 |
| 10.11.4 | The Z-Transform | 467 |

| | | |
|-----------|---------------------------------------------------------------------------------------------|------------|
| 10.12 | The Wavelet Transform | 468 |
| 10.12.1 | The Continuous Wavelet Transform..... | 468 |
| 10.12.2 | Discrete and Orthonormal Wavelets | 471 |
| 10.13 | Applications | 472 |
| 10.13.1 | Numerical Computation of Blackbody Radiation ... | 472 |
| 10.13.2 | Numerical Solution of Schrödinger Equation | 474 |
| 10.14 | Exercises | 476 |
| 11 | Numerical Solution of Ordinary Differential Equations | 479 |
| 11.1 | The Cauchy Problem | 479 |
| 11.2 | One-Step Numerical Methods | 482 |
| 11.3 | Analysis of One-Step Methods | 483 |
| 11.3.1 | The Zero-Stability | 484 |
| 11.3.2 | Convergence Analysis | 486 |
| 11.3.3 | The Absolute Stability | 489 |
| 11.4 | Difference Equations | 492 |
| 11.5 | Multistep Methods | 497 |
| 11.5.1 | Adams Methods..... | 500 |
| 11.5.2 | BDF Methods | 502 |
| 11.6 | Analysis of Multistep Methods | 502 |
| 11.6.1 | Consistency | 502 |
| 11.6.2 | The Root Conditions | 504 |
| 11.6.3 | Stability and Convergence Analysis for Multistep Methods | 505 |
| 11.6.4 | Absolute Stability of Multistep Methods | 509 |
| 11.7 | Predictor-Corrector Methods..... | 511 |
| 11.8 | Runge-Kutta (RK) Methods | 518 |
| 11.8.1 | Derivation of an Explicit RK Method | 521 |
| 11.8.2 | Stepsize Adaptivity for RK Methods..... | 521 |
| 11.8.3 | Implicit RK Methods | 523 |
| 11.8.4 | Regions of Absolute Stability for RK Methods | 525 |
| 11.9 | Systems of ODEs | 526 |
| 11.10 | Stiff Problems..... | 528 |
| 11.11 | Applications | 530 |
| 11.11.1 | Analysis of the Motion of a Frictionless Pendulum .. | 531 |
| 11.11.2 | Compliance of Arterial Walls | 532 |
| 11.12 | Exercises | 536 |
| 12 | Two-Point Boundary Value Problems | 539 |
| 12.1 | A Model Problem | 539 |
| 12.2 | Finite Difference Approximation..... | 541 |
| 12.2.1 | Stability Analysis by the Energy Method | 542 |
| 12.2.2 | Convergence Analysis | 546 |
| 12.2.3 | Finite Differences for Two-Point Boundary Value Problems with Variable Coefficients..... | 548 |

| | | |
|-----------|-------------------------------------------------------------------------------------------------------|------------|
| 12.3 | The Spectral Collocation Method | 550 |
| 12.4 | The Galerkin Method | 552 |
| 12.4.1 | Integral Formulation of Boundary Value Problems . . | 552 |
| 12.4.2 | A Quick Introduction to Distributions | 554 |
| 12.4.3 | Formulation and Properties of the Galerkin Method | 555 |
| 12.4.4 | Analysis of the Galerkin Method | 556 |
| 12.4.5 | The Finite Element Method | 558 |
| 12.4.6 | Implementation Issues | 564 |
| 12.4.7 | Spectral Methods | 566 |
| 12.5 | Advection-Diffusion Equations | 568 |
| 12.5.1 | Galerkin Finite Element Approximation | 569 |
| 12.5.2 | The Relationship between Finite Elements and Finite Differences; the Numerical Viscosity | 572 |
| 12.5.3 | Stabilized Finite Element Methods | 574 |
| 12.6 | A Quick Glance at the Two-Dimensional Case | 580 |
| 12.7 | Applications | 583 |
| 12.7.1 | Lubrication of a Slider | 583 |
| 12.7.2 | Vertical Distribution of Spore Concentration over Wide Regions | 584 |
| 12.8 | Exercises | 586 |
| 13 | Parabolic and Hyperbolic Initial Boundary Value Problems | 589 |
| 13.1 | The Heat Equation | 589 |
| 13.2 | Finite Difference Approximation of the Heat Equation | 591 |
| 13.3 | Finite Element Approximation of the Heat Equation | 593 |
| 13.3.1 | Stability Analysis of the θ -Method | 595 |
| 13.4 | Space-Time Finite Element Methods for the Heat Equation | 601 |
| 13.5 | Hyperbolic Equations: A Scalar Transport Problem | 604 |
| 13.6 | Systems of Linear Hyperbolic Equations | 607 |
| 13.6.1 | The Wave Equation | 608 |
| 13.7 | The Finite Difference Method for Hyperbolic Equations . . . | 609 |
| 13.7.1 | Discretization of the Scalar Equation | 610 |
| 13.8 | Analysis of Finite Difference Methods | 611 |
| 13.8.1 | Consistency | 612 |
| 13.8.2 | Stability | 612 |
| 13.8.3 | The CFL Condition | 613 |
| 13.8.4 | Von Neumann Stability Analysis | 615 |
| 13.9 | Dissipation and Dispersion | 618 |
| 13.9.1 | Equivalent Equations | 619 |
| 13.10 | Finite Element Approximation of Hyperbolic Equations . . . | 624 |
| 13.10.1 | Space Discretization with Continuous and Discontinuous Finite Elements | 625 |

XVIII Contents

| | |
|------------------------------------------------------------------------------------|------------|
| 13.10.2 Time Discretization | 627 |
| 13.11 Applications | 630 |
| 13.11.1 Heat Conduction in a Bar | 630 |
| 13.11.2 A Hyperbolic Model for Blood Flow Interaction with Arterial Walls | 630 |
| 13.12 Exercises | 632 |
| References | 635 |
| Index of MATLAB Programs | 645 |
| Index | 649 |