Contents

Series Preface v

Preface vii

PART I: Getting Started

1. Foundations of Matrix Analysis 1

1.1 Vector Spaces 1
1.2 Matrices 3
1.3 Operations with Matrices 5
1.3.1 Inverse of a Matrix 6
1.3.2 Matrices and Linear Mappings 7
1.3.3 Operations with Block-Partitioned Matrices 7
1.4 Trace and Determinant of a Matrix 8
1.5 Rank and Kernel of a Matrix 9
1.6 Special Matrices 10
1.6.1 Block Diagonal Matrices 10
1.6.2 Trapezoidal and Triangular Matrices 11
1.6.3 Banded Matrices 11
1.7 Eigenvalues and Eigenvectors 12
1.8 Similarity Transformations 14
1.9 The Singular Value Decomposition (SVD) 16
1.10 Scalar Product and Norms in Vector Spaces 17
1.11 Matrix Norms 21

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 . . . 41
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 **57**
3.1 Stability Analysis of Linear Systems . . . 58
3.1.1 The Condition Number of a Matrix . . . 58
3.1.2 Forward *a priori* Analysis . . . 60
3.1.3 Backward *a priori* Analysis . . . 63
3.1.4 *A posteriori* Analysis . . . 64
3.2 Solution of Triangular Systems . . . 65
3.2.1 Implementation of Substitution Methods . . . 65
3.2.2 Rounding Error Analysis . . . 67
3.2.3 Inverse of a Triangular Matrix . . . 67
3.3 The Gaussian Elimination Method (GEM) and LU Factorization . . . 68
3.3.1 GEM as a Factorization Method . . . 72
3.3.2 The Effect of Rounding Errors . . . 76
3.3.3 Implementation of LU Factorization . . . 77
3.3.4 Compact Forms of Factorization . . . 78
3.4 Other Types of Factorization . . . 79
3.4.1 LDM^T Factorization . . . 79
3.4.2 Symmetric and Positive Definite Matrices: The Cholesky Factorization . . . 80
3.4.3 Rectangular Matrices: The QR Factorization . . . 82

3.5 Pivoting . . . 85
3.6 Computing the Inverse of a Matrix . . . 89
3.7 Banded Systems . . . 90
3.7.1 Tridiagonal Matrices . . . 91
3.7.2 Implementation Issues . . . 92
3.8 Block Systems . . . 93
3.8.1 Block LU Factorization . . . 94
3.8.2 Inverse of a Block-Partitioned Matrix . . . 95
3.8.3 Block Tridiagonal Systems . . . 95
3.9 Sparse Matrices . . . 97
3.9.1 The Cuthill-McKee Algorithm . . . 98
3.9.2 Decomposition into Substructures . . . 100
3.9.3 Nested Dissection . . . 103
3.10 Accuracy of the Solution Achieved Using GEM . . . 103
3.11 An Approximate Computation of $K(\mathrm{A})$ . . . 106
3.12 Improving the Accuracy of GEM . . . 109
3.12.1 Scaling . . . 110
3.12.2 Iterative Refinement . . . 111
3.13 Undetermined Systems . . . 112
3.14 Applications . . . 115
3.14.1 Nodal Analysis of a Structured Frame . . . 115
3.14.2 Regularization of a Triangular Grid . . . 118
3.15 Exercises . . . 121

4. Iterative Methods for Solving Linear Systems 123
4.1 On the Convergence of Iterative Methods . . . 123
4.2 Linear Iterative Methods . . . 126
4.2.1 Jacobi, Gauss-Seidel and Relaxation Methods . . . 127
4.2.2 Convergence Results for Jacobi and Gauss-Seidel Methods . . . 129
4.2.3 Convergence Results for the Relaxation Method . . . 131
4.2.4 *A priori* Forward Analysis . . . 132
4.2.5 Block Matrices . . . 133
4.2.6 Symmetric Form of the Gauss-Seidel and SOR Methods . . . 133
4.2.7 Implementation Issues . . . 135
4.3 Stationary and Nonstationary Iterative Methods . . . 136
4.3.1 Convergence Analysis of the Richardson Method . . . 137
4.3.2 Preconditioning Matrices . . . 139
4.3.3 The Gradient Method . . . 146
4.3.4 The Conjugate Gradient Method . . . 150
4.3.5 The Preconditioned Conjugate Gradient Method . . . 156
4.3.6 The Alternating-Direction Method . . . 158
4.4 Methods Based on Krylov Subspace Iterations . . . 159
4.4.1 The Arnoldi Method for Linear Systems . . . 162

4.4.2 The GMRES Method . . . 165
4.4.3 The Lanczos Method for Symmetric Systems . . . 167
4.5 The Lanczos Method for Unsymmetric Systems . . . 168
4.6 Stopping Criteria . . . 171
4.6.1 A Stopping Test Based on the Increment . . . 172
4.6.2 A Stopping Test Based on the Residual . . . 174
4.7 Applications . . . 174
4.7.1 Analysis of an Electric Network . . . 174
4.7.2 Finite Difference Analysis of Beam Bending . . . 177
4.8 Exercises . . . 179

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 . . . 186
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 . . . 200
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 204
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 . . . 210
5.6.5 Implementation of Transformation Matrices . . . 212
5.7 The QR Iteration with Shifting Techniques . . . 215
5.7.1 The QR Method with Single Shift . . . 215
5.7.2 The QR Method with Double Shift . . . 218
5.8 Computing the Eigenvectors and the SVD of a Matrix . . 221
5.8.1 The Hessenberg Inverse Iteration . . . 221
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 . . . 224
5.9.1 Computing the Generalized Real Schur Form . . . 225
5.9.2 Generalized Real Schur Form of Symmetric-Definite Pencils . . . 226
5.10 Methods for Eigenvalues of Symmetric Matrices . . . 227
5.10.1 The Jacobi Method . . . 227
5.10.2 The Method of Sturm Sequences . . . 230

5.11 The Lanczos Method 233
5.12 Applications 235
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 245
6.1 Conditioning of a Nonlinear Equation 246
6.2 A Geometric Approach to Rootfinding 248
6.2.1 The Bisection Method 248
6.2.2 The Methods of Chord, Secant and Regula Falsi and Newton's Method 251
6.2.3 The Dekker-Brent Method 256
6.3 Fixed-Point Iterations for Nonlinear Equations 257
6.3.1 Convergence Results for Some Fixed-Point Methods 260
6.4 Zeros of Algebraic Equations 261
6.4.1 The Horner Method and Deflation 262
6.4.2 The Newton-Horner Method 263
6.4.3 The Muller Method 267
6.5 Stopping Criteria 269
6.6 Post-Processing Techniques for Iterative Methods 272
6.6.1 Aitken's Acceleration 272
6.6.2 Techniques for Multiple Roots 275
6.7 Applications 276
6.7.1 Analysis of the State Equation for a Real Gas . . 276
6.7.2 Analysis of a Nonlinear Electrical Circuit 277
6.8 Exercises 279

7. Nonlinear Systems and Numerical Optimization 281
7.1 Solution of Systems of Nonlinear Equations 282
7.1.1 Newton's Method and Its Variants 283
7.1.2 Modified Newton's Methods 284
7.1.3 Quasi-Newton Methods 288
7.1.4 Secant-Like Methods 288
7.1.5 Fixed-Point Methods 290
7.2 Unconstrained Optimization 294
7.2.1 Direct Search Methods 295
7.2.2 Descent Methods 300
7.2.3 Line Search Techniques 302
7.2.4 Descent Methods for Quadratic Functions 304
7.2.5 Newton-Like Methods for Function Minimization . 307
7.2.6 Quasi-Newton Methods 308

7.2.7 Secant-Like Methods 309
7.3 Constrained Optimization 311
7.3.1 Kuhn-Tucker Necessary Conditions for Nonlinear Programming 313
7.3.2 The Penalty Method 315
7.3.3 The Method of Lagrange Multipliers 317
7.4 Applications 319
7.4.1 Solution of a Nonlinear System Arising from Semiconductor Device Simulation 320
7.4.2 Nonlinear Regularization of a Discretization Grid . 323
7.5 Exercises 325

8. Polynomial Interpolation **327**
8.1 Polynomial Interpolation 328
8.1.1 The Interpolation Error 329
8.1.2 Drawbacks of Polynomial Interpolation on Equally Spaced Nodes and Runge's Counterexample 330
8.1.3 Stability of Polynomial Interpolation 332
8.2 Newton Form of the Interpolating Polynomial 333
8.2.1 Some Properties of Newton Divided Differences . . 335
8.2.2 The Interpolation Error Using Divided Differences 337
8.3 Piecewise Lagrange Interpolation 338
8.4 Hermite-Birkoff Interpolation 341
8.5 Extension to the Two-Dimensional Case 343
8.5.1 Polynomial Interpolation 343
8.5.2 Piecewise Polynomial Interpolation 344
8.6 Approximation by Splines 348
8.6.1 Interpolatory Cubic Splines 349
8.6.2 B-Splines 353
8.7 Splines in Parametric Form 357
8.7.1 Bézier Curves and Parametric B-Splines 359
8.8 Applications 362
8.8.1 Finite Element Analysis of a Clamped Beam . . . 363
8.8.2 Geometric Reconstruction Based on Computer Tomographies 366
8.9 Exercises 368

9. Numerical Integration **371**
9.1 Quadrature Formulae 371
9.2 Interpolatory Quadratures 373
9.2.1 The Midpoint or Rectangle Formula 373
9.2.2 The Trapezoidal Formula 375
9.2.3 The Cavalieri-Simpson Formula 377
9.3 Newton-Cotes Formulae 378
9.4 Composite Newton-Cotes Formulae 383

9.5 Hermite Quadrature Formulae 386
9.6 Richardson Extrapolation 387
9.6.1 Romberg Integration 389
9.7 Automatic Integration 391
9.7.1 Non Adaptive Integration Algorithms 392
9.7.2 Adaptive Integration Algorithms 394
9.8 Singular Integrals 398
9.8.1 Integrals of Functions with Finite Jump Discontinuities 398
9.8.2 Integrals of Infinite Functions 398
9.8.3 Integrals over Unbounded Intervals 401
9.9 Multidimensional Numerical Integration 402
9.9.1 The Method of Reduction Formula 403
9.9.2 Two-Dimensional Composite Quadratures 404
9.9.3 Monte Carlo Methods for Numerical Integration 407
9.10 Applications 408
9.10.1 Computation of an Ellipsoid Surface 408
9.10.2 Computation of the Wind Action on a Sailboat Mast 410
9.11 Exercises 412

PART IV: Transforms, Differentiation and Problem Discretization

10. Orthogonal Polynomials in Approximation Theory 415
10.1 Approximation of Functions by Generalized Fourier Series 415
10.1.1 The Chebyshev Polynomials 417
10.1.2 The Legendre Polynomials 419
10.2 Gaussian Integration and Interpolation 419
10.3 Chebyshev Integration and Interpolation 424
10.4 Legendre Integration and Interpolation 426
10.5 Gaussian Integration over Unbounded Intervals 428
10.6 Programs for the Implementation of Gaussian Quadratures 429
10.7 Approximation of a Function in the Least-Squares Sense . 431
10.7.1 Discrete Least-Squares Approximation 431
10.8 The Polynomial of Best Approximation 433
10.9 Fourier Trigonometric Polynomials 435
10.9.1 The Gibbs Phenomenon 439
10.9.2 The Fast Fourier Transform 440
10.10 Approximation of Function Derivatives 442
10.10.1 Classical Finite Difference Methods 442
10.10.2 Compact Finite Differences 444
10.10.3 Pseudo-Spectral Derivative 448
10.11 Transforms and Their Applications 450

10.11.1 The Fourier Transform 450
10.11.2 (Physical) Linear Systems and Fourier Transform . 453
10.11.3 The Laplace Transform 455
10.11.4 The Z-Transform 457
10.12 The Wavelet Transform 458
10.12.1 The Continuous Wavelet Transform 458
10.12.2 Discrete and Orthonormal Wavelets 461
10.13 Applications 463
10.13.1 Numerical Computation of Blackbody Radiation . 463
10.13.2 Numerical Solution of Schrödinger Equation 464
10.14 Exercises 467

11. Numerical Solution of Ordinary Differential Equations 469
11.1 The Cauchy Problem 469
11.2 One-Step Numerical Methods 472
11.3 Analysis of One-Step Methods 473
11.3.1 The Zero-Stability 475
11.3.2 Convergence Analysis 477
11.3.3 The Absolute Stability 479
11.4 Difference Equations 482
11.5 Multistep Methods 487
11.5.1 Adams Methods 490
11.5.2 BDF Methods 492
11.6 Analysis of Multistep Methods 492
11.6.1 Consistency 493
11.6.2 The Root Conditions 494
11.6.3 Stability and Convergence Analysis for Multistep Methods 495
11.6.4 Absolute Stability of Multistep Methods 499
11.7 Predictor-Corrector Methods 502
11.8 Runge-Kutta Methods 508
11.8.1 Derivation of an Explicit RK Method 511
11.8.2 Stepsize Adaptivity for RK Methods 512
11.8.3 Implicit RK Methods 514
11.8.4 Regions of Absolute Stability for RK Methods . . 516
11.9 Systems of ODEs 517
11.10 Stiff Problems 519
11.11 Applications 521
11.11.1 Analysis of the Motion of a Frictionless Pendulum 522
11.11.2 Compliance of Arterial Walls 523
11.12 Exercises 527

12. Two-Point Boundary Value Problems 531
12.1 A Model Problem 531
12.2 Finite Difference Approximation 533

12.2.1 Stability Analysis by the Energy Method 534
12.2.2 Convergence Analysis 538
12.2.3 Finite Differences for Two-Point Boundary Value Problems with Variable Coefficients 540
12.3 The Spectral Collocation Method 542
12.4 The Galerkin Method 544
12.4.1 Integral Formulation of Boundary-Value Problems 544
12.4.2 A Quick Introduction to Distributions 546
12.4.3 Formulation and Properties of the Galerkin Method 547
12.4.4 Analysis of the Galerkin Method 548
12.4.5 The Finite Element Method 550
12.4.6 Implementation Issues 556
12.4.7 Spectral Methods 559
12.5 Advection-Diffusion Equations 560
12.5.1 Galerkin Finite Element Approximation 561
12.5.2 The Relationship Between Finite Elements and Finite Differences; the Numerical Viscosity 563
12.5.3 Stabilized Finite Element Methods 567
12.6 A Quick Glance to the Two-Dimensional Case 572
12.7 Applications 575
12.7.1 Lubrication of a Slider 575
12.7.2 Vertical Distribution of Spore Concentration over Wide Regions 576
12.8 Exercises 578

13. Parabolic and Hyperbolic Initial Boundary Value Problems **581**
13.1 The Heat Equation 581
13.2 Finite Difference Approximation of the Heat Equation . . 584
13.3 Finite Element Approximation of the Heat Equation . . . 586
13.3.1 Stability Analysis of the θ-Method 588
13.4 Space-Time Finite Element Methods for the Heat Equation 593
13.5 Hyperbolic Equations: A Scalar Transport Problem 597
13.6 Systems of Linear Hyperbolic Equations 599
13.6.1 The Wave Equation 601
13.7 The Finite Difference Method for Hyperbolic Equations . . 602
13.7.1 Discretization of the Scalar Equation 602
13.8 Analysis of Finite Difference Methods 605
13.8.1 Consistency 605
13.8.2 Stability 605
13.8.3 The CFL Condition 606
13.8.4 Von Neumann Stability Analysis 608
13.9 Dissipation and Dispersion 611

13.9.1 Equivalent Equations 614
13.10 Finite Element Approximation of Hyperbolic Equations . . 618
13.10.1 Space Discretization with Continuous and Discontinuous Finite Elements 618
13.10.2 Time Discretization 620
13.11 Applications 623
13.11.1 Heat Conduction in a Bar 623
13.11.2 A Hyperbolic Model for Blood Flow Interaction with Arterial Walls 623
13.12 Exercises 625

References **627**

Index of MATLAB Programs **643**

Index **647**