

Contents

1 Computer Numbers, Error Analysis, Conditioning, Stability of Algorithms and Operations Count	1
1.1 Definition of Errors	1
1.2 Decimal Representation of Numbers	3
1.3 Sources of Errors	6
1.3.1 Input Errors	6
1.3.2 Procedural Errors	7
1.3.3 Error Propagation and the Condition of a Problem	7
1.3.4 The Computational Error and Numerical Stability of an Algorithm	10
1.4 Operations Count, et cetera	11
2 Nonlinear Equations in One Variable	13
2.1 Introduction	13
2.2 Definitions and Theorems on Roots	14
2.3 General Iteration Procedures	15
2.3.1 How to Construct an Iterative Process	15
2.3.2 Existence and Uniqueness of Solutions	16
2.3.3 Convergence and Error Estimates of Iterative Procedures ..	17
2.3.4 Practical Implementation	20
2.4 Order of Convergence of an Iterative Procedure	22
2.4.1 Definitions and Theorems	22
2.4.2 Determining the Order of Convergence Experimentally	24
2.5 Newton's Method	25
2.5.1 Finding Simple Roots	25
2.5.2 A Damped Version of Newton's Method	27
2.5.3 Newton's Method for Multiple Zeros; a Modified Newton's Method	27

2.6 Regula Falsi	28
2.6.1 Regula Falsi for Simple Roots	28
2.6.2 Modified Regula Falsi for Multiple Zeros	30
2.6.3 Simplest Version of the Regula Falsi	30
2.7 Steffensen Method	31
2.7.1 Steffensen Method for Simple Zeros	31
2.7.2 Modified Steffensen Method for Multiple Zeros	31
2.8 Inclusion Methods	32
2.8.1 Bisection Method	32
2.8.2 Pegasus Method	34
2.8.3 Anderson-Björck Method	36
2.8.4 The King and the Anderson-Björck-King Methods, the Illinois Method	39
2.8.5 Zeroin Method	39
2.9 Efficiency of the Methods and Aids for Decision Making	40
3 Roots of Polynomials	43
3.1 Preliminary Remarks	43
3.2 The Horner Scheme	44
3.2.1 First Level Horner Scheme for Real Arguments	44
3.2.2 First Level Horner Scheme for Complex Arguments	45
3.2.3 Complete Horner Scheme for Real Arguments	47
3.2.4 Applications	49
3.3 Methods for Finding all Solutions of Algebraic Equations	49
3.3.1 Preliminaries	49
3.3.2 Muller's Method	51
3.3.3 Bauhuber's Method	54
3.3.4 The Jenkins-Traub Method	55
3.3.5 The Laguerre Method	56
3.4 Hints for Choosing a Method	56
4 Direct Methods for Solving Systems of Linear Equations ..	59
4.1 The Problem	59
4.2 Definitions and Theoretical Background	60
4.3 Solvability Conditions for Systems of Linear Equations	66
4.4 The Factorization Principle	67
4.5 Gauß Algorithm	68
4.5.1 Gauß Algorithm with Column Pivot Search	68

4.5.2 Pivot Strategies	72
4.5.3 Computer Implementation of Gauß Algorithm	73
4.5.4 Gauß Algorithm for Systems with Several Right Hand Sides	76
4.6 Matrix Inversion via Gauß Algorithm	77
4.7 Linear Equations with Symmetric Strongly Nonsingular System Matrices	78
4.7.1 The Cholesky Decomposition	78
4.7.2 The Conjugate Gradient Method	83
4.8 The Gauß - Jordan Method	87
4.9 The Matrix Inverse via Exchange Steps	88
4.10 Linear Systems with Tridiagonal Matrices	89
4.10.1 Systems with Tridiagonal Matrices	89
4.10.2 Systems with Tridiagonal Symmetric Strongly Nonsingular Matrices	92
4.11 Linear Systems with Cyclically Tridiagonal Matrices	94
4.11.1 Systems with a Cyclically Tridiagonal Matrix	94
4.11.2 Systems with Symmetric Cyclically Tridiagonal Strongly Nonsingular Matrices	96
4.12 Linear Systems with Five-Diagonal Matrices	98
4.12.1 Systems with Five-Diagonal Matrices	98
4.12.2 Systems with Five-Diagonal Symmetric Matrices	100
4.13 Linear Systems with Band Matrices	102
4.14 Solving Linear Systems via Householder Transformations	107
4.15 Errors, Conditioning and Iterative Refinement	112
4.15.1 Errors and the Condition Number	112
4.15.2 Condition Estimates	114
4.15.3 Improving the Condition Number	116
4.15.4 Iterative Refinement	117
4.16 Systems of Equations with Block Matrices	119
4.16.1 Preliminary Remarks	119
4.16.2 Gauß Algorithm for Block Matrices	120
4.16.3 Gauß Algorithm for Block Tridiagonal Systems	121
4.16.4 Other Block Methods	121
4.17 The Algorithm of Cuthill-McKee for Sparse Symmetric Matrices	122
4.18 Recommendations for Selecting a Method	127

5 Iterative Methods for Linear Systems	131
5.1 Preliminary Remarks	131
5.2 Vector and Matrix Norms	132
5.3 The Jacobi Method	133
5.4 The Gauß-Seidel Iteration	137
5.5 A Relaxation Method using the Jacobi Method	139
5.6 A Relaxation Method using the Gauß-Seidel Method	140
5.6.1 Iteration Rule	140
5.6.2 Estimate for the Optimal Relaxation Coefficient, an Adaptive SOR Method	141
6 Systems of Nonlinear Equations	143
6.1 General Iterative Methods	143
6.2 Special Iterative Methods	148
6.2.1 Newton Methods for Nonlinear Systems	148
6.2.1.1 The Basic Newton Method	148
6.2.1.2 Damped Newton Method for Systems	149
6.2.2 Regula Falsi for Nonlinear Systems	151
6.2.3 Method of Steepest Descent for Nonlinear Systems	152
6.2.4 Brown's Method for Nonlinear Systems	154
6.3 Choosing a Method	154
7 Eigenvalues and Eigenvectors of Matrices	155
7.1 Basic Concepts	155
7.2 Diagonalizable Matrices and the Conditioning of the Eigenvalue Problem	157
7.3 Vector Iteration	159
7.3.1 The Dominant Eigenvalue and the Associated Eigenvector of a Matrix	159
7.3.2 Determination of the Eigenvalue Closest to Zero	164
7.3.3 Eigenvalues in Between	164
7.4 The Rayleigh Quotient for Hermitian Matrices	166
7.5 The Krylov Method	167
7.5.1 Determining the Eigenvalues	167
7.5.2 Determining the Eigenvectors	169
7.6 Eigenvalues of Positive Definite Tridiagonal Matrices, the QD Algorithm	170
7.7 Transformation to Hessenberg Form, the LR and QR Algorithms	171

7.7.1 Transformation of a Matrix to Upper Hessenberg Form	172
7.7.2 The LR Algorithm	174
7.7.3 The Basic QR Algorithm	175
7.8 Eigenvalues and Eigenvectors of a Matrix via the QR Algorithm	176
7.9 Decision Strategy	178
8 Linear and Nonlinear Approximation	179
8.1 Linear Approximation	180
8.1.1 Statement of the Problem and Best Approximation	180
8.1.2 Linear Continuous Root-Mean-Square Approximation	184
8.1.3 Discrete Linear Root-Mean-Square Approximation	188
8.1.3.1 Normal Equations for Discrete Linear Least Squares	188
8.1.3.2 Discrete Least Squares via Algebraic Polynomials and Orthogonal Polynomials	191
8.1.3.3 Linear Regression, the Least Squares Solution Using Linear Algebraic Polynomials	193
8.1.3.4 Solving Linear Least Squares Problems using Householder Transformations	194
8.1.4 Approximation of Polynomials by Chebyshev Polynomials .	196
8.1.4.1 Best Uniform Approximation	197
8.1.4.2 Approximation by Chebyshev Polynomials	198
8.1.5 Approximation of Periodic Functions and the FFT	204
8.1.5.1 Root-Mean-Square Approximation of Periodic Functions	204
8.1.5.2 Trigonometric Interpolation	205
8.1.5.3 Complex Discrete Fourier Transformation (FFT)	207
8.1.6 Error Estimates for Linear Approximation	209
8.1.6.1 Estimates for the Error in Best Approximation	209
8.1.6.2 Error Estimates for Simultaneous Approximation of a Function and its Derivatives	211
8.1.6.3 Approximation Error Estimates using Linear Projection Operators	213
8.2 Nonlinear Approximation	215
8.2.1 Transformation Method for Nonlinear Least Squares	215
8.2.2 Nonlinear Root-Mean-Square Fitting	217
8.3 Decision Strategy	218

9 Polynomial and Rational Interpolation	219
9.1 The Problem	219
9.2 Lagrange Interpolation Formula	221
9.2.1 Lagrange Formula for Arbitrary Nodes	221
9.2.2 Lagrange Formula for Equidistant Nodes	222
9.3 The Aitken Interpolation Scheme for Arbitrary Nodes	223
9.4 Inverse Interpolation According to Aitken	225
9.5 Newton Interpolation Formula	226
9.5.1 Newton Formula for Arbitrary Nodes	226
9.5.2 Newton Formula for Equidistant Nodes	227
9.6 Remainder of an Interpolation and Estimates of the Interpolation Error	229
9.7 Rational Interpolation	235
9.8 Interpolation for Functions in Several Variables	239
9.8.1 Lagrange Interpolation Formula for Two Variables	239
9.8.2 Shepard Interpolation	241
9.9 Hints for Selecting an Appropriate Interpolation Method	247
10 Interpolating Polynomial Splines for Constructing Smooth Curves	251
10.1 Cubic Polynomial Splines	251
10.1.1 Definition of Interpolating Cubic Spline Functions	252
10.1.2 Computation of Non-Parametric Cubic Splines	254
10.1.3 Computing Parametric Cubic Splines	259
10.1.4 Joined Interpolating Polynomial Splines	266
10.1.5 Convergence and Error Estimates for Interpolating Cubic Splines	272
10.2 Hermite Splines of Fifth Degree	275
10.2.1 Definition of Hermite Splines	275
10.2.2 Computation of Non-Parametric Hermite Splines	276
10.2.3 Computation of Parametric Hermite Splines	280
10.3 Hints for Selecting Appropriate Interpolating or Approximating Splines	282
11 Cubic Fitting Splines for Constructing Smooth Curves ...	287
11.1 The Problem	287
11.2 Definition of Fitting Spline Functions	288
11.3 Non-Parametric Cubic Fitting Splines	289

11.4 Parametric Cubic Fitting Splines	296
11.5 Decision Strategy	297
12 Two-Dimensional Splines, Surface Splines, Bézier Splines, B-Splines	299
12.1 Interpolating Two-Dimensional Cubic Splines for Constructing Smooth Surfaces	299
12.2 Two-Dimensional Interpolating Surface Splines	309
12.3 Bézier Splines	313
12.3.1 Bézier Spline Curves	313
12.3.2 Bézier Spline Surfaces	316
12.3.3 Modified Interpolating Cubic Bézier Splines	324
12.4 B-Splines	325
12.4.1 B-Spline-Curves	325
12.4.2 B-Spline-Surfaces	331
12.5 Hints	335
13 Akima and Renner Subsplines	341
13.1 Akima Subsplines	341
13.2 Renner Subsplines	344
13.3 Rounding of Corners with Akima and Renner Splines	347
13.4 Approximate Computation of Arc Length	349
13.5 Selection Hints	350
14 Numerical Differentiation	353
14.1 The Task	353
14.2 Differentiation Using Interpolating Polynomials	354
14.3 Differentiation via Interpolating Cubic Splines	358
14.4 Differentiation by the Romberg Method	358
14.5 Decision Hints	360
15 Numerical Integration	361
15.1 Preliminary Remarks	361
15.2 Interpolating Quadrature Formulas	364
15.3 Newton-Cotes Formulas	366
15.3.1 The Trapezoidal Rule	367
15.3.2 Simpson's Rule	370

15.3.3	The 3/8 Formula	371
15.3.4	Other Newton-Cotes Formulas	373
15.3.5	The Error Order of Newton-Cotes Formulas	375
15.4	Maclaurin Quadrature Formulas	376
15.4.1	The Tangent Trapezoidal Formula	376
15.4.2	Other Maclaurin Formulas	378
15.5	Euler-Maclaurin Formulas	380
15.6	Chebyshev Quadrature Formulas	382
15.7	Gauß Quadrature Formulas	385
15.8	Calculation of Weights and Nodes of Generalized Gaussian Quadrature Formulas	389
15.9	Clenshaw-Curtis Quadrature Formulas	392
15.10	Romberg Integration	394
15.11	Error Estimates and Computational Errors	397
15.12	Adaptive Quadrature Methods	400
15.13	Convergence of Quadrature Formulas	400
15.14	Hints for Choosing an Appropriate Method	401
16	Numerical Cubature	403
16.1	The Problem	403
16.2	Interpolating Cubature Formulas	406
16.3	Newton-Cotes Cubature Formulas for Rectangular Regions	408
16.4	Newton-Cotes Cubature Formulas for Triangles	413
16.5	Romberg Cubature for Rectangular Regions	414
16.6	Gauß Cubature Formulas for Rectangles	417
16.7	Gauß Cubature Formulas for Triangles	419
16.7.1	Right Triangles with Legs Parallel to the Axis	419
16.7.2	General Triangles	420
16.8	Riemann Double Integrals using Bicubic Splines	421
16.9	Decision Strategy	422
17	Initial Value Problems for Ordinary Differential Equations	423
17.1	The Problem	423
17.2	Principles of the Numerical Methods	424
17.3	One-Step Methods	426
17.3.1	The Euler-Cauchy Polygonal Method	426
17.3.2	The Improved Euler-Cauchy Method	427

17.3.3	The Predictor-Corrector Method of Heun	428
17.3.4	Explicit Runge-Kutta Methods	430
17.3.4.1	Construction of Runge-Kutta Methods	430
17.3.4.2	The Classical Runge-Kutta Method	430
17.3.4.3	A List of Explicit Runge-Kutta Formulas	432
17.3.4.4	Embedding Formulas	436
17.3.5	Implicit Runge-Kutta Methods of Gaussian Type	449
17.3.6	Consistence and Convergence of One-Step Methods	451
17.3.7	Error Estimation and Step Size Control	452
17.3.7.1	Error Estimation	452
17.3.7.2	Automatic Step Size Control, Adaptive Methods for Initial Value Problems	454
17.4	Multi-Step Methods	457
17.4.1	The Principle of Multi-Step Methods	457
17.4.2	The Adams-Bashforth Method	458
17.4.3	The Predictor-Corrector Method of Adams-Moulton	460
17.4.4	The Adams-Störmer Method	465
17.4.5	Error Estimates for Multi-Step Methods	466
17.4.6	Computational Error of One-Step and Multi-Step Methods	467
17.5	Bulirsch-Stoer-Gragg Extrapolation	468
17.6	Stability	471
17.6.1	Preliminary Remarks	471
17.6.2	Stability of Differential Equations	472
17.6.3	Stability of the Numerical Method	473
17.7	Stiff Systems of Differential Equations	477
17.7.1	The Problem	477
17.7.2	Criteria for the Stiffness of a System	478
17.7.3	Gear's Method for Integrating Stiff Systems	479
17.8	Suggestions for Choosing among the Methods	484
18	Boundary Value Problems for Ordinary Differential Equations	489
18.1	Statement of the Problem	489
18.2	Reduction of Boundary Value Problems to Initial Value Problems	490
18.2.1	Boundary Value Problems for Nonlinear Differential Equations of Second Order	490
18.2.2	Boundary Value Problems for Systems of Differential Equations of First Order	492

18.2.3 The Multiple Shooting Method	494
18.3 Difference Methods	497
18.3.1 The Ordinary Difference Method	497
18.3.2 Higher Order Difference Methods	504
18.3.3 Iterative Solution of Linear Systems for Special Boundary Value Problems	506
18.3.4 Linear Eigenvalue Problems	507
A Appendix: Standard FORTRAN 77 Subroutines	509
A.1 Preface of the Appendix	511
A.2 Information on Campus and Site Licenses, as well as on Other Software Packages	513
A.3 Contents of the Enclosed CD	516
Contents of the Appendix	517
A.4 FORTRAN 77 Subroutines	521
B Bibliography	575
Literature for Other Topics	593
- Numerical Treatment of Partial Differential Equations	593
- Finite Element Method	594
C Index	597