

Contents

List of Figures	xv
List of Tables	xix
List of Conventions	xxi
Preface	xxiii
1 Principles of Numerical Calculations	1
1.1 Common Ideas and Concepts	1
1.1.1 Fixed-Point Iteration	2
1.1.2 Newton's Method	5
1.1.3 Linearization and Extrapolation	9
1.1.4 Finite Difference Approximations	11
Review Questions	15
Problems and Computer Exercises	15
1.2 Some Numerical Algorithms	16
1.2.1 Solving a Quadratic Equation	16
1.2.2 Recurrence Relations	17
1.2.3 Divide and Conquer Strategy	20
1.2.4 Power Series Expansions	22
Review Questions	23
Problems and Computer Exercises	23
1.3 Matrix Computations	26
1.3.1 Matrix Multiplication	26
1.3.2 Solving Linear Systems by LU Factorization	28
1.3.3 Sparse Matrices and Iterative Methods	38
1.3.4 Software for Matrix Computations	41
Review Questions	43
Problems and Computer Exercises	43
1.4 The Linear Least Squares Problem	44
1.4.1 Basic Concepts in Probability and Statistics	45
1.4.2 Characterization of Least Squares Solutions	46
1.4.3 The Singular Value Decomposition	50
1.4.4 The Numerical Rank of a Matrix	52
Review Questions	54

Problems and Computer Exercises	54
1.5 Numerical Solution of Differential Equations	55
1.5.1 Euler's Method	55
1.5.2 An Introductory Example	56
1.5.3 Second Order Accurate Methods	59
1.5.4 Adaptive Choice of Step Size	61
Review Questions	63
Problems and Computer Exercises	63
1.6 Monte Carlo Methods	64
1.6.1 Origin of Monte Carlo Methods	64
1.6.2 Generating and Testing Pseudorandom Numbers	66
1.6.3 Random Deviates for Other Distributions	73
1.6.4 Reduction of Variance	77
Review Questions	81
Problems and Computer Exercises	82
Notes and References	83
2 How to Obtain and Estimate Accuracy	87
2.1 Basic Concepts in Error Estimation	87
2.1.1 Sources of Error	87
2.1.2 Absolute and Relative Errors	90
2.1.3 Rounding and Chopping	91
Review Questions	93
2.2 Computer Number Systems	93
2.2.1 The Position System	93
2.2.2 Fixed- and Floating-Point Representation	95
2.2.3 IEEE Floating-Point Standard	99
2.2.4 Elementary Functions	102
2.2.5 Multiple Precision Arithmetic	104
Review Questions	105
Problems and Computer Exercises	105
2.3 Accuracy and Rounding Errors	107
2.3.1 Floating-Point Arithmetic	107
2.3.2 Basic Rounding Error Results	113
2.3.3 Statistical Models for Rounding Errors	116
2.3.4 Avoiding Overflow and Cancellation	118
Review Questions	122
Problems and Computer Exercises	122
2.4 Error Propagation	126
2.4.1 Numerical Problems, Methods, and Algorithms	126
2.4.2 Propagation of Errors and Condition Numbers	127
2.4.3 Perturbation Analysis for Linear Systems	134
2.4.4 Error Analysis and Stability of Algorithms	137
Review Questions	142
Problems and Computer Exercises	142

2.5 Automatic Control of Accuracy and Verified Computing	145
2.5.1 Running Error Analysis	145
2.5.2 Experimental Perturbations	146
2.5.3 Interval Arithmetic	147
2.5.4 Range of Functions	150
2.5.5 Interval Matrix Computations	153
Review Questions	154
Problems and Computer Exercises	155
Notes and References	155
3 Series, Operators, and Continued Fractions	157
3.1 Some Basic Facts about Series	157
3.1.1 Introduction	157
3.1.2 Taylor’s Formula and Power Series	162
3.1.3 Analytic Continuation	171
3.1.4 Manipulating Power Series	173
3.1.5 Formal Power Series	181
Review Questions	184
Problems and Computer Exercises	185
3.2 More about Series	191
3.2.1 Laurent and Fourier Series	191
3.2.2 The Cauchy–FFT Method	193
3.2.3 Chebyshev Expansions	198
3.2.4 Perturbation Expansions	203
3.2.5 Ill-Conditioned Series	206
3.2.6 Divergent or Semiconvergent Series	212
Review Questions	215
Problems and Computer Exercises	215
3.3 Difference Operators and Operator Expansions	220
3.3.1 Properties of Difference Operators	220
3.3.2 The Calculus of Operators	225
3.3.3 The Peano Theorem	237
3.3.4 Approximation Formulas by Operator Methods	242
3.3.5 Single Linear Difference Equations	251
Review Questions	261
Problems and Computer Exercises	261
3.4 Acceleration of Convergence	271
3.4.1 Introduction	271
3.4.2 Comparison Series and Aitken Acceleration	272
3.4.3 Euler’s Transformation	278
3.4.4 Complete Monotonicity and Related Concepts	284
3.4.5 Euler–Maclaurin’s Formula	292
3.4.6 Repeated Richardson Extrapolation	302
Review Questions	309
Problems and Computer Exercises	309

3.5	Continued Fractions and Padé Approximants	321
3.5.1	Algebraic Continued Fractions	321
3.5.2	Analytic Continued Fractions	326
3.5.3	The Padé Table	329
3.5.4	The Epsilon Algorithm	336
3.5.5	The qd Algorithm	339
	Review Questions	345
	Problems and Computer Exercises	345
	Notes and References	348
4	Interpolation and Approximation	351
4.1	The Interpolation Problem	351
4.1.1	Introduction	351
4.1.2	Bases for Polynomial Interpolation	352
4.1.3	Conditioning of Polynomial Interpolation	355
	Review Questions	357
	Problems and Computer Exercises	357
4.2	Interpolation Formulas and Algorithms	358
4.2.1	Newton's Interpolation Formula	358
4.2.2	Inverse Interpolation	366
4.2.3	Barycentric Lagrange Interpolation	367
4.2.4	Iterative Linear Interpolation	371
4.2.5	Fast Algorithms for Vandermonde Systems	373
4.2.6	The Runge Phenomenon	377
	Review Questions	380
	Problems and Computer Exercises	380
4.3	Generalizations and Applications	381
4.3.1	Hermite Interpolation	381
4.3.2	Complex Analysis in Polynomial Interpolation	385
4.3.3	Rational Interpolation	389
4.3.4	Multidimensional Interpolation	395
4.3.5	Analysis of a Generalized Runge Phenomenon	398
	Review Questions	407
	Problems and Computer Exercises	407
4.4	Piecewise Polynomial Interpolation	410
4.4.1	Bernštejn Polynomials and Bézier Curves	411
4.4.2	Spline Functions	417
4.4.3	The B-Spline Basis	426
4.4.4	Least Squares Splines Approximation	434
	Review Questions	436
	Problems and Computer Exercises	437
4.5	Approximation and Function Spaces	439
4.5.1	Distance and Norm	440
4.5.2	Operator Norms and the Distance Formula	444
4.5.3	Inner Product Spaces and Orthogonal Systems	450

Contents	xi
<hr/>	
4.5.4 Solution of the Approximation Problem	454
4.5.5 Mathematical Properties of Orthogonal Polynomials	457
4.5.6 Expansions in Orthogonal Polynomials	466
4.5.7 Approximation in the Maximum Norm	471
Review Questions	478
Problems and Computer Exercises	479
4.6 Fourier Methods	482
4.6.1 Basic Formulas and Theorems	483
4.6.2 Discrete Fourier Analysis	487
4.6.3 Periodic Continuation of a Function	491
4.6.4 Convergence Acceleration of Fourier Series	492
4.6.5 The Fourier Integral Theorem	494
4.6.6 Sampled Data and Aliasing	497
Review Questions	500
Problems and Computer Exercises	500
4.7 The Fast Fourier Transform	503
4.7.1 The FFT Algorithm	503
4.7.2 Discrete Convolution by FFT	509
4.7.3 FFTs of Real Data	510
4.7.4 Fast Trigonometric Transforms	512
4.7.5 The General Case FFT	515
Review Questions	516
Problems and Computer Exercises	517
Notes and References	518
5 Numerical Integration	521
5.1 Interpolatory Quadrature Rules	521
5.1.1 Introduction	521
5.1.2 Treating Singularities	525
5.1.3 Some Classical Formulas	527
5.1.4 Superconvergence of the Trapezoidal Rule	531
5.1.5 Higher-Order Newton–Cotes’ Formulas	533
5.1.6 Fejér and Clenshaw–Curtis Rules	538
Review Questions	542
Problems and Computer Exercises	542
5.2 Integration by Extrapolation	546
5.2.1 The Euler–Maclaurin Formula	546
5.2.2 Romberg’s Method	548
5.2.3 Oscillating Integrands	554
5.2.4 Adaptive Quadrature	560
Review Questions	564
Problems and Computer Exercises	564
5.3 Quadrature Rules with Free Nodes	565
5.3.1 Method of Undetermined Coefficients	565
5.3.2 Gauss–Christoffel Quadrature Rules	568

5.3.3	Gauss Quadrature with Preassigned Nodes	573
5.3.4	Matrices, Moments, and Gauss Quadrature	576
5.3.5	Jacobi Matrices and Gauss Quadrature	580
	Review Questions	585
	Problems and Computer Exercises	585
5.4	Multidimensional Integration	587
5.4.1	Analytic Techniques	588
5.4.2	Repeated One-Dimensional Integration	589
5.4.3	Product Rules	590
5.4.4	Irregular Triangular Grids	594
5.4.5	Monte Carlo Methods	599
5.4.6	Quasi-Monte Carlo and Lattice Methods	601
	Review Questions	604
	Problems and Computer Exercises	605
	Notes and References	606
6	Solving Scalar Nonlinear Equations	609
6.1	Some Basic Concepts and Methods	609
6.1.1	Introduction	609
6.1.2	The Bisection Method	610
6.1.3	Limiting Accuracy and Termination Criteria	614
6.1.4	Fixed-Point Iteration	618
6.1.5	Convergence Order and Efficiency	621
	Review Questions	624
	Problems and Computer Exercises	624
6.2	Methods Based on Interpolation	626
6.2.1	Method of False Position	626
6.2.2	The Secant Method	628
6.2.3	Higher-Order Interpolation Methods	631
6.2.4	A Robust Hybrid Method	634
	Review Questions	635
	Problems and Computer Exercises	636
6.3	Methods Using Derivatives	637
6.3.1	Newton's Method	637
6.3.2	Newton's Method for Complex Roots	644
6.3.3	An Interval Newton Method	646
6.3.4	Higher-Order Methods	647
	Review Questions	652
	Problems and Computer Exercises	653
6.4	Finding a Minimum of a Function	656
6.4.1	Introduction	656
6.4.2	Unimodal Functions and Golden Section Search	657
6.4.3	Minimization by Interpolation	660
	Review Questions	661
	Problems and Computer Exercises	661

Contents	xiii
<hr/>	
6.5 Algebraic Equations	662
6.5.1 Some Elementary Results	662
6.5.2 Ill-Conditioned Algebraic Equations	665
6.5.3 Three Classical Methods	668
6.5.4 Deflation and Simultaneous Determination of Roots	671
6.5.5 A Modified Newton Method	675
6.5.6 Sturm Sequences	677
6.5.7 Finding Greatest Common Divisors	680
Review Questions	682
Problems and Computer Exercises	683
Notes and References	685
Bibliography	687
Index	707
A Online Appendix: Introduction to Matrix Computations	A-1
A.1 Vectors and Matrices	A-1
A.1.1 Linear Vector Spaces	A-1
A.1.2 Matrix and Vector Algebra	A-3
A.1.3 Rank and Linear Systems	A-5
A.1.4 Special Matrices	A-6
A.2 Submatrices and Block Matrices	A-8
A.2.1 Block Gaussian Elimination	A-10
A.3 Permutations and Determinants	A-12
A.4 Eigenvalues and Norms of Matrices	A-16
A.4.1 The Characteristic Equation	A-16
A.4.2 The Schur and Jordan Normal Forms	A-17
A.4.3 Norms of Vectors and Matrices	A-18
Review Questions	A-21
Problems	A-22
B Online Appendix: A MATLAB Multiple Precision Package	B-1
B.1 The Mulprec Package	B-1
B.1.1 Number Representation	B-1
B.1.2 The Mulprec Function Library	B-3
B.1.3 Basic Arithmetic Operations	B-3
B.1.4 Special Mulprec Operations	B-4
B.2 Function and Vector Algorithms	B-4
B.2.1 Elementary Functions	B-4
B.2.2 Mulprec Vector Algorithms	B-5
B.2.3 Miscellaneous	B-6
B.2.4 Using Mulprec	B-6
Computer Exercises	B-6

C	Online Appendix: Guide to Literature	C-1
C.1	Introduction	C-1
C.2	Textbooks in Numerical Analysis	C-1
C.3	Handbooks and Collections	C-5
C.4	Encyclopedias, Tables, and Formulas	C-6
C.5	Selected Journals	C-8
C.6	Algorithms and Software	C-9
C.7	Public Domain Software	C-10