

# Contents

<b>List of Figures</b>	<b>xv</b>
<b>List of Tables</b>	<b>xix</b>
<b>List of Conventions</b>	<b>xxi</b>
<b>Preface</b>	<b>xxiii</b>
<b>1 Principles of Numerical Calculations</b>	<b>1</b>
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
<b>2 How to Obtain and Estimate Accuracy . . . . .</b>	<b>87</b>
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 . . . . .	133
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
<b>3</b>	<b>Series, Operators, and Continued Fractions</b>	<b>157</b>
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
<b>4</b>	<b>Interpolation and Approximation</b> . . . . .	<b>351</b>
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	Multivariate 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
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 Fast Fourier 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
<b>5 Numerical Integration</b> . . . . .	<b>521</b>
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 Multivariate 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
<b>6</b>	<b>Solving Scalar Nonlinear Equations</b>	<b>609</b>
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 Interpolating Methods . . . . .	632
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
6.5	Algebraic Equations . . . . .	662
6.5.1	Some Elementary Results . . . . .	662
6.5.2	The Condition of 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

Contents	xiii
<b>Bibliography</b>	<b>687</b>
<b>Index</b>	<b>707</b>