

CONTENTS

Both section and page numbers are given for the topics below. The reader is recommended to use section numbers (at the top of the pages of the text proper) when looking up a given topic, since a better idea of the structure of the book will be obtained.

In general, review questions and/or problems follow after each one-decimal sub-section.

PREFACE	xvii
----------------	------

CONVENTIONS	xix
--------------------	-----

1 SOME GENERAL PRINCIPLES OF NUMERICAL CALCULATION	1
1.1. Introduction	1
1.2. Some Common Ideas and Concepts in Numerical Methods	2
1.3. Numerical Problems and Algorithms	13
1.3.1. Definitions	13
1.3.2. Recursive Formulas; Horner's Rule	14
1.3.3. An Example of Numerical Instability	16
2 HOW TO OBTAIN AND ESTIMATE ACCURACY IN NUMERICAL CALCULATIONS	21
2.1. Basic Concepts in Error Estimation	21
2.1.1. Introduction	21
2.1.2. Sources of Error	22
2.1.3. Absolute and Relative Errors	23
2.1.4. Rounding and Chopping	24

2.2	Propagation of Errors	26
2.2.1.	Simple Examples of Error Analysis	26
2.2.2.	The General Formula for Error Propagation; Maximum Error and Standard Error	29
2.2.3.	On the Practical Application of Error Estimation	34
2.2.4.	The Use of Experimental Perturbations	36
2.2.5.	Automatic Control of Accuracy	37
2.3.	Number Systems; Floating and Fixed Representation	42
2.3.1.	The Position System	42
2.3.2.	Floating and Fixed Representation	43
2.3.3.	Floating Decimal Point	44
2.3.4.	Fixed Decimal Point	46
2.3.5.	Round-off Errors in Computation with Floating Arithmetic Operations	46
2.4.	Backward Error Analysis; Condition Numbers	51
2.4.1.	Backward Error Analysis	51
2.4.2.	Condition Numbers for Problems and Algorithms	53
2.4.3.	Geometrical Illustration of Error Analysis	56

3 NUMERICAL USES OF SERIES 60

3.1.	Elementary Uses of Series	60
3.1.1.	Simple Examples	60
3.1.2.	Estimating the Remainder	62
3.1.3.	Power Series	65
3.2.	Acceleration of Convergence	71
3.2.1.	Slowly Converging Alternating Series	71
3.2.2.	Slowly Converging Series with Positive Terms	73
3.2.3.	Other Simple Ways to Accelerate Convergence	74
3.2.4.	Ill-Conditioned Series	75
3.2.5.	Numerical Use of Divergent Series	77

4 APPROXIMATION OF FUNCTIONS 81

4.1.	Basic Concepts in Approximation	81
4.1.1.	Introduction	81
4.1.2.	The Idea of a Function Space	84
4.1.3.	Norms and Seminorms	85
4.1.4.	Approximation of Functions as a Geometric Problem in Function Space	87
4.2.	The Approximation of Functions by the Method of Least Squares	88
4.2.1.	Statement of the Problems	88
4.2.2.	Orthogonal Systems	89
4.2.3.	Solution of the Approximation Problem	92
4.3.	Polynomials	97
4.3.1.	Basic Terminology; the Weierstrass Approximation Theorem	97
4.3.2.	Triangle Families of Polynomials	98

4.3.3.	A Triangle Family and Its Application to Interpolation	99
4.3.4.	Equidistant Interpolation and the Runge Phenomenon	101
4.4.	Orthogonal Polynomials and Applications	104
4.4.1.	Tchebycheff Polynomials	104
4.4.2.	Tchebycheff Interpolation and Smoothing	106
4.4.3.	General Theory of Orthogonal Polynomials	108
4.4.4.	Legendre Polynomials and Gram Polynomials	113
4.5.	Complementary Observations on Polynomial Approximation	117
4.5.1.	Summary of the Use of Polynomials	117
4.5.2.	Some Inequalities for $E_n(f)$ with Applications to the Computation of Linear Functionals	120
4.5.3.	Approximation in the Maximum Norm	124
4.5.4.	Economization of Power Series; Standard Functions	125
4.5.5.	Some Statistical Aspects of the Method of Least Squares	126
4.6.	Spline Functions	131

5**NUMERICAL LINEAR ALGEBRA**

5.1.	Introduction	137
5.2.	Basic Concepts of Linear Algebra	138
5.2.1.	Fundamental Definitions	138
5.2.2.	Partitioned Matrices	140
5.2.3.	Linear Vector Spaces	141
5.2.4.	Eigenvalues and Similarity Transformations	142
5.2.5.	Singular-Value Decomposition and Pseudo-Inverse	143
5.3.	Direct Methods for Solving Systems of Linear Equations	146
5.3.1.	Triangular Systems	146
5.3.2.	Gaussian Elimination	147
5.3.3.	Pivoting Strategies	150
5.3.4.	<i>LU</i> -Decomposition	152
5.3.5.	Compact Schemes for Gaussian Elimination	157
5.3.6.	Inverse Matrices	159
5.4.	Special Matrices	162
5.4.1.	Symmetric Positive-Definite Matrices	162
5.4.2.	Band Matrices	165
5.4.3.	Large-Scale Linear Systems	168
5.4.4.	Other Sparse Matrices	169
5.5.	Error Analysis for Linear Systems	174
5.5.1.	An Ill-Conditioned Example	174
5.5.2.	Vector and Matrix Norms	175
5.5.3.	Perturbation Analysis	176
5.5.4.	Rounding Errors in Gaussian Elimination	177
5.5.5.	Scaling of Linear Systems	181
5.5.6.	Iterative Improvement of a Solution	183
5.6.	Iterative Methods	188
5.7.	Ondetermined Linear Systems	196
5.7.1.	The Normal Equations	197
5.7.2.	Orthogonalization Methods	201

5.7.3. Improvement of Least-Squares Solutions	204
5.7.4. Least-Squares Problems with Linear Constraints	205
5.8. Computation of Eigenvalues and Eigenvectors	208
5.8.1. The Power Method	209
5.8.2. Methods Based on Similarity Transformations	211
5.8.3. Eigenvalues by Equation Solving	215
5.8.4. The <i>QR</i> -Algorithm	216
6 NONLINEAR EQUATIONS	218
6.1. Introduction	218
6.2. Initial Approximations; Starting Methods	219
6.2.1. Introduction	219
6.2.2. The Bisection Method	220
6.3. Newton-Raphson's Method	222
6.4. The Secant Method	227
6.4.1. Description of the Method	227
6.4.2. Error Analysis for the Secant Method	228
6.4.3. Regula Falsi	230
6.4.4. Other Related Methods	230
6.5. General Theory of Iteration Methods	233
6.6. Error Estimation and Attainable Accuracy in Iteration Methods	238
6.6.1. Error Estimation	238
6.6.2. Attainable Accuracy; Termination Criteria	240
6.7. Multiple Roots	242
6.8. Algebraic Equations	243
6.8.1. Introduction	243
6.8.2. Deflation	245
6.8.3. Ill-Conditioned Algebraic Equations	246
6.9. Systems of Nonlinear Equations	248
6.9.1. Iteration	249
6.9.2. Newton-Raphson's Method and Some Modifications	249
6.9.3. Other Methods	251
7 FINITE DIFFERENCES WITH APPLICATIONS TO NUMERICAL INTEGRATION, DIFFERENTIATION, AND INTERPOLATION	255
7.1. Difference Operators and Their Simplest Properties	255
7.2. Simple Methods for Deriving Approximation Formulas and Error Estimates	263
7.2.1. Statement of the Problems and Some Typical Examples	263
7.2.2. Repeated Richardson Extrapolation	269
7.3. Interpolation	275
7.3.1. Introduction	275
7.3.2. When is Linear Interpolation Sufficient?	276

7.3.3.	Newton's General Interpolation Formula	277
7.3.4.	Formulas for Equidistant Interpolation	279
7.3.5.	Complementary Remarks on Interpolation	282
7.3.6.	Lagrange's Interpolation Formula	284
7.3.7.	Hermite Interpolation	285
7.3.8.	Inverse Interpolation	286
7.4.	Numerical Integration	290
7.4.1.	The Rectangle Rule, Trapezoidal Rule, and Romberg's Method	291
7.4.2.	The Truncation Error of the Trapezoidal Rule	293
7.4.3.	Some Difficulties and Possibilities in Numerical Integration	294
7.4.4.	The Euler-Maclaurin Summation Formula	297
7.4.5.	Uses of the Euler-Maclaurin Formula	300
7.4.6.	Other Methods for Numerical Integration	302
7.5.	Numerical Differentiation	307
7.6.	The Calculus of Operators	311
7.6.1.	Operator Algebra	311
7.6.2.	Operator Series with Applications	312
7.7.	Functions of Several Variables	318
7.7.1.	Working with One Variable at a Time	319
7.7.2.	Rectangular Grids	319
7.7.3.	Irregular Triangular Grids	322

8

DIFFERENTIAL EQUATIONS

8.1.	Theoretical Background	330
8.1.1.	Initial-Value Problems for Ordinary Differential Equations	330
8.1.2.	Error Propagation	333
8.1.3.	Other Differential Equation Problems	337
8.2.	Euler's Method, with Repeated Richardson Extrapolation	338
8.3.	Other Methods for Initial-Value Problems in Ordinary Differential Equations	342
8.3.1.	The Modified Midpoint Method	342
8.3.2.	The Power-Series Method	345
8.3.3.	Runge-Kutta Methods	346
8.3.4.	Implicit Methods	347
8.3.5.	Stiff Problems	349
8.3.6.	Control of Step Size	350
8.3.7.	A Finite-Difference Method for a Second-Order Equation	352
8.4.	Orientation on Boundary and Eigenvalue Problems for Ordinary Differential Equations	359
8.4.1.	Introduction	359
8.4.2.	The Shooting Method	361
8.4.3.	The Band Matrix Method	363
8.4.4.	Numerical Example of an Eigenvalue Problem	367
8.5.	Difference Equations	368
8.5.1.	Homogeneous Linear Difference Equations with Constant Coefficients	368

8.5.2. General Linear Difference Equations	370
8.5.3. Analysis of a Numerical Method with the Help of a Test Problem	372
8.5.4. Linear Multistep Methods	375
8.6. Partial Differential Equations	383
8.6.1. Introduction	383
8.6.2. An Example of an Initial-Value Problem	384
8.6.3. An Example of a Boundary-Value Problem	389
8.6.4. Methods of Undetermined Coefficients and Variational Methods	392
8.6.5. Finite-Element Methods	395
8.6.6. Integral Equations	397
9 FOURIER METHODS	405
9.1. Introduction	405
9.2. Basic Formulas and Theorems in Fourier Analysis	406
9.2.1. Functions of One Variable	406
9.2.2. Functions of Several Variables	411
9.3. Fast Fourier Analysis	413
9.3.1. An Important Special Case	413
9.3.2. Fast Fourier Analysis, General Case	414
9.4. Periodic Continuation of a Nonperiodic Function	417
9.5. The Fourier Integral Theorem	419
10 OPTIMIZATION	422
10.1. Statement of the Problem, Definitions, and Normal Form	422
10.2. The Simplex Method	426
10.3. Duality	435
10.4. The Transportation Problem and Some Other Optimization Problems	436
10.5. Nonlinear Optimization Problems	438
10.5.1. Basic Concepts and Introductory Examples	438
10.5.2. Line Search	440
10.5.3. Algorithms for Unconstrained Optimization	441
10.5.4. Overdetermined Nonlinear Systems	443
10.5.5. Constrained Optimization	444
11 THE MONTE CARLO METHOD AND SIMULATION	448
11.1. Introduction	448
11.2. Random Digits and Random Numbers	449
11.3. Applications; Reduction of Variance	455
11.4. Pseudorandom Numbers	463

12	SOLUTIONS TO PROBLEMS	465
13	BIBLIOGRAPHY AND PUBLISHED ALGORITHMS	536
13.1.	Introduction	536
13.2.	General Literature in Numerical Analysis	536
13.3.	Tables, Collections of Formulas, and Problems	539
13.4.	Error Analysis and Approximation of Functions	540
13.5.	Linear Algebra and Nonlinear Systems of Equations	541
13.6.	Interpolation, Numerical Integration, and Numerical Treatment of Differential Equations	543
13.7.	Optimization; Simulation	545
13.8.	Reviews, Abstracts and Other Periodicals	547
13.9.	Survey of Published Algorithms	548
	Index by Subject to Algorithms, 1960-1970	548
	APPENDIX TABLES	563
	INDEX	565