Contents

Preface to the C Edition xi

Preface xiii

List of Computer Programs xvii

1 PRELIMINARIES 1

1.0 Introduction 1
1.1 Program Organization and Control Structures 4
1.2 Some C Conventions for Scientific Computing 14
1.3 Error, Accuracy, and Stability 24

2 SOLUTION OF LINEAR ALGEBRAIC EQUATIONS 28

2.0 Introduction 28
2.1 Gauss-Jordan Elimination 32
2.2 Gaussian Elimination with Backsubstitution 37
2.3 *LU* Decomposition 39
2.4 Inverse of a Matrix 45
2.5 Determinant of a Matrix 46
2.6 Tridiagonal Systems of Equations 47
2.7 Iterative Improvement of a Solution to Linear Equations 49
2.8 Vandermonde Matrices and Toeplitz Matrices 51
2.9 Singular Value Decomposition 60
2.10 Sparse Linear Systems 72
2.11 Is Matrix Inversion an N^3 Process? 81

3 INTERPOLATION AND EXTRAPOLATION 85

3.0 Introduction 85
3.1 Polynomial Interpolation and Extrapolation 88
3.2 Rational Function Interpolation and Extrapolation 91
3.3 Cubic Spline Interpolation 94
3.4 How to Search an Ordered Table 98
3.5 Coefficients of the Interpolating Polynomial 101
3.6 Interpolation in Two or More Dimensions 104

4 INTEGRATION OF FUNCTIONS 111

4.0 Introduction 111
4.1 Classical Formulas for Equally-Spaced Abscissas 112
4.2 Elementary Algorithms 119
4.3 Romberg Integration 123
4.4 Improper Integrals 125
4.5 Gaussian Quadratures 131
4.6 Multidimensional Integrals 137

5 *EVALUATION OF FUNCTIONS* 142

5.0 Introduction 142
5.1 Series and Their Convergence 143
5.2 Evaluation of Continued Fractions 146
5.3 Polynomials and Rational Functions 148
5.4 Recurrence Relations and Clenshaw's Recurrence Formula 152
5.5 Quadratic and Cubic Equations 156
5.6 Chebyshev Approximation 158
5.7 Derivatives or Integrals of a Chebyshev-approximated Function 162
5.8 Polynomial Approximation from Chebyshev Coefficients 164

6 *SPECIAL FUNCTIONS* 166

6.0 Introduction 166
6.1 Gamma Function, Beta Function, Factorials, and Binomial Coefficients 167
6.2 Incomplete Gamma Function, Error Function, Chi-Square Probability Function, Cumulative Poisson Distribution 171
6.3 Incomplete Beta Function, Student's Distribution, F-Distribution, Cumulative Binomial Distribution 178
6.4 Bessel Functions of Integer Order 182
6.5 Modified Bessel Functions of Integer Order 189
6.6 Spherical Harmonics 194
6.7 Elliptic Integrals and Jacobian Elliptic Functions 197

7 *RANDOM NUMBERS* 204

7.0 Introduction 204
7.1 Uniform Deviates 205
7.2 Transformation Method: Exponential and Normal Deviates 214
7.3 Rejection Method: Gamma, Poisson, Binomial Deviates 218
7.4 Generation of Random Bits 224
7.5 The Data Encryption Standard 228
7.6 Monte Carlo Integration 237

8 *SORTING* 242

8.0 Introduction 242
8.1 Straight Insertion and Shell's Method 243
8.2 Heapsort 245
8.3 Indexing and Ranking 248
8.4 Quicksort 251
8.5 Determination of Equivalence Classes 252

9 *ROOT FINDING AND NONLINEAR SETS OF EQUATIONS* 255

9.0 Introduction 255
9.1 Bracketing and Bisection 258
9.2 Secant Method and False Position Method 263

9.3 Van Wijngaarden–Dekker–Brent Method 267
9.4 Newton-Raphson Method Using Derivative 269
9.5 Roots of Polynomials 275
9.6 Newton-Raphson Method for Nonlinear Systems of Equations 286

10 MINIMIZATION OR MAXIMIZATION OF FUNCTIONS 290

10.0 Introduction 290
10.1 Golden Section Search in One Dimension 293
10.2 Parabolic Interpolation and Brent's Method in One Dimension 299
10.3 One-Dimensional Search with First Derivatives 302
10.4 Downhill Simplex Method in Multidimensions 305
10.5 Direction Set (Powell's) Methods in Multidimensions 309
10.6 Conjugate Gradient Methods in Multidimensions 317
10.7 Variable Metric Methods in Multidimensions 324
10.8 Linear Programming and the Simplex Method 329
10.9 Combinatorial Minimization: Method of Simulated Annealing 343

11 EIGENSYSTEMS 353

11.0 Introduction 353
11.1 Jacobi Transformations of a Symmetric Matrix 360
11.2 Reduction of a Symmetric Matrix to Tridiagonal Form: Givens and Householder Reductions 367
11.3 Eigenvalues and Eigenvectors of a Tridiagonal Matrix 374
11.4 Hermitian Matrices 381
11.5 Reduction of a General Matrix to Hessenberg Form 382
11.6 The QR Algorithm for Real Hessenberg Matrices 387
11.7 Improving Eigenvalues and/or Finding Eigenvectors by Inverse Iteration 394

12 FOURIER TRANSFORM SPECTRAL METHODS 398

12.0 Introduction 398
12.1 Fourier Transform of Discretely Sampled Data 403
12.2 Fast Fourier Transform (FFT) 407
12.3 FFT of Real Functions, Sine and Cosine Transforms 414
12.4 Convolution and Deconvolution Using the FFT 425
12.5 Correlation and Autocorrelation Using the FFT 432
12.6 Optimal (Wiener) Filtering with the FFT 434
12.7 Power Spectrum Estimation Using the FFT 437
12.8 Power Spectrum Estimation by the Maximum Entropy (All Poles) Method 447
12.9 Digital Filtering in the Time Domain 452
12.10 Linear Prediction and Linear Predictive Coding 461
12.11 FFT in Two or More Dimensions 467

13 STATISTICAL DESCRIPTION OF DATA 471

13.0 Introduction 471
13.1 Moments of a Distribution: Mean, Variance, Skewness, and so forth 472
13.2 Efficient Search for the Median 476
13.3 Estimation of the Mode for Continuous Data 479
13.4 Do Two Distributions Have the Same Means or Variances? 481
13.5 Are Two Distributions Different? 487
13.6 Contingency Table Analysis of Two Distributions 494
13.7 Linear Correlation 503
13.8 Nonparametric or Rank Correlation 507
13.9 Smoothing of Data 514

14 MODELING OF DATA 517

14.0 Introduction 517
14.1 Least Squares as a Maximum Likelihood Estimator 518
14.2 Fitting Data to a Straight Line 523
14.3 General Linear Least Squares 528
14.4 Nonlinear Models 540
14.5 Confidence Limits on Estimated Model Parameters 548
14.6 Robust Estimation 558

15 INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS 566

15.0 Introduction 566
15.1 Runge-Kutta Method 569
15.2 Adaptive Stepsize Control for Runge-Kutta 574
15.3 Modified Midpoint Method 580
15.4 Richardson Extrapolation and the Bulirsch-Stoer Method 582
15.5 Predictor-Corrector Methods 589
15.6 Stiff Sets of Equations 592

16 TWO POINT BOUNDARY VALUE PROBLEMS 598

16.0 Introduction 598
16.1 The Shooting Method 602
16.2 Shooting to a Fitting Point 606
16.3 Relaxation Methods 609
16.4 A Worked Example: Spheroidal Harmonics 621
16.5 Automated Allocation of Mesh Points 630
16.6 Handling Internal Boundary Conditions or Singular Points 632

17 PARTIAL DIFFERENTIAL EQUATIONS 636

17.0 Introduction 636
17.1 Flux-Conservative Initial Value Problems 644
17.2 Diffusive Initial Value Problems 656
17.3 Initial Value Problems in Multidimensions 663

17.4 Fourier and Cyclic Reduction Methods for Boundary Value Problems 667
17.5 Relaxation Methods for Boundary Value Problems 673
17.6 Operator Splitting Methods and ADI 681

APPENDIX A: References 689

APPENDIX B: Table of Program Dependencies 694

APPENDIX C: Table of Prototype Declarations 699

APPENDIX D: Utility Routines (nrutil.c) 705

APPENDIX E: Complex Arithmetic (complex.c) 710

Index 713