

# Contents

<b>Preface to the Third Edition (2007)</b>	<b>xi</b>
<b>Preface to the Second Edition (1992)</b>	<b>xiv</b>
<b>Preface to the First Edition (1985)</b>	<b>xvii</b>
<b>License and Legal Information</b>	<b>xix</b>
<b>1 Preliminaries</b>	<b>1</b>
1.0 Introduction . . . . .	1
1.1 Error, Accuracy, and Stability . . . . .	8
1.2 C Family Syntax . . . . .	12
1.3 Objects, Classes, and Inheritance . . . . .	17
1.4 Vector and Matrix Objects . . . . .	24
1.5 Some Further Conventions and Capabilities . . . . .	30
<b>2 Solution of Linear Algebraic Equations</b>	<b>37</b>
2.0 Introduction . . . . .	37
2.1 Gauss-Jordan Elimination . . . . .	41
2.2 Gaussian Elimination with Backsubstitution . . . . .	46
2.3 <i>LU</i> Decomposition and Its Applications . . . . .	48
2.4 Tridiagonal and Band-Diagonal Systems of Equations . . . . .	56
2.5 Iterative Improvement of a Solution to Linear Equations . . . . .	61
2.6 Singular Value Decomposition . . . . .	65
2.7 Sparse Linear Systems . . . . .	75
2.8 Vandermonde Matrices and Toeplitz Matrices . . . . .	93
2.9 Cholesky Decomposition . . . . .	100
2.10 <i>QR</i> Decomposition . . . . .	102
2.11 Is Matrix Inversion an $N^3$ Process? . . . . .	106
<b>3 Interpolation and Extrapolation</b>	<b>110</b>
3.0 Introduction . . . . .	110
3.1 Preliminaries: Searching an Ordered Table . . . . .	114
3.2 Polynomial Interpolation and Extrapolation . . . . .	118
3.3 Cubic Spline Interpolation . . . . .	120
3.4 Rational Function Interpolation and Extrapolation . . . . .	124

3.5	Coefficients of the Interpolating Polynomial . . . . .	129
3.6	Interpolation on a Grid in Multidimensions . . . . .	132
3.7	Interpolation on Scattered Data in Multidimensions . . . . .	139
3.8	Laplace Interpolation . . . . .	150
<b>4</b>	<b>Integration of Functions</b> . . . . .	<b>155</b>
4.0	Introduction . . . . .	155
4.1	Classical Formulas for Equally Spaced Abscissas . . . . .	156
4.2	Elementary Algorithms . . . . .	162
4.3	Romberg Integration . . . . .	166
4.4	Improper Integrals . . . . .	167
4.5	Quadrature by Variable Transformation . . . . .	172
4.6	Gaussian Quadratures and Orthogonal Polynomials . . . . .	179
4.7	Adaptive Quadrature . . . . .	194
4.8	Multidimensional Integrals . . . . .	196
<b>5</b>	<b>Evaluation of Functions</b> . . . . .	<b>201</b>
5.0	Introduction . . . . .	201
5.1	Polynomials and Rational Functions . . . . .	201
5.2	Evaluation of Continued Fractions . . . . .	206
5.3	Series and Their Convergence . . . . .	209
5.4	Recurrence Relations and Clenshaw's Recurrence Formula . . . . .	219
5.5	Complex Arithmetic . . . . .	225
5.6	Quadratic and Cubic Equations . . . . .	227
5.7	Numerical Derivatives . . . . .	229
5.8	Chebyshev Approximation . . . . .	233
5.9	Derivatives or Integrals of a Chebyshev-Approximated Function . . . . .	240
5.10	Polynomial Approximation from Chebyshev Coefficients . . . . .	241
5.11	Economization of Power Series . . . . .	243
5.12	Padé Approximants . . . . .	245
5.13	Rational Chebyshev Approximation . . . . .	247
5.14	Evaluation of Functions by Path Integration . . . . .	251
<b>6</b>	<b>Special Functions</b> . . . . .	<b>255</b>
6.0	Introduction . . . . .	255
6.1	Gamma Function, Beta Function, Factorials, Binomial Coefficients . . . . .	256
6.2	Incomplete Gamma Function and Error Function . . . . .	259
6.3	Exponential Integrals . . . . .	266
6.4	Incomplete Beta Function . . . . .	270
6.5	Bessel Functions of Integer Order . . . . .	274
6.6	Bessel Functions of Fractional Order, Airy Functions, Spherical Bessel Functions . . . . .	283
6.7	Spherical Harmonics . . . . .	292
6.8	Fresnel Integrals, Cosine and Sine Integrals . . . . .	297
6.9	Dawson's Integral . . . . .	302
6.10	Generalized Fermi-Dirac Integrals . . . . .	304
6.11	Inverse of the Function $x \log(x)$ . . . . .	307
6.12	Elliptic Integrals and Jacobian Elliptic Functions . . . . .	309

6.13	Hypergeometric Functions . . . . .	318
6.14	Statistical Functions . . . . .	320
<b>7</b>	<b>Random Numbers</b> . . . . .	<b>340</b>
7.0	Introduction . . . . .	340
7.1	Uniform Deviates . . . . .	341
7.2	Completely Hashing a Large Array . . . . .	358
7.3	Deviates from Other Distributions . . . . .	361
7.4	Multivariate Normal Deviates . . . . .	378
7.5	Linear Feedback Shift Registers . . . . .	380
7.6	Hash Tables and Hash Memories . . . . .	386
7.7	Simple Monte Carlo Integration . . . . .	397
7.8	Quasi- (that is, Sub-) Random Sequences . . . . .	403
7.9	Adaptive and Recursive Monte Carlo Methods . . . . .	410
<b>8</b>	<b>Sorting and Selection</b> . . . . .	<b>419</b>
8.0	Introduction . . . . .	419
8.1	Straight Insertion and Shell's Method . . . . .	420
8.2	Quicksort . . . . .	423
8.3	Heapsort . . . . .	426
8.4	Indexing and Ranking . . . . .	428
8.5	Selecting the $M$ th Largest . . . . .	431
8.6	Determination of Equivalence Classes . . . . .	439
<b>9</b>	<b>Root Finding and Nonlinear Sets of Equations</b> . . . . .	<b>442</b>
9.0	Introduction . . . . .	442
9.1	Bracketing and Bisection . . . . .	445
9.2	Secant Method, False Position Method, and Ridders' Method . . . . .	449
9.3	Van Wijngaarden-Dekker-Brent Method . . . . .	454
9.4	Newton-Raphson Method Using Derivative . . . . .	456
9.5	Roots of Polynomials . . . . .	463
9.6	Newton-Raphson Method for Nonlinear Systems of Equations . . . . .	473
9.7	Globally Convergent Methods for Nonlinear Systems of Equations . . . . .	477
<b>10</b>	<b>Minimization or Maximization of Functions</b> . . . . .	<b>487</b>
10.0	Introduction . . . . .	487
10.1	Initially Bracketing a Minimum . . . . .	490
10.2	Golden Section Search in One Dimension . . . . .	492
10.3	Parabolic Interpolation and Brent's Method in One Dimension . . . . .	496
10.4	One-Dimensional Search with First Derivatives . . . . .	499
10.5	Downhill Simplex Method in Multidimensions . . . . .	502
10.6	Line Methods in Multidimensions . . . . .	507
10.7	Direction Set (Powell's) Methods in Multidimensions . . . . .	509
10.8	Conjugate Gradient Methods in Multidimensions . . . . .	515
10.9	Quasi-Newton or Variable Metric Methods in Multidimensions . . . . .	521
10.10	Linear Programming: The Simplex Method . . . . .	526
10.11	Linear Programming: Interior-Point Methods . . . . .	537
10.12	Simulated Annealing Methods . . . . .	549
10.13	Dynamic Programming . . . . .	555

<b>11 Eigensystems</b>	<b>563</b>
11.0 Introduction	563
11.1 Jacobi Transformations of a Symmetric Matrix	570
11.2 Real Symmetric Matrices	576
11.3 Reduction of a Symmetric Matrix to Tridiagonal Form: Givens and Householder Reductions	578
11.4 Eigenvalues and Eigenvectors of a Tridiagonal Matrix	583
11.5 Hermitian Matrices	590
11.6 Real Nonsymmetric Matrices	590
11.7 The $QR$ Algorithm for Real Hessenberg Matrices	596
11.8 Improving Eigenvalues and/or Finding Eigenvectors by Inverse Iteration	597
<b>12 Fast Fourier Transform</b>	<b>600</b>
12.0 Introduction	600
12.1 Fourier Transform of Discretely Sampled Data	605
12.2 Fast Fourier Transform (FFT)	608
12.3 FFT of Real Functions	617
12.4 Fast Sine and Cosine Transforms	620
12.5 FFT in Two or More Dimensions	627
12.6 Fourier Transforms of Real Data in Two and Three Dimensions	631
12.7 External Storage or Memory-Local FFTs	637
<b>13 Fourier and Spectral Applications</b>	<b>640</b>
13.0 Introduction	640
13.1 Convolution and Deconvolution Using the FFT	641
13.2 Correlation and Autocorrelation Using the FFT	648
13.3 Optimal (Wiener) Filtering with the FFT	649
13.4 Power Spectrum Estimation Using the FFT	652
13.5 Digital Filtering in the Time Domain	667
13.6 Linear Prediction and Linear Predictive Coding	673
13.7 Power Spectrum Estimation by the Maximum Entropy (All-Poles) Method	681
13.8 Spectral Analysis of Unevenly Sampled Data	685
13.9 Computing Fourier Integrals Using the FFT	692
13.10 Wavelet Transforms	699
13.11 Numerical Use of the Sampling Theorem	717
<b>14 Statistical Description of Data</b>	<b>720</b>
14.0 Introduction	720
14.1 Moments of a Distribution: Mean, Variance, Skewness, and So Forth	721
14.2 Do Two Distributions Have the Same Means or Variances?	726
14.3 Are Two Distributions Different?	730
14.4 Contingency Table Analysis of Two Distributions	741
14.5 Linear Correlation	745
14.6 Nonparametric or Rank Correlation	748
14.7 Information-Theoretic Properties of Distributions	754
14.8 Do Two-Dimensional Distributions Differ?	762

14.9 Savitzky-Golay Smoothing Filters	766
<b>15 Modeling of Data</b>	<b>773</b>
15.0 Introduction	773
15.1 Least Squares as a Maximum Likelihood Estimator	776
15.2 Fitting Data to a Straight Line	780
15.3 Straight-Line Data with Errors in Both Coordinates	785
15.4 General Linear Least Squares	788
15.5 Nonlinear Models	799
15.6 Confidence Limits on Estimated Model Parameters	807
15.7 Robust Estimation	818
15.8 Markov Chain Monte Carlo	824
15.9 Gaussian Process Regression	836
<b>16 Classification and Inference</b>	<b>840</b>
16.0 Introduction	840
16.1 Gaussian Mixture Models and k-Means Clustering	842
16.2 Viterbi Decoding	850
16.3 Markov Models and Hidden Markov Modeling	856
16.4 Hierarchical Clustering by Phylogenetic Trees	868
16.5 Support Vector Machines	883
<b>17 Integration of Ordinary Differential Equations</b>	<b>899</b>
17.0 Introduction	899
17.1 Runge-Kutta Method	907
17.2 Adaptive Stepsize Control for Runge-Kutta	910
17.3 Richardson Extrapolation and the Bulirsch-Stoer Method	921
17.4 Second-Order Conservative Equations	928
17.5 Stiff Sets of Equations	931
17.6 Multistep, Multivalued, and Predictor-Corrector Methods	942
17.7 Stochastic Simulation of Chemical Reaction Networks	946
<b>18 Two-Point Boundary Value Problems</b>	<b>955</b>
18.0 Introduction	955
18.1 The Shooting Method	959
18.2 Shooting to a Fitting Point	962
18.3 Relaxation Methods	964
18.4 A Worked Example: Spheroidal Harmonics	971
18.5 Automated Allocation of Mesh Points	981
18.6 Handling Internal Boundary Conditions or Singular Points	983
<b>19 Integral Equations and Inverse Theory</b>	<b>986</b>
19.0 Introduction	986
19.1 Fredholm Equations of the Second Kind	989
19.2 Volterra Equations	992
19.3 Integral Equations with Singular Kernels	995
19.4 Inverse Problems and the Use of A Priori Information	1001
19.5 Linear Regularization Methods	1006
19.6 Backus-Gilbert Method	1014

19.7	Maximum Entropy Image Restoration . . . . .	1016
<b>20</b>	<b>Partial Differential Equations</b>	<b>1024</b>
20.0	Introduction . . . . .	1024
20.1	Flux-Conservative Initial Value Problems . . . . .	1031
20.2	Diffusive Initial Value Problems . . . . .	1043
20.3	Initial Value Problems in Multidimensions . . . . .	1049
20.4	Fourier and Cyclic Reduction Methods for Boundary Value Problems . . . . .	1053
20.5	Relaxation Methods for Boundary Value Problems . . . . .	1059
20.6	Multigrid Methods for Boundary Value Problems . . . . .	1066
20.7	Spectral Methods . . . . .	1083
<b>21</b>	<b>Computational Geometry</b>	<b>1097</b>
21.0	Introduction . . . . .	1097
21.1	Points and Boxes . . . . .	1099
21.2	KD Trees and Nearest-Neighbor Finding . . . . .	1101
21.3	Triangles in Two and Three Dimensions . . . . .	1111
21.4	Lines, Line Segments, and Polygons . . . . .	1117
21.5	Spheres and Rotations . . . . .	1128
21.6	Triangulation and Delaunay Triangulation . . . . .	1131
21.7	Applications of Delaunay Triangulation . . . . .	1141
21.8	Quadtrees and Octrees: Storing Geometrical Objects . . . . .	1149
<b>22</b>	<b>Less-Numerical Algorithms</b>	<b>1160</b>
22.0	Introduction . . . . .	1160
22.1	Plotting Simple Graphs . . . . .	1160
22.2	Diagnosing Machine Parameters . . . . .	1163
22.3	Gray Codes . . . . .	1166
22.4	Cyclic Redundancy and Other Checksums . . . . .	1168
22.5	Huffman Coding and Compression of Data . . . . .	1175
22.6	Arithmetic Coding . . . . .	1181
22.7	Arithmetic at Arbitrary Precision . . . . .	1185
<b>Index</b>		<b>1195</b>