

Computational Methods for Numerical Analysis with R

James P. Howard, II

The Johns Hopkins University
Applied Physics Laboratory
Laurel, Maryland, USA



CRC Press

Taylor & Francis Group

Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business
A CHAPMAN & HALL BOOK

Contents

List of Figures	xiii
List of Tables	xv
List of R Functions	xvii
Preface	xix
1 Introduction to Numerical Analysis	1
1.1 Numerical Analysis	1
1.1.1 The Goals of Numerical Analysis	1
1.1.2 Numerical Analysis in R	3
1.1.3 Efficiency	5
1.2 Data Types in R	8
1.2.1 Data Types	8
1.2.2 Data Structures	11
1.3 Elementary Problems	16
1.3.1 Summation Algorithms	16
1.3.2 Evaluating Polynomials	20
1.3.3 The n th Root Algorithm	24
Comments	26
Exercises	27
2 Error Analysis	29
2.1 True Values	29
2.1.1 Accuracy	30
2.1.2 Precision	32
2.2 Internal Data Storage	35
2.2.1 Binary Numbers	35
2.2.2 Floating Point Numbers	37
2.3 Numerical Error	42
2.3.1 Round-Off Error and Machine ϵ	42
2.3.2 Loss of Significance	44
2.3.3 Overflow and Underflow	48
2.3.4 Error Propagation and Stability	50

2.4	Applications	53
2.4.1	Simple Division Algorithms	53
2.4.2	Binary Long Division	55
	Comments	57
	Exercises	58
3	Linear Algebra	59
3.1	Vectors and Matrices	59
3.1.1	Vector and Matrix Operations	59
3.1.2	Elementary Row Operations	64
3.2	Gaussian Elimination	67
3.2.1	Row Echelon Form	67
3.2.2	Tridiagonal Matrices	73
3.3	Matrix Decomposition	76
3.3.1	LU Decomposition	76
3.3.2	Cholesky Decomposition	80
3.4	Iterative Methods	82
3.4.1	Jacobi Iteration	83
3.4.2	Gauss–Seidel Iteration	86
3.5	Applications	89
3.5.1	Least Squares	89
	Comments	91
	Exercises	92
4	Interpolation and Extrapolation	95
4.1	Polynomial Interpolation	95
4.1.1	Linear Interpolation	95
4.1.2	Higher-Order Polynomial Interpolation	97
4.2	Piecewise Interpolation	102
4.2.1	Piecewise Linear Interpolation	103
4.2.2	Cubic Spline Interpolation	105
4.2.3	Bézier Curves	110
4.3	Multidimensional Interpolation	115
4.3.1	Bilinear Interpolation	115
4.3.2	Nearest Neighbor Interpolation	119
4.4	Applications	122
4.4.1	Time Series Interpolation	122
4.4.2	Computer Graphics	125
	Comments	130
	Exercises	131

5	Differentiation and Integration	133
5.1	Numerical Differentiation	133
5.1.1	Finite Differences	133
5.1.2	The Second Derivative	137
5.2	Newton–Cotes Integration	138
5.2.1	Multipanel Interpolation Rules	139
5.2.2	Newton–Cotes Errors	145
5.2.3	Newton–Cotes Forms, Generally	147
5.3	Gaussian Integration	149
5.3.1	The Gaussian Method	149
5.3.2	Implementation Details	151
5.4	More Techniques	153
5.4.1	Adaptive Integrators	153
5.4.2	Romberg’s Method	156
5.4.3	Monte Carlo Methods	159
5.5	Applications	163
5.5.1	Revolved Volumes	163
5.5.2	Gini Coefficients	168
	Comments	170
	Exercises	173
6	Root Finding and Optimization	175
6.1	One-Dimensional Root Finding	175
6.1.1	Bisection Method	175
6.1.2	Newton–Raphson Method	179
6.1.3	Secant Method	183
6.2	Minimization and Maximization	185
6.2.1	Golden Section Search	185
6.2.2	Gradient Descent	188
6.3	Multidimensional Optimization	192
6.3.1	Multidimensional Gradient Descent	192
6.3.2	Hill Climbing	195
6.3.3	Simulated Annealing	197
6.4	Applications	200
6.4.1	Least Squares	200
6.4.2	The Traveling Salesperson	203
	Comments	208
	Exercises	210
7	Differential Equations	213
7.1	Initial Value Problems	213
7.1.1	Euler Method	213

7.1.2	Runge–Kutta Methods, Generally	219
7.1.3	Linear Multistep Methods	224
7.2	Systems of Ordinary Differential Equations	227
7.2.1	Solution Systems and Initial Value Problems	228
7.2.2	Boundary Value Problems	231
7.3	Partial Differential Equations	234
7.3.1	The Heat Equation	234
7.3.2	The Wave Equation	238
7.4	Applications	242
7.4.1	Carbon Dating	242
7.4.2	Lotka–Volterra Equations	244
	Comments	245
	Exercises	247
	Suggested Reading	249
	Index	253