

Contents

<i>Preface</i>	<i>page ix</i>
1 Types and sources of numerical error	1
1.1 Introduction	1
1.2 Representation of floating-point numbers	4
1.2.1 How computers store numbers	7
1.2.2 Binary to decimal system	7
1.2.3 Decimal to binary system	9
1.2.4 Binary representation of floating-point numbers	10
1.3 Methods used to measure error	16
1.4 Significant digits	18
1.5 Round-off errors generated by floating-point operations	20
1.6 Taylor series and truncation error	26
1.6.1 Order of magnitude estimation of truncation error	28
1.6.2 Convergence of a series	32
1.6.3 Finite difference formulas for numerical differentiation	33
1.7 Criteria for convergence	39
1.8 End of Chapter 1: key points to consider	40
1.9 Problems	40
References	46
2 Systems of linear equations	47
2.1 Introduction	47
2.2 Fundamentals of linear algebra	53
2.2.1 Vectors and matrices	53
2.2.2 Matrix operations	56
2.2.3 Vector and matrix norms	64
2.2.4 Linear combinations of vectors	66
2.2.5 Vector spaces and basis vectors	69
2.2.6 Rank, determinant, and inverse of matrices	71
2.3 Matrix representation of a system of linear equations	75
2.4 Gaussian elimination with backward substitution	76
2.4.1 Gaussian elimination without pivoting	76
2.4.2 Gaussian elimination with pivoting	84
2.5 LU factorization	87
2.5.1 LU factorization without pivoting	88
2.5.2 LU factorization with pivoting	93
2.5.3 The MATLAB <code>lu</code> function	95
2.6 The MATLAB backslash (<code>\</code>) operator	96
2.7 III-conditioned problems and the condition number	97
2.8 Linear regression	101

2.9	Curve fitting using linear least-squares approximation	107
2.9.1	The normal equations	109
2.9.2	Coefficient of determination and quality of fit	115
2.10	Linear least-squares approximation of transformed equations	118
2.11	Multivariable linear least-squares regression	123
2.12	The MATLAB function polyfit	124
2.13	End of Chapter 2: key points to consider	125
2.14	Problems	127
	References	139
3	Probability and statistics	141
3.1	Introduction	141
3.2	Characterizing a population: descriptive statistics	144
3.2.1	Measures of central tendency	145
3.2.2	Measures of dispersion	146
3.3	Concepts from probability	147
3.3.1	Random sampling and probability	149
3.3.2	Combinatorics: permutations and combinations	154
3.4	Discrete probability distributions	157
3.4.1	Binomial distribution	159
3.4.2	Poisson distribution	163
3.5	Normal distribution	166
3.5.1	Continuous probability distributions	167
3.5.2	Normal probability density	169
3.5.3	Expectations of sample-derived statistics	171
3.5.4	Standard normal distribution and the z statistic	175
3.5.5	Confidence intervals using the z statistic and the t statistic	177
3.5.6	Non-normal samples and the central-limit theorem	183
3.6	Propagation of error	186
3.6.1	Addition/subtraction of random variables	187
3.6.2	Multiplication/division of random variables	188
3.6.3	General functional relationship between two random variables	190
3.7	Linear regression error	191
3.7.1	Error in model parameters	193
3.7.2	Error in model predictions	196
3.8	End of Chapter 3: key points to consider	199
3.9	Problems	202
	References	208
4	Hypothesis testing	209
4.1	Introduction	209
4.2	Formulating a hypothesis	210
4.2.1	Designing a scientific study	211
4.2.2	Null and alternate hypotheses	217
4.3	Testing a hypothesis	219
4.3.1	The p value and assessing statistical significance	220
4.3.2	Type I and type II errors	226
4.3.3	Types of variables	228
4.3.4	Choosing a hypothesis test	230

4.4	Parametric tests and assessing normality	231
4.5	The z test	235
4.5.1	One-sample z test	235
4.5.2	Two-sample z test	241
4.6	The t test	244
4.6.1	One-sample and paired sample t tests	244
4.6.2	Independent two-sample t test	249
4.7	Hypothesis testing for population proportions	251
4.7.1	Hypothesis testing for a single population proportion	256
4.7.2	Hypothesis testing for two population proportions	257
4.8	One-way ANOVA	260
4.9	Chi-square tests for nominal scale data	274
4.9.1	Goodness-of-fit test	276
4.9.2	Test of independence	281
4.9.3	Test of homogeneity	285
4.10	More on non-parametric (distribution-free) tests	288
4.10.1	Sign test	289
4.10.2	Wilcoxon signed-rank test	292
4.10.3	Wilcoxon rank-sum test	296
4.11	End of Chapter 4: key points to consider	299
4.12	Problems	299
	References	308
5	Root-finding techniques for nonlinear equations	310
5.1	Introduction	310
5.2	Bisection method	312
5.3	Regula-falsi method	319
5.4	Fixed-point iteration	320
5.5	Newton's method	327
5.5.1	Convergence issues	329
5.6	Secant method	336
5.7	Solving systems of nonlinear equations	338
5.8	MATLAB function <code>fzero</code>	346
5.9	End of Chapter 5: key points to consider	348
5.10	Problems	349
	References	353
6	Numerical quadrature	354
6.1	Introduction	354
6.2	Polynomial interpolation	361
6.3	Newton–Cotes formulas	371
6.3.1	Trapezoidal rule	372
6.3.2	Simpson's 1/3 rule	380
6.3.3	Simpson's 3/8 rule	384
6.4	Richardson's extrapolation and Romberg integration	387
6.5	Gaussian quadrature	391
6.6	End of Chapter 6: key points to consider	402
6.7	Problems	403
	References	408

7 Numerical integration of ordinary differential equations	409
7.1 Introduction	409
7.2 Euler's methods	416
7.2.1 Euler's forward method	417
7.2.2 Euler's backward method	428
7.2.3 Modified Euler's method	431
7.3 Runge–Kutta (RK) methods	434
7.3.1 Second-order RK methods	434
7.3.2 Fourth-order RK methods	438
7.4 Adaptive step size methods	440
7.5 Multistep ODE solvers	451
7.5.1 Adams methods	452
7.5.2 Predictor–corrector methods	454
7.6 Stability and stiff equations	456
7.7 Shooting method for boundary-value problems	461
7.7.1 Linear ODEs	463
7.7.2 Nonlinear ODEs	464
7.8 End of Chapter 7: key points to consider	472
7.9 Problems	473
References	478
8 Nonlinear model regression and optimization	480
8.1 Introduction	480
8.2 Unconstrained single-variable optimization	487
8.2.1 Newton's method	488
8.2.2 Successive parabolic interpolation	492
8.2.3 Golden section search method	495
8.3 Unconstrained multivariable optimization	500
8.3.1 Steepest descent or gradient method	502
8.3.2 Multidimensional Newton's method	509
8.3.3 Simplex method	513
8.4 Constrained nonlinear optimization	523
8.5 Nonlinear error analysis	530
8.6 End of Chapter 8: key points to consider	533
8.7 Problems	534
References	538
9 Basic algorithms of bioinformatics	539
9.1 Introduction	539
9.2 Sequence alignment and database searches	540
9.3 Phylogenetic trees using distance-based methods	554
9.4 End of Chapter 9: key points to consider	557
9.5 Problems	558
References	558
<i>Appendix A Introduction to MATLAB</i>	560
<i>Appendix B Location of nodes for Gauss–Legendre quadrature</i>	576
<i>Index for MATLAB commands</i>	578
<i>Index</i>	579