

# Contents

List of Figures	xvii
List of Tables	xix
Preface to Second Edition	xxi
Preface to First Edition	xxv
About the Dedication	xxix
<b>1 Principles of Finite Precision Computation</b>	<b>1</b>
1.1 Notation and Background	2
1.2 Relative Error and Significant Digits	3
1.3 Sources of Errors	5
1.4 Precision Versus Accuracy	6
1.5 Backward and Forward Errors	6
1.6 Conditioning	8
1.7 Cancellation	9
1.8 Solving a Quadratic Equation	10
1.9 Computing the Sample Variance	11
1.10 Solving Linear Equations	12
1.10.1 GEPP Versus Cramer's Rule	13
1.11 Accumulation of Rounding Errors	14
1.12 Instability Without Cancellation	14
1.12.1 The Need for Pivoting	15
1.12.2 An Innocuous Calculation?	15
1.12.3 An Infinite Sum	16
1.13 Increasing the Precision	17
1.14 Cancellation of Rounding Errors	19
1.14.1 Computing $(e^x - 1)/x$	19
1.14.2 QR Factorization	21
1.15 Rounding Errors Can Be Beneficial	22
1.16 Stability of an Algorithm Depends on the Problem	24
1.17 Rounding Errors Are Not Random	25
1.18 Designing Stable Algorithms	26
1.19 Misconceptions	28
1.20 Rounding Errors in Numerical Analysis	28
1.21 Notes and References	28
Problems	31

<b>2</b>	<b>Floating Point Arithmetic</b>	<b>35</b>
2.1	Floating Point Number System . . . . .	36
2.2	Model of Arithmetic . . . . .	40
2.3	IEEE Arithmetic . . . . .	41
2.4	Aberrant Arithmetics . . . . .	43
2.5	Exact Subtraction . . . . .	45
2.6	Fused Multiply-Add Operation . . . . .	46
2.7	Choice of Base and Distribution of Numbers . . . . .	47
2.8	Statistical Distribution of Rounding Errors . . . . .	48
2.9	Alternative Number Systems . . . . .	49
2.10	Elementary Functions . . . . .	50
2.11	Accuracy Tests . . . . .	51
2.12	Notes and References . . . . .	52
	Problems . . . . .	57
<b>3</b>	<b>Basics</b>	<b>61</b>
3.1	Inner and Outer Products . . . . .	62
3.2	The Purpose of Rounding Error Analysis . . . . .	65
3.3	Running Error Analysis . . . . .	65
3.4	Notation for Error Analysis . . . . .	67
3.5	Matrix Multiplication . . . . .	69
3.6	Complex Arithmetic . . . . .	71
3.7	Miscellany . . . . .	73
3.8	Error Analysis Demystified . . . . .	74
3.9	Other Approaches . . . . .	76
3.10	Notes and References . . . . .	76
	Problems . . . . .	77
<b>4</b>	<b>Summation</b>	<b>79</b>
4.1	Summation Methods . . . . .	80
4.2	Error Analysis . . . . .	81
4.3	Compensated Summation . . . . .	83
4.4	Other Summation Methods . . . . .	88
4.5	Statistical Estimates of Accuracy . . . . .	88
4.6	Choice of Method . . . . .	89
4.7	Notes and References . . . . .	90
	Problems . . . . .	91
<b>5</b>	<b>Polynomials</b>	<b>93</b>
5.1	Horner's Method . . . . .	94
5.2	Evaluating Derivatives . . . . .	96
5.3	The Newton Form and Polynomial Interpolation . . . . .	99
5.4	Matrix Polynomials . . . . .	102
5.5	Notes and References . . . . .	102
	Problems . . . . .	104

<b>6</b>	<b>Norms</b>	<b>105</b>
6.1	Vector Norms . . . . .	106
6.2	Matrix Norms . . . . .	107
6.3	The Matrix $p$ -Norm . . . . .	112
6.4	Singular Value Decomposition . . . . .	114
6.5	Notes and References . . . . .	114
	Problems . . . . .	115
<b>7</b>	<b>Perturbation Theory for Linear Systems</b>	<b>119</b>
7.1	Normwise Analysis . . . . .	120
7.2	Componentwise Analysis . . . . .	122
7.3	Scaling to Minimize the Condition Number . . . . .	125
7.4	The Matrix Inverse . . . . .	127
7.5	Extensions . . . . .	128
7.6	Numerical Stability . . . . .	129
7.7	Practical Error Bounds . . . . .	130
7.8	Perturbation Theory by Calculus . . . . .	132
7.9	Notes and References . . . . .	132
	Problems . . . . .	134
<b>8</b>	<b>Triangular Systems</b>	<b>139</b>
8.1	Backward Error Analysis . . . . .	140
8.2	Forward Error Analysis . . . . .	142
8.3	Bounds for the Inverse . . . . .	147
8.4	A Parallel Fan-In Algorithm . . . . .	149
8.5	Notes and References . . . . .	151
	8.5.1 LAPACK . . . . .	153
	Problems . . . . .	153
<b>9</b>	<b>LU Factorization and Linear Equations</b>	<b>157</b>
9.1	Gaussian Elimination and Pivoting Strategies . . . . .	158
9.2	LU Factorization . . . . .	160
9.3	Error Analysis . . . . .	163
9.4	The Growth Factor . . . . .	166
9.5	Diagonally Dominant and Banded Matrices . . . . .	170
9.6	Tridiagonal Matrices . . . . .	174
9.7	More Error Bounds . . . . .	176
9.8	Scaling and Choice of Pivoting Strategy . . . . .	177
9.9	Variants of Gaussian Elimination . . . . .	179
9.10	A Posteriori Stability Tests . . . . .	180
9.11	Sensitivity of the LU Factorization . . . . .	181
9.12	Rank-Revealing LU Factorizations . . . . .	182
9.13	Historical Perspective . . . . .	183
9.14	Notes and References . . . . .	187
	9.14.1 LAPACK . . . . .	191
	Problems . . . . .	192

<b>10 Cholesky Factorization</b>	<b>195</b>
10.1 Symmetric Positive Definite Matrices . . . . .	196
10.1.1 Error Analysis . . . . .	197
10.2 Sensitivity of the Cholesky Factorization . . . . .	201
10.3 Positive Semidefinite Matrices . . . . .	201
10.3.1 Perturbation Theory . . . . .	203
10.3.2 Error Analysis . . . . .	205
10.4 Matrices with Positive Definite Symmetric Part . . . . .	208
10.5 Notes and References . . . . .	209
10.5.1 LAPACK . . . . .	210
Problems . . . . .	211
<b>11 Symmetric Indefinite and Skew-Symmetric Systems</b>	<b>213</b>
11.1 Block $LDL^T$ Factorization for Symmetric Matrices . . . . .	214
11.1.1 Complete Pivoting . . . . .	215
11.1.2 Partial Pivoting . . . . .	216
11.1.3 Rook Pivoting . . . . .	219
11.1.4 Tridiagonal Matrices . . . . .	221
11.2 Aasen's Method . . . . .	222
11.2.1 Aasen's Method Versus Block $LDL^T$ Factorization . . . . .	224
11.3 Block $LDL^T$ Factorization for Skew-Symmetric Matrices . . . . .	225
11.4 Notes and References . . . . .	226
11.4.1 LAPACK . . . . .	228
Problems . . . . .	228
<b>12 Iterative Refinement</b>	<b>231</b>
12.1 Behaviour of the Forward Error . . . . .	232
12.2 Iterative Refinement Implies Stability . . . . .	235
12.3 Notes and References . . . . .	240
12.3.1 LAPACK . . . . .	242
Problems . . . . .	242
<b>13 Block LU Factorization</b>	<b>245</b>
13.1 Block Versus Partitioned LU Factorization . . . . .	246
13.2 Error Analysis of Partitioned LU Factorization . . . . .	249
13.3 Error Analysis of Block LU Factorization . . . . .	250
13.3.1 Block Diagonal Dominance . . . . .	251
13.3.2 Symmetric Positive Definite Matrices . . . . .	255
13.4 Notes and References . . . . .	256
13.4.1 LAPACK . . . . .	257
Problems . . . . .	257
<b>14 Matrix Inversion</b>	<b>259</b>
14.1 Use and Abuse of the Matrix Inverse . . . . .	260
14.2 Inverting a Triangular Matrix . . . . .	262
14.2.1 Unblocked Methods . . . . .	262
14.2.2 Block Methods . . . . .	265
14.3 Inverting a Full Matrix by LU Factorization . . . . .	267

14.3.1	Method A . . . . .	267
14.3.2	Method B . . . . .	268
14.3.3	Method C . . . . .	269
14.3.4	Method D . . . . .	270
14.3.5	Summary . . . . .	271
14.4	Gauss–Jordan Elimination . . . . .	273
14.5	Parallel Inversion Methods . . . . .	278
14.6	The Determinant . . . . .	279
14.6.1	Hyman’s Method . . . . .	280
14.7	Notes and References . . . . .	281
14.7.1	LAPACK . . . . .	282
	Problems . . . . .	283
<b>15</b>	<b>Condition Number Estimation</b>	<b>287</b>
15.1	How to Estimate Componentwise Condition Numbers . . . . .	288
15.2	The $p$ -Norm Power Method . . . . .	289
15.3	LAPACK 1-Norm Estimator . . . . .	292
15.4	Block 1-Norm Estimator . . . . .	294
15.5	Other Condition Estimators . . . . .	295
15.6	Condition Numbers of Tridiagonal Matrices . . . . .	299
15.7	Notes and References . . . . .	301
15.7.1	LAPACK . . . . .	303
	Problems . . . . .	303
<b>16</b>	<b>The Sylvester Equation</b>	<b>305</b>
16.1	Solving the Sylvester Equation . . . . .	307
16.2	Backward Error . . . . .	308
16.2.1	The Lyapunov Equation . . . . .	311
16.3	Perturbation Result . . . . .	313
16.4	Practical Error Bounds . . . . .	315
16.5	Extensions . . . . .	316
16.6	Notes and References . . . . .	317
16.6.1	LAPACK . . . . .	318
	Problems . . . . .	318
<b>17</b>	<b>Stationary Iterative Methods</b>	<b>321</b>
17.1	Survey of Error Analysis . . . . .	323
17.2	Forward Error Analysis . . . . .	325
17.2.1	Jacobi’s Method . . . . .	328
17.2.2	Successive Overrelaxation . . . . .	329
17.3	Backward Error Analysis . . . . .	330
17.4	Singular Systems . . . . .	331
17.4.1	Theoretical Background . . . . .	331
17.4.2	Forward Error Analysis . . . . .	333
17.5	Stopping an Iterative Method . . . . .	335
17.6	Notes and References . . . . .	337
	Problems . . . . .	337

<b>18 Matrix Powers</b>	<b>339</b>
18.1 Matrix Powers in Exact Arithmetic . . . . .	340
18.2 Bounds for Finite Precision Arithmetic . . . . .	346
18.3 Application to Stationary Iteration . . . . .	351
18.4 Notes and References . . . . .	351
Problems . . . . .	352
<b>19 QR Factorization</b>	<b>353</b>
19.1 Householder Transformations . . . . .	354
19.2 QR Factorization . . . . .	355
19.3 Error Analysis of Householder Computations . . . . .	357
19.4 Pivoting and Row-Wise Stability . . . . .	362
19.5 Aggregated Householder Transformations . . . . .	363
19.6 Givens Rotations . . . . .	365
19.7 Iterative Refinement . . . . .	368
19.8 Gram–Schmidt Orthogonalization . . . . .	369
19.9 Sensitivity of the QR Factorization . . . . .	373
19.10 Notes and References . . . . .	374
19.10.1 LAPACK . . . . .	377
Problems . . . . .	378
<b>20 The Least Squares Problem</b>	<b>381</b>
20.1 Perturbation Theory . . . . .	382
20.2 Solution by QR Factorization . . . . .	384
20.3 Solution by the Modified Gram–Schmidt Method . . . . .	386
20.4 The Normal Equations . . . . .	386
20.5 Iterative Refinement . . . . .	388
20.6 The Seminormal Equations . . . . .	391
20.7 Backward Error . . . . .	392
20.8 Weighted Least Squares Problems . . . . .	395
20.9 The Equality Constrained Least Squares Problem . . . . .	396
20.9.1 Perturbation Theory . . . . .	396
20.9.2 Methods . . . . .	397
20.10 Proof of Wedin’s Theorem . . . . .	400
20.11 Notes and References . . . . .	402
20.11.1 LAPACK . . . . .	405
Problems . . . . .	405
<b>21 Underdetermined Systems</b>	<b>407</b>
21.1 Solution Methods . . . . .	408
21.2 Perturbation Theory and Backward Error . . . . .	409
21.3 Error Analysis . . . . .	411
21.4 Notes and References . . . . .	413
21.4.1 LAPACK . . . . .	414
Problems . . . . .	414

<b>22 Vandermonde Systems</b>	<b>415</b>
22.1 Matrix Inversion . . . . .	416
22.2 Primal and Dual Systems . . . . .	418
22.3 Stability . . . . .	423
22.3.1 Forward Error . . . . .	424
22.3.2 Residual . . . . .	425
22.3.3 Dealing with Instability . . . . .	426
22.4 Notes and References . . . . .	428
Problems . . . . .	430
<b>23 Fast Matrix Multiplication</b>	<b>433</b>
23.1 Methods . . . . .	434
23.2 Error Analysis . . . . .	438
23.2.1 Winograd's Method . . . . .	439
23.2.2 Strassen's Method . . . . .	440
23.2.3 Bilinear Noncommutative Algorithms . . . . .	443
23.2.4 The 3M Method . . . . .	444
23.3 Notes and References . . . . .	446
Problems . . . . .	448
<b>24 The Fast Fourier Transform and Applications</b>	<b>451</b>
24.1 The Fast Fourier Transform . . . . .	452
24.2 Circulant Linear Systems . . . . .	454
24.3 Notes and References . . . . .	456
Problems . . . . .	457
<b>25 Nonlinear Systems and Newton's Method</b>	<b>459</b>
25.1 Newton's Method . . . . .	460
25.2 Error Analysis . . . . .	461
25.3 Special Cases and Experiments . . . . .	462
25.4 Conditioning . . . . .	464
25.5 Stopping an Iterative Method . . . . .	467
25.6 Notes and References . . . . .	468
Problems . . . . .	469
<b>26 Automatic Error Analysis</b>	<b>471</b>
26.1 Exploiting Direct Search Optimization . . . . .	472
26.2 Direct Search Methods . . . . .	474
26.3 Examples of Direct Search . . . . .	477
26.3.1 Condition Estimation . . . . .	477
26.3.2 Fast Matrix Inversion . . . . .	478
26.3.3 Roots of a Cubic . . . . .	479
26.4 Interval Analysis . . . . .	481
26.5 Other Work . . . . .	484
26.6 Notes and References . . . . .	486
Problems . . . . .	487

<b>27 Software Issues in Floating Point Arithmetic</b>	<b>489</b>
27.1 Exploiting IEEE Arithmetic . . . . .	490
27.2 Subtleties of Floating Point Arithmetic . . . . .	493
27.3 Cray Peculiarities . . . . .	493
27.4 Compilers . . . . .	494
27.5 Determining Properties of Floating Point Arithmetic . . . . .	494
27.6 Testing a Floating Point Arithmetic . . . . .	495
27.7 Portability . . . . .	496
27.7.1 Arithmetic Parameters . . . . .	496
27.7.2 $2 \times 2$ Problems in LAPACK . . . . .	497
27.7.3 Numerical Constants . . . . .	498
27.7.4 Models of Floating Point Arithmetic . . . . .	498
27.8 Avoiding Underflow and Overflow . . . . .	499
27.9 Multiple Precision Arithmetic . . . . .	501
27.10 Extended and Mixed Precision BLAS . . . . .	503
27.11 Patriot Missile Software Problem . . . . .	503
27.12 Notes and References . . . . .	504
Problems . . . . .	505
<b>28 A Gallery of Test Matrices</b>	<b>511</b>
28.1 The Hilbert and Cauchy Matrices . . . . .	512
28.2 Random Matrices . . . . .	515
28.3 “Randsvd” Matrices . . . . .	517
28.4 The Pascal Matrix . . . . .	518
28.5 Tridiagonal Toeplitz Matrices . . . . .	521
28.6 Companion Matrices . . . . .	522
28.7 Notes and References . . . . .	523
28.7.1 LAPACK . . . . .	525
Problems . . . . .	525
<b>A Solutions to Problems</b>	<b>527</b>
<b>B Acquiring Software</b>	<b>573</b>
B.1 Internet . . . . .	574
B.2 Netlib . . . . .	574
B.3 MATLAB . . . . .	575
B.4 NAG Library and NAGWare F95 Compiler . . . . .	575
<b>C Program Libraries</b>	<b>577</b>
C.1 Basic Linear Algebra Subprograms . . . . .	578
C.2 EISPACK . . . . .	579
C.3 LINPACK . . . . .	579
C.4 LAPACK . . . . .	579
C.4.1 Structure of LAPACK . . . . .	580
<b>D The Matrix Computation Toolbox</b>	<b>583</b>
<b>Bibliography</b>	<b>587</b>



**Name Index**

**657**

**Subject Index**

**667**