Contents

PREFACE xv
ACKNOWLEDGMENTS xix

SECTION I **Preliminaries**

CHAPTER 1 ▪ Mathematics Review 3

1.1 PRELIMINARIES: NUMBERS AND SETS 3
1.2 VECTOR SPACES 4
1.2.1 Defining Vector Spaces 4
1.2.2 Span, Linear Independence, and Bases 5
1.2.3 Our Focus: $\mathbb{R}^n$ 7
1.3 LINEARITY 9
1.3.1 Matrices 10
1.3.2 Scalars, Vectors, and Matrices 12
1.3.3 Matrix Storage and Multiplication Methods 13
1.3.4 Model Problem: $A\vec{x} = \vec{b}$ 14
1.4 NON-LINEARITY: DIFFERENTIAL CALCULUS 15
1.4.1 Differentiation in One Variable 16
1.4.2 Differentiation in Multiple Variables 17
1.4.3 Optimization 20
1.5 EXERCISES 23

CHAPTER 2 ▪ Numerics and Error Analysis 27

2.1 STORING NUMBERS WITH FRACTIONAL PARTS 27
2.1.1 Fixed-Point Representations 28
2.1.2 Floating-Point Representations 29
2.1.3 More Exotic Options 31
2.2 UNDERSTANDING ERROR 32
2.2.1 Classifying Error 33
2.2.2 Conditioning, Stability, and Accuracy 35
2.3 PRACTICAL ASPECTS 36
2.3.1 Computing Vector Norms 37

2.3.2 Larger-Scale Example: Summation 38
2.4 EXERCISES 39

SECTION II **Linear Algebra**

CHAPTER 3 ▪ Linear Systems and the LU Decomposition 47

3.1 SOLVABILITY OF LINEAR SYSTEMS 47
3.2 AD-HOC SOLUTION STRATEGIES 49
3.3 ENCODING ROW OPERATIONS 51
3.3.1 Permutation 51
3.3.2 Row Scaling 52
3.3.3 Elimination 52
3.4 GAUSSIAN ELIMINATION 54
3.4.1 Forward-Substitution 55
3.4.2 Back-Substitution 56
3.4.3 Analysis of Gaussian Elimination 56
3.5 LU FACTORIZATION 58
3.5.1 Constructing the Factorization 59
3.5.2 Using the Factorization 60
3.5.3 Implementing LU 61
3.6 EXERCISES 61

CHAPTER 4 ▪ Designing and Analyzing Linear Systems 65

4.1 SOLUTION OF SQUARE SYSTEMS 65
4.1.1 Regression 66
4.1.2 Least-Squares 68
4.1.3 Tikhonov Regularization 70
4.1.4 Image Alignment 71
4.1.5 Deconvolution 73
4.1.6 Harmonic Parameterization 74
4.2 SPECIAL PROPERTIES OF LINEAR SYSTEMS 75
4.2.1 Positive Definite Matrices and the Cholesky Factorization 75
4.2.2 Sparsity 79
4.2.3 Additional Special Structures 80
4.3 SENSITIVITY ANALYSIS 81
4.3.1 Matrix and Vector Norms 81
4.3.2 Condition Numbers 84
4.4 EXERCISES 86

CHAPTER 5 ▪ Column Spaces and QR 91

5.1 THE STRUCTURE OF THE NORMAL EQUATIONS 91
5.2 ORTHOGONALITY 92
5.3 STRATEGY FOR NON-ORTHOGONAL MATRICES 93
5.4 GRAM-SCHMIDT ORTHOGONALIZATION 94
5.4.1 Projections 94
5.4.2 Gram-Schmidt Algorithm 96
5.5 HOUSEHOLDER TRANSFORMATIONS 99
5.6 REDUCED QR FACTORIZATION 103
5.7 EXERCISES 103

CHAPTER 6 ▪ Eigenvectors 107

6.1 MOTIVATION 107
6.1.1 Statistics 108
6.1.2 Differential Equations 109
6.1.3 Spectral Embedding 110
6.2 PROPERTIES OF EIGENVECTORS 112
6.2.1 Symmetric and Positive Definite Matrices 114
6.2.2 Specialized Properties 116
6.2.2.1 Characteristic Polynomial 116
6.2.2.2 Jordan Normal Form 116
6.3 COMPUTING A SINGLE EIGENVALUE 117
6.3.1 Power Iteration 117
6.3.2 Inverse Iteration 118
6.3.3 Shifting 119
6.4 FINDING MULTIPLE EIGENVALUES 120
6.4.1 Deflation 120
6.4.2 QR Iteration 121
6.4.3 Krylov Subspace Methods 126
6.5 SENSITIVITY AND CONDITIONING 126
6.6 EXERCISES 127

CHAPTER 7 ▪ Singular Value Decomposition 131

7.1 DERIVING THE SVD 131
7.1.1 Computing the SVD 133
7.2 APPLICATIONS OF THE SVD 134
7.2.1 Solving Linear Systems and the Pseudoinverse 134

7.2.2 Decomposition into Outer Products and Low-Rank Approximations 135
7.2.3 Matrix Norms 136
7.2.4 The Procrustes Problem and Point Cloud Alignment 137
7.2.5 Principal Component Analysis (PCA) 139
7.2.6 Eigenfaces 140
7.3 EXERCISES 141

SECTION III **Nonlinear Techniques**

CHAPTER 8 ▪ Nonlinear Systems 147

8.1 ROOT-FINDING IN A SINGLE VARIABLE 147
8.1.1 Characterizing Problems 147
8.1.2 Continuity and Bisection 148
8.1.3 Fixed Point Iteration 149
8.1.4 Newton's Method 151
8.1.5 Secant Method 153
8.1.6 Hybrid Techniques 155
8.1.7 Single-Variable Case: Summary 155
8.2 MULTIVARIABLE PROBLEMS 156
8.2.1 Newton's Method 156
8.2.2 Making Newton Faster: Quasi-Newton and Broyden 156
8.3 CONDITIONING 158
8.4 EXERCISES 158

CHAPTER 9 ▪ Unconstrained Optimization 163

9.1 UNCONSTRAINED OPTIMIZATION: MOTIVATION 163
9.2 OPTIMALITY 165
9.2.1 Differential Optimality 166
9.2.2 Alternative Conditions for Optimality 168
9.3 ONE-DIMENSIONAL STRATEGIES 169
9.3.1 Newton's Method 170
9.3.2 Golden Section Search 170
9.4 MULTIVARIABLE STRATEGIES 173
9.4.1 Gradient Descent 173
9.4.2 Newton's Method in Multiple Variables 174
9.4.3 Optimization without Hessians: BFGS 175
9.5 EXERCISES 178
9.6 APPENDIX: DERIVATION OF BFGS UPDATE 182

CHAPTER 10 ▪ Constrained Optimization 185

10.1 MOTIVATION 186
10.2 THEORY OF CONSTRAINED OPTIMIZATION 189
10.2.1 Optimality 189
10.2.2 KKT Conditions 189
10.3 OPTIMIZATION ALGORITHMS 192
10.3.1 Sequential Quadratic Programming (SQP) 193
10.3.1.1 Equality Constraints 193
10.3.1.2 Inequality Constraints 193
10.3.2 Barrier Methods 194
10.4 CONVEX PROGRAMMING 194
10.4.1 Linear Programming 196
10.4.2 Second-Order Cone Programming 197
10.4.3 Semidefinite Programming 199
10.4.4 Integer Programs and Relaxations 200
10.5 EXERCISES 201

CHAPTER 11 ▪ Iterative Linear Solvers 207

11.1 GRADIENT DESCENT 208
11.1.1 Gradient Descent for Linear Systems 208
11.1.2 Convergence 209
11.2 CONJUGATE GRADIENTS 211
11.2.1 Motivation 212
11.2.2 Suboptimality of Gradient Descent 214
11.2.3 Generating A-Conjugate Directions 215
11.2.4 Formulating the Conjugate Gradients Algorithm 217
11.2.5 Convergence and Stopping Conditions 219
11.3 PRECONDITIONING 219
11.3.1 CG with Preconditioning 220
11.3.2 Common Preconditioners 221
11.4 OTHER ITERATIVE ALGORITHMS 222
11.5 EXERCISES 223

CHAPTER 12 ▪ Specialized Optimization Methods 227

12.1 NONLINEAR LEAST-SQUARES 227
12.1.1 Gauss-Newton 228
12.1.2 Levenberg-Marquardt 229
12.2 ITERATIVELY REWEIGHTED LEAST-SQUARES 230

12.3 COORDINATE DESCENT AND ALTERNATION 231
12.3.1 Identifying Candidates for Alternation 231
12.3.2 Augmented Lagrangians and ADMM 235
12.4 GLOBAL OPTIMIZATION 240
12.4.1 Graduated Optimization 241
12.4.2 Randomized Global Optimization 243
12.5 ONLINE OPTIMIZATION 244
12.6 EXERCISES 248

SECTION IV **Functions, Derivatives, and Integrals**

CHAPTER 13 ▪ Interpolation 257

13.1 INTERPOLATION IN A SINGLE VARIABLE 258
13.1.1 Polynomial Interpolation 258
13.1.2 Alternative Bases 262
13.1.3 Piecewise Interpolation 263
13.2 MULTIVARIABLE INTERPOLATION 265
13.2.1 Nearest-Neighbor Interpolation 265
13.2.2 Barycentric Interpolation 266
13.2.3 Grid-Based Interpolation 268
13.3 THEORY OF INTERPOLATION 269
13.3.1 Linear Algebra of Functions 269
13.3.2 Approximation via Piecewise Polynomials 272
13.4 EXERCISES 272

CHAPTER 14 ▪ Integration and Differentiation 277

14.1 MOTIVATION 278
14.2 QUADRATURE 279
14.2.1 Interpolatory Quadrature 280
14.2.2 Quadrature Rules 281
14.2.3 Newton-Cotes Quadrature 282
14.2.4 Gaussian Quadrature 286
14.2.5 Adaptive Quadrature 287
14.2.6 Multiple Variables 289
14.2.7 Conditioning 290
14.3 DIFFERENTIATION 290
14.3.1 Differentiating Basis Functions 291
14.3.2 Finite Differences 291
14.3.3 Richardson Extrapolation 293

14.3.4 Choosing the Step Size 294
14.3.5 Automatic Differentiation 295
14.3.6 Integrated Quantities and Structure Preservation 296
14.4 EXERCISES 298

CHAPTER 15 ▪ Ordinary Differential Equations 303

15.1 MOTIVATION 304
15.2 THEORY OF ODES 305
15.2.1 Basic Notions 305
15.2.2 Existence and Uniqueness 307
15.2.3 Model Equations 309
15.3 TIME-STEPPING SCHEMES 311
15.3.1 Forward Euler 311
15.3.2 Backward Euler 313
15.3.3 Trapezoidal Method 314
15.3.4 Runge-Kutta Methods 315
15.3.5 Exponential Integrators 316
15.4 MULTIVALUE METHODS 318
15.4.1 Newmark Integrators 318
15.4.2 Staggered Grid and Leapfrog 321
15.5 COMPARISON OF INTEGRATORS 322
15.6 EXERCISES 324

CHAPTER 16 ▪ Partial Differential Equations 329

16.1 MOTIVATION 330
16.2 STATEMENT AND STRUCTURE OF PDES 335
16.2.1 Properties of PDEs 335
16.2.2 Boundary Conditions 336
16.3 MODEL EQUATIONS 338
16.3.1 Elliptic PDEs 338
16.3.2 Parabolic PDEs 339
16.3.3 Hyperbolic PDEs 340
16.4 REPRESENTING DERIVATIVE OPERATORS 341
16.4.1 Finite Differences 342
16.4.2 Collocation 346
16.4.3 Finite Elements 347
16.4.4 Finite Volumes 350
16.4.5 Other Methods 351
16.5 SOLVING PARABOLIC AND HYPERBOLIC EQUATIONS 352

16.5.1 Semidiscrete Methods 352
16.5.2 Fully Discrete Methods 353
16.6 NUMERICAL CONSIDERATIONS 354
16.6.1 Consistency, Convergence, and Stability 354
16.6.2 Linear Solvers for PDE 354
16.7 EXERCISES 355

Index 369