

Contents

Preface	xi
1 Vectors	1
1.1 Vectors	1
1.2 Subspaces	4
1.3 Span and Linear Independence	7
1.4 Basis and Dimension	11
2 Inner Product, Orthogonality, Norm	19
2.1 Inner Products	20
2.2 Inequalities	26
2.2.1 The Cauchy–Schwarz Inequality	26
2.2.2 The Triangle Inequality	28
2.3 Orthogonal Vectors and Orthogonal Bases	29
2.4 Orthogonal Projection and the Closest Point	33
2.5 The Gram–Schmidt Process	36
2.6 Orthogonal Subspaces and Complements	42
2.7 Norms	45
2.7.1 Basic Examples	45
2.7.2 Spheres and Balls	46
2.7.3 Equivalence of Norms	47
2.7.4 Metrics and Distance	49
3 Matrices	53
3.1 Matrices and Matrix Arithmetic	53
3.2 Transposes and Symmetric Matrices	60
3.3 Linear Systems and Vectors	62
3.4 Image, Kernel, Rank, Nullity	65
3.5 Superposition Principles for Linear Systems	69
3.6 Matrix Inverses	73
3.7 Linear and Affine Functions	76
3.7.1 Linear Functions	76
3.7.2 Affine Functions	79
4 How Matrices Interact with Inner Products and Norms	81
4.1 Symmetric Positive Definite Matrices	81
4.2 Gram Matrices	86
4.3 Adjoints	90
4.3.1 Self-Adjoint and Positive Definite Matrices	91
4.4 The Fundamental Matrix Subspaces	94
4.4.1 Applications to Self-Adjoint Matrices	95
4.4.2 Applications to Linear Systems	96
4.5 Orthogonal and Norm–Preserving Matrices	100
4.5.1 Rigid Motions	103
4.6 Projection Matrices	104

4.7	The General QR Factorization and the Solution of Linear Systems	107
4.7.1	The QR Factorization of a Matrix	108
4.7.2	Solutions to Linear Systems and Least Squares	111
4.8	Matrix Norms	115
4.8.1	Natural Matrix Norms	115
4.8.2	The Frobenius Inner Product and Norm	118
5	Eigenvalues and Singular Values	121
5.1	Eigenvalues and Eigenvectors	122
5.2	Eigenvector Bases	127
5.2.1	Powers of Matrices and the Spectral Radius	131
5.2.2	Connections with Matrix Norms	133
5.3	Eigenvalues of Self-Adjoint Matrices	135
5.3.1	The Spectral Theorem	138
5.3.2	Powers of Self-Adjoint Matrices	139
5.3.3	The Schur Product Theorem	141
5.3.4	Generalized Eigenvalues and Eigenvectors	142
5.4	Optimization Principles	144
5.4.1	Intermediate Eigenvalues and the Min-Max Theorem	147
5.4.2	Eigenvalue Inequalities	151
5.5	Linear Iterative Systems	153
5.5.1	Affine Iterative Systems	155
5.5.2	Markov Processes	156
5.6	Numerical Computation of Eigenvalues	161
5.6.1	The Power Method	161
5.6.2	Orthogonal Iteration	165
5.7	Singular Values	172
5.7.1	The Singular Value Decomposition	173
5.7.2	The Euclidean Matrix Norm	176
5.7.3	Condition Number and Rank	177
6	Basics of Optimization	181
6.1	The Objective Function	182
6.2	Minimization of Quadratic Functions	185
6.2.1	Unconstrained Minimization	186
6.2.2	Least Squares	188
6.2.3	Constrained Minimization	190
6.3	The Gradient and Critical Points	193
6.3.1	The Gradient	193
6.3.2	Critical Points	197
6.4	Gradient Descent	199
6.4.1	Proximal Gradient Descent	203
6.5	The Conjugate Gradient Method	205
6.6	The Second Derivative Test	210
6.7	Convex Functions	215
6.7.1	Some Inequalities	220
6.7.2	Strong Convexity	222
6.8	Lipschitz Continuity	227
6.9	Basic Convergence Results	233
6.10	Newton's Method	239

7	Introduction to Machine Learning and Data	247
7.1	Basics of Machine Learning and Data	247
7.1.1	Mean, Variance, and Covariance	250
7.1.2	Labels and Learning from Data	255
7.1.3	Fully Supervised Learning	256
7.1.4	Overfitting and Generalization	257
7.1.5	The Train–Test Split and Hyperparameters	259
7.1.6	Semi-supervised and Unsupervised Learning	260
7.2	Linear Regression	261
7.2.1	Ridge Regression	263
7.2.2	Lasso Regression	266
7.2.3	Optimization Aspects	269
7.2.4	Kernel Regression	271
7.3	Support Vector Machines (SVM)	273
7.3.1	Optimization Aspects	277
7.3.2	Multiclass Support Vector Machines	277
7.3.3	Kernel Support Vector Machines	280
7.4	k–Nearest Neighbor Classification	282
7.4.1	Computational Aspects	286
7.5	k–Means Clustering	287
7.6	Kernel Methods	298
7.6.1	Kernel Regression	304
7.6.2	Kernel Support Vector Machines	305
8	Principal Component Analysis	311
8.1	The Principal Components	311
8.1.1	Kernel Principal Component Analysis	319
8.2	The Best Approximating Subspace	322
8.2.1	Robust Subspace Recovery	330
8.3	PCA-based Compression	333
8.4	Linear Discriminant Analysis	339
8.5	Multidimensional Scaling (MDS)	346
9	Graph Theory and Graph-based Learning	357
9.1	Graphs and Digraphs	358
9.1.1	Graphs in Applications	364
9.1.2	Similarity Graphs	367
9.2	The Incidence Matrix	372
9.3	The Graph Laplacian	378
9.4	Binary Spectral Clustering	386
9.4.1	Community Detection	391
9.5	Distances on Graphs	397
9.5.1	Computing the Shortest Path Distance	399
9.5.2	Computing Shortest Paths via Dynamic Programming	404
9.5.3	ISOMAP and Metric Multidimensional Scaling	405
9.6	Diffusion on Graphs and Digraphs	410
9.6.1	Jump Diffusion and PageRank	418
9.7	Diffusion Maps and Spectral Embeddings	426
9.7.1	Diffusion Distance	426
9.7.2	Spectral Clustering	433

9.8	t-SNE Embedding	437
9.9	Graph-based Semi-supervised Learning	446
9.9.1	Laplacian Regularization	448
9.9.2	Label Propagation and Hard Constraints	452
9.10	The Discrete Fourier Transform	455
9.10.1	Complexification	459
9.10.2	Roots of Unity	462
9.10.3	The Complex Discrete Fourier Transform	463
9.10.4	Sampling, Trigonometric Interpolation, and Aliasing	465
9.10.5	Convolution and the DFT	469
9.10.6	The Fast Fourier Transform	476
10	Neural Networks and Deep Learning	483
10.1	Fully Connected Networks	484
10.1.1	Training and Optimization	488
10.1.2	Approximation of Functions	490
10.1.3	Classification	491
10.1.4	Connection to Kernel Methods	494
10.2	Backpropagation and Automatic Differentiation	496
10.3	Convolutional Neural Networks	501
10.3.1	Transfer Learning	508
10.4	Graph Convolutional Neural Networks	510
10.4.1	Convolution on Graphs	511
10.4.2	Numerical Experiments	514
10.5	Transformers and Large Language Models	517
10.5.1	The Attention Mechanism	519
10.5.2	Positional Encoding	521
10.5.3	Experiments with Character-based Models	525
10.6	Universal Approximation	526
10.6.1	Polynomials	528
10.6.2	Trigonometric Polynomials	529
10.6.3	Piecewise Affine Functions	530
10.6.4	Two Layer Neural Networks	532
10.6.5	Two Layer ReLU Networks	534
10.6.6	Deep ReLU Networks	537
10.6.7	Approximating Multivariate Functions	541
11	Advanced Optimization	547
11.1	Linear Convergence of Gradient Descent	547
11.2	The Heavy Ball Method	552
11.3	Krylov Subspace Methods and Conjugate Gradients	556
11.4	Nesterov's Accelerated Gradient Descent	562
11.5	Stochastic Gradient Descent	567
11.6	Continuum Analysis of Optimization	577
11.7	Optimizing Neural Networks	584
	Bibliography	593
	Index	609