A frequent challenge faced by beginners in machine learning is the extensive background requirement in linear algebra and optimization. This makes the learning curve very steep. This book, therefore, reverses the focus by teaching linear algebra and optimization as the primary topics of interest, and solutions to machine learning problems as applications of these methods. Therefore, the book also provides significant exposure to machine learning. The chapters of this book belong to two categories:

1. **Linear algebra and its applications**: These chapters focus on the basics of linear algebra together with their common applications to singular value decomposition, similarity matrices (kernel methods), and graph analysis. Numerous machine learning applications have been used as examples, such as spectral clustering, kernel-based classification, and outlier detection.

2. **Optimization and its applications**: Basic methods in optimization such as gradient descent, Newton's method, and coordinate descent are discussed. Constrained optimization methods are introduced as well. Machine learning applications such as linear regression, SVMs, logistic regression, matrix factorization, recommender systems, and K-means clustering are discussed in detail. A general view of optimization in computational graphs is discussed together with its applications to backpropagation in neural networks.

Exercises are included both within the text of the chapters and at the end of the chapters. The book is written for a diverse audience, including graduate students, researchers, and practitioners.

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Linear Algebra and Optimization for Machine Learning
To my wife Lata, my daughter Sayani,
and all my mathematics teachers
# Contents

1 Linear Algebra and Optimization: An Introduction 1

1.1 Introduction ................................... 1

1.2 Scalars, Vectors, and Matrices .......................... 2
  1.2.1 Basic Operations with Scalars and Vectors .......... 3
  1.2.2 Basic Operations with Vectors and Matrices ...... 8
  1.2.3 Special Classes of Matrices .......................... 12
  1.2.4 Matrix Powers, Polynomials, and the Inverse .......... 14
  1.2.5 The Matrix Inversion Lemma: Inverting the Sum of Matrices .... 17
  1.2.6 Frobenius Norm, Trace, and Energy ................. 19

1.3 Matrix Multiplication as a Decomposable Operator ... 21
  1.3.1 Matrix Multiplication as Decomposable Row and Column Operators ................................ 21
  1.3.2 Matrix Multiplication as Decomposable Geometric Operators .... 25

1.4 Basic Problems in Machine Learning ..................... 27
  1.4.1 Matrix Factorization .......................... 27
  1.4.2 Clustering ................................ 28
  1.4.3 Classification and Regression Modeling ................. 29
  1.4.4 Outlier Detection .......................... 30

1.5 Optimization for Machine Learning .......................... 31
  1.5.1 The Taylor Expansion for Function Simplification .... 31
  1.5.2 Example of Optimization in Machine Learning .......... 33
  1.5.3 Optimization in Computational Graphs .......... 34

1.6 Summary .................................... 35

1.7 Further Reading .................................. 35

1.8 Exercises ..................................... 36

2 Linear Transformations and Linear Systems 41

2.1 Introduction ................................... 41
  2.1.1 What Is a Linear Transform? ..................... 42

2.2 The Geometry of Matrix Multiplication ................. 43
2.3 Vector Spaces and Their Geometry ........................................... 51
  2.3.1 Coordinates in a Basis System ........................................... 55
  2.3.2 Coordinate Transformations Between Basis Sets ..................... 57
  2.3.3 Span of a Set of Vectors .................................................. 59
  2.3.4 Machine Learning Example: Discrete Wavelet Transform ........... 60
  2.3.5 Relationships Among Subspaces of a Vector Space .................. 61
2.4 The Linear Algebra of Matrix Rows and Columns ......................... 63
2.5 The Row Echelon Form of a Matrix ......................................... 64
  2.5.1 LU Decomposition ......................................................... 66
  2.5.2 Application: Finding a Basis Set ....................................... 67
  2.5.3 Application: Matrix Inversion ......................................... 67
  2.5.4 Application: Solving a System of Linear Equations ................. 68
2.6 The Notion of Matrix Rank .................................................. 70
  2.6.1 Effect of Matrix Operations on Rank ................................... 71
2.7 Generating Orthogonal Basis Sets .......................................... 73
  2.7.1 Gram-Schmidt Orthogonalization and QR Decomposition ......... 73
  2.7.2 QR Decomposition ......................................................... 74
  2.7.3 The Discrete Cosine Transform ......................................... 77
2.8 An Optimization-Centric View of Linear Systems ......................... 79
  2.8.1 Moore-Penrose Pseudoinverse .......................................... 81
  2.8.2 The Projection Matrix .................................................... 82
2.9 Ill-Conditioned Matrices and Systems .................................... 85
2.10 Inner Products: A Geometric View ........................................ 86
2.11 Complex Vector Spaces ...................................................... 87
  2.11.1 The Discrete Fourier Transform ....................................... 89
2.12 Summary ................................................................. 90
2.13 Further Reading .......................................................... 91
2.14 Exercises ................................................................. 91
3 Eigenvectors and Diagonalizable Matrices ................................ 97
  3.1 Introduction ............................................................... 97
  3.2 Determinants ............................................................... 98
  3.3 Diagonalizable Transformations and Eigenvectors ....................... 103
    3.3.1 Complex Eigenvalues .................................................. 107
    3.3.2 Left Eigenvectors and Right Eigenvectors ......................... 108
    3.3.3 Existence and Uniqueness of Diagonalization ...................... 109
    3.3.4 Existence and Uniqueness of Triangulization ..................... 111
    3.3.5 Similar Matrix Families Sharing Eigenvalues .................... 113
    3.3.6 Diagonalizable Matrix Families Sharing Eigenvectors ........... 115
    3.3.7 Symmetric Matrices .................................................... 115
    3.3.8 Positive Semidefinite Matrices ...................................... 117
    3.3.9 Cholesky Factorization: Symmetric LU Decomposition .......... 119
  3.4 Machine Learning and Optimization Applications ....................... 120
    3.4.1 Fast Matrix Operations in Machine Learning ..................... 121
    3.4.2 Examples of Diagonalizable Matrices in Machine Learning ....... 121
    3.4.3 Symmetric Matrices in Quadratic Optimization ................... 124
    3.4.4 Diagonalization Application: Variable Separation for ... 128
       Optimization ............................................................. 128
    3.4.5 Eigenvectors in Norm-Constrained Quadratic Programming ...... 130
## 5.6.3 Convergence Problems and Solutions with Non-quadratic Functions

5.6.3.1 Trust Region Method

## 5.7 Computationally Efficient Variations of Newton Method

5.7.1 Conjugate Gradient Method

5.7.2 Quasi-Newton Methods and BFGS

## 5.8 Non-differentiable Optimization Functions

5.8.1 The Subgradient Method

5.8.1.1 Application: $L_1$-Regularization

5.8.1.2 Combining Subgradients with Coordinate Descent

5.8.2 Proximal Gradient Method

5.8.2.1 Application: Alternative for $L_1$-Regularized Regression

5.8.3 Designing Surrogate Loss Functions for Combinatorial Optimization

5.8.3.1 Application: Ranking Support Vector Machine

5.8.3.2 Proximal Gradient Method

## 5.9 Summary

## 5.10 Further Reading

## 5.11 Exercises

## 6 Constrained Optimization and Duality

6.1 Introduction

6.2 Primal Gradient Descent Methods

6.2.1 Linear Equality Constraints

6.2.1.1 Convex Quadratic Program with Equality Constraints

6.2.1.2 Application: Linear Regression with Equality Constraints

6.2.1.3 Application: Newton Method with Equality Constraints

6.2.2 Linear Inequality Constraints

6.2.2.1 The Special Case of Box Constraints

6.2.2.2 General Conditions for Projected Gradient Descent to Work

6.2.3 Sequential Quadratic Programming

6.3 Primal Coordinate Descent

6.3.1 Coordinate Descent for Convex Optimization Over Convex Set

6.3.2 Machine Learning Application: Box Regression

6.4 Lagrangian Relaxation and Duality

6.4.1 Kuhn-Tucker Optimality Conditions

6.4.2 General Procedure for Using Duality

6.4.2.1 Inferring the Optimal Primal Solution from Optimal Dual Solution

6.4.3 Application: Formulating the SVM Dual

6.4.3.1 Inferring the Optimal Primal Solution from Optimal Dual Solution
CONTENTS

6.4.4 Optimization Algorithms for the SVM Dual ........................................ 279
  6.4.4.1 Gradient Descent ........................................ 279
  6.4.4.2 Coordinate Descent ...................................... 280
6.4.5 Getting the Lagrangian Relaxation of Unconstrained Problems ............ 281
  6.4.5.1 Machine Learning Application: Dual of Linear Regression ...................... 283
6.5 Penalty-Based and Primal-Dual Methods ............................................. 286
  6.5.1 Penalty Method with Single Constraint ...................................... 286
  6.5.2 Penalty Method: General Formulation ...................................... 287
  6.5.3 Barrier and Interior Point Methods ...................................... 288
6.6 Norm-Constrained Optimization .................................................... 290
6.7 Primal Versus Dual Methods ........................................................ 292
6.8 Summary ......................................................................................... 293
6.9 Further Reading .............................................................................. 294
6.10 Exercises ......................................................................................... 294

7 Singular Value Decomposition .................................................................. 299
  7.1 Introduction ..................................................................................... 300
  7.2 SVD: A Linear Algebra Perspective .................................................. 300
    7.2.1 Singular Value Decomposition of a Square Matrix ....................... 300
    7.2.2 Square SVD to Rectangular SVD via Padding ............................... 304
    7.2.3 Several Definitions of Rectangular Singular Value Decomposition .... 305
    7.2.4 Truncated Singular Value Decomposition .................................... 307
      7.2.4.1 Relating Truncation Loss to Singular Values ......................... 309
      7.2.4.2 Geometry of Rank-k Truncation ...................................... 311
      7.2.4.3 Example of Truncated SVD ........................................... 311
    7.2.5 Two Interpretations of SVD ..................................................... 313
    7.2.6 Is Singular Value Decomposition Unique? .................................... 315
    7.2.7 Two-Way Versus Three-Way Decompositions ................................. 316
  7.3 SVD: An Optimization Perspective .................................................. 317
    7.3.1 A Maximization Formulation with Basis Orthogonality .................. 318
    7.3.2 A Minimization Formulation with Residuals .................................. 319
    7.3.3 Generalization to Matrix Factorization Methods ............................. 320
    7.3.4 Principal Component Analysis .................................................. 320
  7.4 Applications of Singular Value Decomposition .................................... 323
    7.4.1 Dimensionality Reduction ....................................................... 323
    7.4.2 Noise Removal ......................................................................... 324
    7.4.3 Finding the Four Fundamental Subspaces in Linear Algebra ............ 325
    7.4.4 Moore-Penrose Pseudoinverse .................................................. 325
      7.4.4.1 Ill-Conditioned Square Matrices ....................................... 326
    7.4.5 Solving Linear Equations and Linear Regression ............................ 327
    7.4.6 Feature Preprocessing and Whitening in Machine Learning ............ 327
    7.4.7 Outlier Detection ....................................................................... 328
    7.4.8 Feature Engineering .................................................................... 329
  7.5 Numerical Algorithms for SVD .......................................................... 330
  7.6 Summary .......................................................................................... 332
  7.7 Further Reading ............................................................................... 332
  7.8 Exercises ......................................................................................... 333
8 Matrix Factorization
8.1 Introduction ................................... 339
8.2 Optimization-Based Matrix Factorization ................................. 341
  8.2.1 Example: K-Means as Constrained Matrix Factorization .... 342
8.3 Unconstrained Matrix Factorization .................................. 342
  8.3.1 Gradient Descent with Fully Specified Matrices .... 343
  8.3.2 Application to Recommender Systems ................ 346
    8.3.2.1 Stochastic Gradient Descent ................. 348
    8.3.2.2 Coordinate Descent ..................... 348
    8.3.2.3 Block Coordinate Descent: Alternating Least Squares . 349
8.4 Nonnegative Matrix Factorization .................................. 350
  8.4.1 Optimization Problem with Frobenius Norm ................ 350
    8.4.1.1 Projected Gradient Descent with Box Constraints ... 351
  8.4.2 Solution Using Duality ................................ 351
  8.4.3 Interpretability of Nonnegative Matrix Factorization ...... 353
  8.4.4 Example of Nonnegative Matrix Factorization ............ 353
  8.4.5 The I-Divergence Objective Function ................. 356
8.5 Weighted Matrix Factorization .................................. 356
  8.5.1 Practical Use Cases of Nonnegative and Sparse Matrices ...... 357
  8.5.2 Stochastic Gradient Descent ................................ 359
    8.5.2.1 Why Negative Sampling Is Important ........... 360
  8.5.3 Application: Recommendations with Implicit Feedback Data ... 360
  8.5.4 Application: Link Prediction in Adjacency Matrices ...... 360
  8.5.5 Application: Word-Word Context Embedding with GloVe ... 361
8.6 Nonlinear Matrix Factorizations .................................. 362
  8.6.1 Logistic Matrix Factorization ................................ 362
    8.6.1.1 Gradient Descent Steps for Logistic Matrix Factorization .......... 363
  8.6.2 Maximum Margin Matrix Factorization ...................... 364
8.7 Generalized Low-Rank Models ................................... 365
  8.7.1 Handling Categorical Entries ........................... 367
  8.7.2 Handling Ordinal Entries ................................ 367
8.8 Shared Matrix Factorization .................................. 369
  8.8.1 Gradient Descent Steps for Shared Factorization .......... 370
  8.8.2 How to Set Up Shared Models in Arbitrary Scenarios .... 370
8.9 Factorization Machines .................................. 371
8.10 Summary .................................... 375
8.11 Further Reading .................................. 375
8.12 Exercises ..................................... 375

9 The Linear Algebra of Similarity
9.1 Introduction ................................... 379
9.2 Equivalence of Data and Similarity Matrices ................... 379
  9.2.1 From Data Matrix to Similarity Matrix and Back .... 380
  9.2.2 When Is Data Recovery from a Similarity Matrix Useful? .. 381
  9.2.3 What Types of Similarity Matrices Are “Valid”? ...... 382
  9.2.4 Symmetric Matrix Factorization as an Optimization Model ... 383
  9.2.5 Kernel Methods: The Machine Learning Terminology ...... 383
9.3 Efficient Data Recovery from Similarity Matrices 
  9.3.1 Nyström Sampling ................................ 385
  9.3.2 Matrix Factorization with Stochastic Gradient Descent 386
  9.3.3 Asymmetric Similarity Decompositions ............... 388
9.4 Linear Algebra Operations on Similarity Matrices .............. 389
  9.4.1 Energy of Similarity Matrix and Unit Ball Normalization 390
  9.4.2 Norm of the Mean and Variance .................. 390
  9.4.3 Centering a Similarity Matrix .................... 391
    9.4.3.1 Application: Kernel PCA .................. 391
  9.4.4 From Similarity Matrix to Distance Matrix and Back .... 392
    9.4.4.1 Application: ISOMAP .................... 393
9.5 Machine Learning with Similarity Matrices .................. 394
  9.5.1 Feature Engineering from Similarity Matrix .......... 395
    9.5.1.1 Kernel Clustering ........................ 395
    9.5.1.2 Kernel Outlier Detection .................. 396
    9.5.1.3 Kernel Classification ..................... 396
  9.5.2 Direct Use of Similarity Matrix .................... 397
    9.5.2.1 Kernel K-Means .......................... 397
    9.5.2.2 Kernel SVM ............................. 398
9.6 The Linear Algebra of the Representer Theorem ............... 399
9.7 Similarity Matrices and Linear Separability ................. 403
  9.7.1 Transformations That Preserve Positive Semi-definiteness 405
9.8 Summary .................................... 407
9.9 Further Reading .................................. 407
9.10 Exercises ..................................... 407

10 The Linear Algebra of Graphs Somewhere around page 411
10.1 Introduction ................................... 411
10.2 Graph Basics and Adjacency Matrices .................... 411
10.3 Powers of Adjacency Matrices .......................... 416
10.4 The Perron-Frobenius Theorem .......................... 419
10.5 The Right Eigenvectors of Graph Matrices ............... 423
  10.5.1 The Kernel View of Spectral Clustering ............ 423
    10.5.1.1 Relating Shi-Malik and Ng-Jordan-Weiss Embeddings . 425
  10.5.2 The Laplacian View of Spectral Clustering ......... 426
    10.5.2.1 Graph Laplacian ........................ 426
    10.5.2.2 Optimization Model with Laplacian ........... 428
  10.5.3 The Matrix Factorization View of Spectral Clustering . 430
    10.5.3.1 Machine Learning Application: Directed Link Prediction . . . . 430
  10.5.4 Which View of Spectral Clustering Is Most Informative? 431
10.6 The Left Eigenvectors of Graph Matrices .................. 431
  10.6.1 PageRank as Left Eigenvector of Transition Matrix . 433
  10.6.2 Related Measures of Prestige and Centrality ........ 434
  10.6.3 Application of Left Eigenvectors to Link Prediction . 435
10.7 Eigenvectors of Reducible Matrices ........................ 436
  10.7.1 Undirected Graphs ............................ 436
  10.7.2 Directed Graphs ............................. 436
10.8 Machine Learning Applications ......................................................... 439
  10.8.1 Application to Vertex Classification ........................................ 440
  10.8.2 Applications to Multidimensional Data ..................................... 442
10.9 Summary ....................................................................................... 443
10.10 Further Reading ........................................................................... 443
10.11 Exercises ....................................................................................... 444

11 Optimization in Computational Graphs .............................................. 447
  11.1 Introduction ................................................................................ 447
  11.2 The Basics of Computational Graphs ............................................. 448
  11.2.1 Neural Networks as Directed Computational Graphs ................ 451
  11.3 Optimization in Directed Acyclic Graphs ....................................... 453
    11.3.1 The Challenge of Computational Graphs .................................. 453
    11.3.2 The Broad Framework for Gradient Computation .................... 455
    11.3.3 Computing Node-to-Node Derivatives Using Brute Force .......... 456
    11.3.4 Dynamic Programming for Computing Node-to-Node Derivatives 459
      11.3.4.1 Example of Computing Node-to-Node Derivatives .......... 461
    11.3.5 Converting Node-to-Node Derivatives into Loss-to-Weight Derivatives . 464
      11.3.5.1 Example of Computing Loss-to-Weight Derivatives .... 465
    11.3.6 Computational Graphs with Vector Variables ......................... 466
  11.4 Application: Backpropagation in Neural Networks ............................... 468
    11.4.1 Derivatives of Common Activation Functions .......................... 470
    11.4.2 Vector-Centric Backpropagation .......................................... 471
    11.4.3 Example of Vector-Centric Backpropagation ........................... 473
  11.5 A General View of Computational Graphs ...................................... 475
  11.6 Summary ....................................................................................... 478
  11.7 Further Reading .......................................................................... 478
  11.8 Exercises ...................................................................................... 478

Bibliography ....................................................................................... 483

Index ..................................................................................................... 491
“Mathematics is the language with which God wrote the universe.”– Galileo

A frequent challenge faced by beginners in machine learning is the extensive background required in linear algebra and optimization. One problem is that the existing linear algebra and optimization courses are not specific to machine learning; therefore, one would typically have to complete more course material than is necessary to pick up machine learning. Furthermore, certain types of ideas and tricks from optimization and linear algebra recur more frequently in machine learning than other application-centric settings. Therefore, there is significant value in developing a view of linear algebra and optimization that is better suited to the specific perspective of machine learning.

It is common for machine learning practitioners to pick up missing bits and pieces of linear algebra and optimization via “osmosis” while studying the solutions to machine learning applications. However, this type of unsystematic approach is unsatisfying, because the primary focus on machine learning gets in the way of learning linear algebra and optimization in a generalizable way across new situations and applications. Therefore, we have inverted the focus in this book, with linear algebra and optimization as the primary topics of interest and solutions to machine learning problems as the applications of this machinery. In other words, the book goes out of its way to teach linear algebra and optimization with machine learning examples. By using this approach, the book focuses on those aspects of linear algebra and optimization that are more relevant to machine learning and also teaches the reader how to apply them in the machine learning context. As a side benefit, the reader will pick up knowledge of several fundamental problems in machine learning. At the end of the process, the reader will become familiar with many of the basic linear-algebra- and optimization-centric algorithms in machine learning. Although the book is not intended to provide exhaustive coverage of machine learning, it serves as a “technical starter” for the key models and optimization methods in machine learning. Even for seasoned practitioners of machine learning, a systematic introduction to fundamental linear algebra and optimization methodologies can be useful in terms of providing a fresh perspective.

The chapters of the book are organized as follows:

1. Linear algebra and its applications: The chapters focus on the basics of linear algebra together with their common applications to singular value decomposition, matrix factorization, similarity matrices (kernel methods), and graph analysis. Numerous machine learning applications have been used as examples, such as spectral clustering,
kernel-based classification, and outlier detection. The tight integration of linear algebra methods with examples from machine learning differentiates this book from generic volumes on linear algebra. The focus is clearly on the most relevant aspects of linear algebra for machine learning and to teach readers how to apply these concepts.

2. Optimization and its applications: Much of machine learning is posed as an optimization problem in which we try to maximize the accuracy of regression and classification models. The “parent problem” of optimization-centric machine learning is least-squares regression. Interestingly, this problem arises in both linear algebra and optimization and is one of the key connecting problems of the two fields. Least-squares regression is also the starting point for support vector machines, logistic regression, and recommender systems. Furthermore, the methods for dimensionality reduction and matrix factorization also require the development of optimization methods. A general view of optimization in computational graphs is discussed together with its applications to backpropagation in neural networks.

This book contains exercises both within the text of the chapter and at the end of the chapter. The exercises within the text of the chapter should be solved as one reads the chapter in order to solidify the concepts. This will lead to slower progress, but a better understanding. For in-chapter exercises, hints for the solution are given in order to help the reader along. The exercises at the end of the chapter are intended to be solved as refreshers after completing the chapter.

Throughout this book, a vector or a multidimensional data point is annotated with a bar, such as $\bar{X}$ or $\bar{y}$. A vector or multidimensional point may be denoted by either small letters or capital letters, as long as it has a bar. Vector dot products are denoted by centered dots, such as $\bar{X} \cdot \bar{Y}$. A matrix is denoted in capital letters without a bar, such as $R$. Throughout the book, the $n \times d$ matrix corresponding to the entire training data set is denoted by $D$, with $n$ data points and $d$ dimensions. The individual data points in $D$ are therefore $d$-dimensional row vectors and are often denoted by $\bar{X}_1, \ldots, \bar{X}_n$. Conversely, vectors with one component for each data point are usually $n$-dimensional column vectors. An example is the $n$-dimensional column vector $\bar{y}$ of class variables of $n$ data points. An observed value $y_i$ is distinguished from a predicted value $\hat{y}_i$ by a circumflex at the top of the variable.

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Charu C. Aggarwal
I would like to thank my family for their love and support during the busy time spent in writing this book. Knowledge of the very basics of optimization (e.g., calculus) and linear algebra (e.g., vectors and matrices) starts in high school and increases over the course of many years of undergraduate/graduate education as well as during the postgraduate years of research. As such, I feel indebted to a large number of teachers and collaborators over the years. This section is, therefore, a rather incomplete attempt to express my gratitude.

My initial exposure to vectors, matrices, and optimization (calculus) occurred during my high school years, where I was ably taught these subjects by S. Adhikari and P. C. Pathrose. Indeed, my love of mathematics started during those years, and I feel indebted to both these individuals for instilling the love of these subjects in me. During my undergraduate study in computer science at IIT Kanpur, I was taught several aspects of linear algebra and optimization by Dr. R. Ahuja, Dr. B. Bhatia, and Dr. S. Gupta. Even though linear algebra and mathematical optimization are distinct (but interrelated) subjects, Dr. Gupta’s teaching style often provided an integrated view of these topics. I was able to fully appreciate the value of such an integrated view when working in machine learning. For example, one can approach many problems such as solving systems of equations or singular value decomposition either from a linear algebra viewpoint or from an optimization viewpoint, and both perspectives provide complementary views in different machine learning applications. Dr. Gupta’s courses on linear algebra and mathematical optimization had a profound influence on me in choosing mathematical optimization as my field of study during my PhD years; this choice was relatively unusual for undergraduate computer science majors at that time. Finally, I had the good fortune to learn about linear and nonlinear optimization methods from several luminaries on these subjects during my graduate years at MIT. In particular, I feel indebted to my PhD thesis advisor James B. Orlin for his guidance during my early years. In addition, Nagui Halim has provided a lot of support for all my book-writing projects over the course of a decade and deserves a lot of credit for my work in this respect. My manager, Horst Samulowitz, has supported my work over the past year, and I would like to thank him for his help.

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