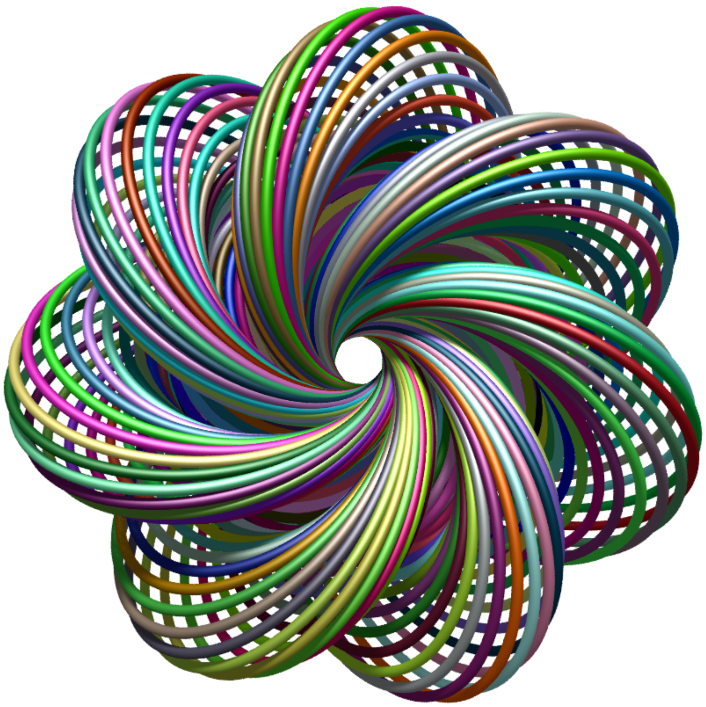
Essentials of Mathematical Methods:

Foundations, Principles, and Algorithms

Yuguang Yang

version 3.0



God used beautiful mathematics in creating the world. –Paul Dirac

Dedicated to
those who appreciate the power of mathematical methods
and enjoy learning it.

License statement

You are free to redistribute the material in any medium or format under the following terms:

- **Attribution**: You must give appropriate credit, provide a link to the license, and indicate if changes were made. You may do so in any reasonable manner, but not in any way that suggests the licensor endorses you or your use.
- **NonCommercial**: You may not use the material for commercial purposes.

* The licensor cannot revoke these freedoms as long as you follow the license terms.
* This license is created via creative commons (https://creativecommons.org)
* If you have any questions regarding the license, please contact the author.

Preface

Objective

Today, mathematical methods, models, and computational algorithms are playing increasingly significant roles in addressing major challenges arising from scientific research and technological developments. Although many novel methods and algorithms, such as deep learning and artificial intelligence, are emerging and reshaping various areas at an unprecedented pace, their core ideas and working mechanisms are inherently related to and deeply rooted in some essential mathematical foundations and principles. By performing an in-depth survey on the underlying foundations, principles, and algorithms, this book aims to navigate the vast landscape of mathematical methods widely used in diverse scientific and engineering domains.

This book starts with a survey of mathematical foundations, including essential concepts and theorems in real analysis, linear algebra, and related fundamentals. Then it examines a broad spectrum of applied mathematical methods, ranging from traditional ones such as optimizations and dynamical system modeling, to state-of-the-art such as machine learning, deep learning, and reinforcement learning. The emphasis is placed on methods for stochastic and dynamical system modeling, optimal decision-making, and statistical learning. For each topic, this book organizes fundamental definitions, theorems, methods, and algorithms in a logical and illuminating way.

Features and Highlights

- Comprehensive, essential, and self-contained.
- Concepts, theorems, and discussions are developed to suit real-world applications.
- Key references and resources are provided on each topic.
- Comparisons and discussions on similar definitions and theorems.
- An evolving book with regular updates on Github.

Acknowledgment

This book evolved from my study notes during my PhD studies at the Johns Hopkins University (JHU). I want to thank the following professors at JHU for their courses and valuable discussion: Daniel Robinson, Teresa Lebair, Andrea Prosperetti, Gregory Chirikjian, Michael Kahadan, James C. Spall, Marin Kobilarov, Suchi Saria, Michael Dimitz, Sean Sun, Ari Turner, Gregory Eyink, Amitabh Basu, John Miller and David Audley. I also want to thank Rachael Zhang for her editorial assistance.

Yuguang Yang, Fall 2019
yangyutu123@gmail.com

Notations

- $\mathbb{R}$: real numbers.
- $\mathbb{R}_+$: nonnegative real numbers.
- $\mathbb{R}_{++}$: positive real numbers.
- $\bar{\mathbb{R}}$: extended real numbers.
- $\mathbb{C}$: complex numbers.
- $\mathbb{F}$: real or complex numbers.
- $\mathbb{Q}$: rational numbers.
- $\mathbb{Z}$: integer numbers.
- $\mathbb{P}$: positive numbers.
- $\mathcal{P}_n$: polynomial of degree of n.
- $\mathbb{N}$: natural numbers.
- $\mathcal{R}(A)$: the range of matrix A.
- $\mathcal{N}(A)$: the null space of matrix A.
- V: vector space.
- $det(A)$: the determinant of matrix A.
- $rank(A)$: the rank of matrix A.
- $\|\cdot\|_2$: Euclidean 2 norm of a vector of a matrix.
- $\|\cdot\|_F$: Frobenius norm of a matrix.
- $\rho(A)$: the spectral radius of matrix A.
- $Tr(A)$: the trace of matrix A.
- $L^2[a,b]$: Lebesgue integrable function on $[a,b]$.
- $L^1[a,b]$: Lebesgue integrable function on $[a,b]$.
- $N(0,1)$: standard Gaussian distribution.
- $N(\mu,\sigma^2)$: Gaussian distribution with mean μ and variance σ^2.
- $MN(\mu,\Sigma)$: multivariate Gaussian distribution with mean vector μ and covariance matrix Σ.
- $\mathbf{1}(x), I(x)$ indicator function.
- $E[X], \mathbf{E}[X], \mathbb{E}[X]$ expectation of random variable X.
- $Var[X]$ variance of random variable X.

CONTENTS

i mathematical foundations

1 SETS, SEQUENCES, AND SERIES 2

2 METRIC SPACE 36

3 ADVANCED CALCULUS 58

4 LINEAR ALGEBRA AND MATRIX ANALYSIS 138

5 BASIC FUNCTIONAL ANALYSIS 268

ii mathematical optimization methods

6 UNCONSTRAINED NONLINEAR OPTIMIZATION 315

7 CONSTRAINED NONLINEAR OPTIMIZATION 359

8 LINEAR OPTIMIZATION 405

9 CONVEX ANALYSIS AND CONVEX OPTIMIZATION 428

10 BASIC GAME THEORY 477

iii classical statistical methods

11 PROBABILITY THEORY 499

12 STATISTICAL DISTRIBUTIONS 603

13 STATISTICAL ESTIMATION THEORY 657

14 MULTIVARIATE STATISTICAL METHODS 716

15 LINEAR REGRESSION ANALYSIS 806

16 MONTE CARLO METHODS 900

iv dynamics modeling methods

17 MODELS AND ESTIMATION IN LINEAR SYSTEMS 936

18 STOCHASTIC PROCESS 1010

19 STOCHASTIC CALCULUS 1047

20 MARKOV CHAIN AND RANDOM WALK 1095

21 TIME SERIES ANALYSIS 1144

v statistical learning methods

22 SUPERVISED LEARNING PRINCIPLES 1223

23 LINEAR MODELS FOR REGRESSION 1268

24 LINEAR MODELS FOR CLASSIFICATION 1287

25 GENERATIVE MODELS 1338

26 K NEAREST NEIGHBORS 1360

27 TREE METHODS 1366

28 ENSEMBLE AND BOOSTING METHODS 1390

29 UNSUPERVISED STATISTICAL LEARNING 1420

30 NEURAL NETWORK AND DEEP LEARNING 1483

vi optimal control and reinforcement learning methods

31 CLASSICAL OPTIMAL CONTROL THEORY 1593

32 REINFORCEMENT LEARNING 1611

vii appendix

A SUPPLEMENTAL MATHEMATICAL FACTS 1691

Alphabetical Index 1721

LIST OF ALGORITHMS

1 A generic line search algorithm 324

2 Backtracking-Armijo line search algorithm 335

3 Steepest decent Backtracking-Armijo line search algorithm 338

4 Modified Newton Backtracking-Armijo line search algorithm 338

5 Quasi Newton with Wolfe line search algorithm 338

6 A generic trust-region algorithm 340

7 A linear conjugate algorithm 349

8 Iteratively reweighted least squares for p norm least square 352

9 Gauss-Newton method for nonlinear least-square algorithm 354

10 Levenberg-Marquardt method for nonlinear least-square algorithm 355

11 Newton method for root finding 356

12 Primal active-set method for strictly convex quadratic programming 378

13 First order gradient projection algorithm 381

14 The Simplex algorithm (non-degenerate system) 419

15 Primal-dual long-step path-following algorithm 424

16 A generic subgradient algorithm 463

17 Gradient projection algorithm with constant step size 470

18 Gradient projection algorithm with adaptive size 471

19 Proximal gradient algorithm 472

20 Iterative Shrinkage-Thresholding Algorithm with constant step size for L1 optimization 474

21 Iterative reweighed estimation for multivariate normal distribution 723

22 Alternating sparse canonical correlation analysis algorithm 743

23 EM algorithm for least square with nonconstant variance 869

24 Accept-Reject algorithm for random number generation. 904

25 Importance sampling for Monte Carlo integration. 913

26 MCMC Metropolis-Hasting algorithm 917

27 MCMC Gibbs sampling algorithm 919

28 Recursive linear least square estimation of dynamical systems. 1001

29 Recursive nonlinear least square of dynamical systems 1003

30 Kalman filtering 1007

31 Extended Kalman filter 1008

32 Coordinate descent for Lasso regression. 1279

33 Iteratively reweighted least squares for logistic regression 1293

34 Perceptron learning algorithm 1323

35 Soft margin SVM algorithm 1332

36 Multinomial Naive Bayes classification 1347

37 KNN classification and regression algorithm 1361

38 A generic decision tree generation algorithm 1374

39 ID3 classification decision tree algorithm 1379

40 A regression tree growth algorithm 1387

41 A basic bagging algorithm 1396

42 Generic Adaboost classifier algorithm 1402

43 Adaboost regressor algorithm 1405

44 A generic additive model algorithm 1407

45 Generic gradient boosting algorithm 1410

46 Gradient tree boosting algorithm 1411

47 XGBoost algorithm 1417

48 Iterative reweighted least square PCA with outliers algorithm 1432

49 Random sample consensus PCA with outliers algorithm 1432

50 Orthogonal Matching Pursuit 1434

51 K-SVD for dictionary learning. 1436

52 Online dictionary learning 1437

53 Stochastic gradient descent for matrix factorization based recommender systems. 1447

54 Isomap algorithm 1456
55 Kernel PCA algorithm 1457
56 Laplacian Eigenmap algorithm 1462
57 Diffusion map algorithm 1465
58 K-means algorithm. 1470
59 DBSCAN algorithm 1473
60 General spectral clustering algorithm 1475
61 Gaussian mixture model EM algorithm 1479
62 Full batch gradient descent algorithm 1499
63 Minibatch stochastic gradient descent algorithm 1500
64 Adam stochastic gradient descent algorithm. 1505
65 Solve forward backward stochastic differential equation via deep learning. . 1527
66 Minibatch stochastic gradient descent training of GAN. 1580
67 Minibatch stochastic gradient descent training of conditional GAN. 1587
68 Minibatch stochastic gradient descent training of Wasserstein GAN. 1589
69 The policy iteration algorithm for MDP 1618
70 Value iteration algorithm for a finite state MDP 1620
71 First-visit MC value function estimation 1627
72 MC-based reinforcement learning control 1629
73 TD(0) estimation of a value function. 1630
74 SARSA learning 1631
75 Q-learning algorithm 1632
76 TD(n) estimation of a value function. 1635
77 *n*-step SARSA learning 1636
78 A generic batch policy-gradient algorithm (REINFORCE) 1647
79 A basic Monte-Carlo policy-gradient algorithm 1648
80 Actor-Critic policy-gradient method 1650
81 Policy-gradient method with a value function baseline 1655
82 Neural Fitted Q Iteration (NFQ) 1660
83 Deep Q-learning with experience replay 1662

84 Asynchronous Deep Q-Learning for each thread 1667
85 Deep Q-learning with universal value function approximator 1668
86 Deep deterministic policy gradient algorithm (DDPG) 1671
87 Twin-delayed deep deterministic policy gradient (TD3) 1673
88 Trust Region Policy Optimization 1675
89 Proximal Policy Optimization 1678
90 Soft Actor-Critic (SAC) policy optimization 1681
91 Isotropic multivariate Gaussian evolution strategies for reinforcement learning 1683
92 Isotropic multivariate Gaussian parallelized evolution strategies for reinforcement learning 1683
93 Q learning with prioritized experience replay 1685
94 Deep Q-learning with hindsight experience replay 1686

LIST OF FIGURES

Figure 3.1.1 An example 3D curve generated by $z = t, x = t\cos(t), y = t\sin(t)$. 69

Figure 3.1.2 An example smooth surface generated by $z = x\exp(-2x^2 - y^2)$ 72

Figure 4.9.1 Demonstration of SVD for matrices of different shapes. The dashed lines highlight the compact form SVD. 207

Figure 4.12.1 Illustration of different quadratic forms. 228

Figure 6.1.1 Demonstration of local minimizer (red, green, and blue), strict lcoal minimizer (red and blue), and global minimizer (blue). 318

Figure 6.1.2 A complex objective function in unconstrained optimization. 319

Figure 6.1.3 Illustration of different cases in unconstrained quadratic optimization. 323

Figure 6.2.1 Drawbacks of steepest gradient descent. 326

Figure 6.2.2 Demonstration on the step choices on the iterative algorithm. (a) Large step size. (b) Small step size. 331

Figure 6.2.3 Armijo sufficient decrease condition. 335

Figure 6.3.1 Demonstration of the dogleg path as an approximation to the exact solution path in the trust-region subproblem. 343

Figure 6.4.1 Demonstration of coordinate descent procedures when A is diagonal and non-diagonal. 346

Figure 7.1.1 Demonstration of KKT condition at a local minimal for $f(x_1, x_2) = x_1^2 + x_2^2$ under constraint $x_1 + x_2 = 1$. 363

Figure 7.2.1 Demonstration of KKT condition at a local minimal for $f(x_1, x_2) = x_1^2 + x_2^2$ under constraint $x_1 + x_2 \geq 1$. 373

Figure 8.2.1 The geometry of linear programming. (a) The feasible region is an open space extending to infinity if A is not full column rank. (b-d) Example feasible regions if $rank(A) = n, m \geq n$. Red arrows are direction of $-c$. When moving along $-c$ in the feasible region, the objective function will decrease. 409

Figure 8.2.2 Demonstration on multiple minimizers forming a convex set. 411

Figure 8.3.1 Overview of geometry approach to linear programming. 413

Figure 9.1.1 Example 2D affine hull and 3D affine hull. 430

Figure 9.1.2 Affine subspace and linear subspace. 432

Figure 9.2.1 (left) A convex set. (right) A non-convex set. 436

Figure 9.2.2 (left) The affine hull of two points in a plane is a line passing through them. (right) The convex hull of two points in a plane is a line segment containing them them. 438

Figure 9.2.3 An illustration of separating hyperplane theorem for two convex bodies. 440

Figure 9.2.4 An illustration of Farkas' lemma. (left) When b lies outside the cone (that is, $Ax = b, x \geq 0$ has no solution), there exists a hyperplane, characterized by normal vector y, seperating b and the cone. (right) When b lies inside the cone (that is, $Ax = b, x \geq 0$ has a solution), there does not exist a hyperplane, characterized by normal vector y, seperating b and the cone. 443

Figure 9.2.5 An illustration of Farkas' lemma variant where the cone is open set. (left) When b lies outside the cone (that is, $Ax = b, x > 0$ has no solution), there exists a hyperplane, characterized by normal vector y, seperating b and the cone. (right) When b lies inside the cone (that is, $Ax = b, x > 0$ has a solution), there does not exist a hyperplane, characterized by normal vector y, seperating b and the cone. 443

Figure 9.3.1 Demonstration of convex functions. (a) A convex function satisfying $f(\alpha x_1 + (1-\alpha)x_2) \leq \alpha f(x_1) + (1-\alpha)f(x_2)$. (b) A non-convex function where the green points does not satisfy the relation. 445

Figure 9.3.2 The epigraph (green area) of a convex function. 447

Figure 9.3.3 Illustration of linear underestimator. 450

Figure 9.5.1 Demonstration of optimality condition $\nabla f(x^*)^T(x - x^*) \geq 0, \forall x \in X$ when x^* lies on the boundary of X. 460

Figure 11.1.1 An illustration of measurable functions. 506

Figure 11.11.1 Visualization of central limit theorem. Samples are drawn from uniform and lognormal distributions. Sample means $\overline{X}_n$ converge to normal distribution in distribution when n is large. 576

Figure 12.1.1 Comparison of Laplace distribution and normal distribution. 613

Figure 12.1.2 Density of $LN(0,1)$ and $LN(0,0.5)$. Note the positive skewness. 620

Figure 12.1.3 Density of $NLN(0,1)$ and $NLN(0,0.5)$. Note the negative skewness. 621

Figure 12.2.1 Distributions with left-skewness (black) and right-skewness (red). 642

Figure 12.2.2 Distributions with zero excess Kurtosis (Normal distribution, black), positive excess kurtosis (Laplace distribution, red), and negative excess Kurtosis (Uniform distribution, blue). 643

Figure 12.2.3 Percentile points at $\alpha = 0.1, 0.2, ..., 0.9$ for a standard normal distribution. 645

Figure 12.2.4 QQ plot of different sample distributions against standard normal distribution, including standard normal $N(0,1)$, shifted-scaled normal $N(50,5)$, Student's t with degree 1, and lognormal $LN(0,1)$. Red solid lines are the fitted linear lines. 647

Figure 13.1.1 Statistical estimation and inference scheme. 660

Figure 13.1.2 An example of biased estimator with smaller variance than unbiased estimator 665

Figure 13.1.3 Visualization of log-likelihood function for normal distributed samples. 673

Figure 13.6.1 Demonstration for rejection regions for upper-tailed one-sided hypothesis (a), two-sided hypothesis(b), and lower-tailed one-sided hypothesis (c). 700

Figure 13.7.1 QQ plot with different sample distributions, including normal, Laplace ($b = 4$), Uniform $U([-1,1])$, Lognormal $LN(0,1)$. Red solid lines are the fitted linear lines. 709

Figure 14.2.1 Principal components for 2D samples. 727

Figure 14.2.2 PCA eigenface analysis. 735

Figure 14.2.3 PCA eigen-digit analysis for MNIST dataset. 736

Figure 14.2.4 Demonstration of interest rate curve dynamics. 738

Figure 14.2.5 Demonstration of first three dominating PCA factor in the swap rate curve daily change. 738

Figure 14.4.1 Gaussian copula with different correlations. 760

Figure 14.4.2 Student T copula with different correlations. 764

Figure 14.4.3 Generated correlated default time via Gaussian copula with different correlations. The hazard rate for both parties is $h(t) = 0.01$. 781

Figure 14.5.1 Correlation structure for the Gaussian copula implied by the factor model. 792

Figure 14.5.2 Factor model using (a) external factors or (b) internal factors. 793

Figure 14.5.3 Scatter plot of AAPL return vs. market excess return, SMB excess return and HML excess return. 797

Figure 14.6.1 A fully connected graphical model representing the joint distribution $P(X_1, ..., X_N)$. 800

Figure 14.6.2 Graphical model examples. 802

Figure 14.6.3 d-separation examples. 804

Figure 15.1.1 Demonstration of simple linear regression model $y = \beta_1 x + \beta_0 + \epsilon$ and multiple linear regression model $y = \beta_1 x_1 + \beta_2 x_2 + \beta_0 + \epsilon$. Scatter points are observed data. The solid line in the left and the plane in the right are the mean responses. 809

Figure 15.3.1 Demo of heteroskedasticity in linear regression. The noises are larger at larger x values. 867

Figure 15.3.2 Demonstrations on linear regression with auto-correlated error. Observations are generated by $y_i = x_i + \epsilon_i, \epsilon_i = \rho\epsilon_{i-1} + z, z \sim N(0,1)$. 872

Figure 15.3.3 Illustration of an outlier, a high-leverage point, and a influential point. Left subfigure shows a red-colored outlier, which does not have high leverage and large influence on the regression result. Middle subfigure shows a red-colored high-leverage point, which is not an outlier or influential point due to its weak influence on the regression result. Right subfigure shows an influential point that is both an outlier and a high-leverage point. 877

Figure 15.3.4 Visual scatter and box plots to identify outliers. 878

Figure 15.3.5 Different function choice for M-estimation linear regression 883

Figure 15.3.6 Common linear regression diagnosis plots 886

Figure 15.4.1 Diagnosis plots for a toy linear regression example 889

Figure 15.4.2 Diagnosis plots for the Boston Housing example 891

Figure 16.4.1 Brownian motion interpolation Demo. 925

Figure 18.1.1 An illustration of a random walk mapping a sample point, ω, to a trajectory parameterized by time, where red trajectory sample point HHT, and blue trajectory has sample point THT. 1014

Figure 18.3.1 Sample trajectories of Brownian motion process. 1019

Figure 18.4.1 Variance of X_t in a Brownian bridge 1029

Figure 18.5.1 A typical realized trajectory from the Poisson process with jumps at T_1, T_2, and T_3. 1034

Figure 19.4.1 The variance function $Var[X(t)]$ for Brownian motion (red) and OU process(black) with $a = 0.5, \sigma = 1$. 1081

Figure 19.4.2 Representative trajectories from three OU processes with different k. k has the unit of inverse year. Mean level $\mu = 50$ and volatility $\sigma = 20$. 1083

Figure 20.1.1 Example Markov chains. Arrows and numbers are transition directions and probabilities. 1098

Figure 20.1.2 Markov chain diagram for a random walk on the state space $\mathbb{Z}$. 1099

Figure 20.2.1 Demonstration accessibility in a Markov chain. In chain (a), states A and B are accessible to each other or they can communicate. In chain (b), state A can access B but B cannot access A. 1101

Figure 20.2.2 Demonstration of partitioning state space by communicating classes. Green and orange states belong to different communicating classes. Note that a communicating class can consist of only one state. 1102

Figure 20.2.3 Classification of communicating classes into recurrent class and state space by communicating classes. Green states form a communicating class belonging to the transient class. Orange states form a communicating class belonging to the recurrent/closed/adsorbing class. 1109
Figure 20.2.4 Example periodic and aperiodic Markov chains. 1111
Figure 21.1.1 Example time series including a white noise process (upper left), a seasonable time series with periodicity 20, the US new privately owned housing [source], and the US GDP time series[source]. 1146
Figure 21.1.2 Demonstration on using STL to decompose an example CO2 concentration time series. 1151
Figure 21.2.1 Example trajectories of AR(1) models ($X_t = aX_{t-1} + Z_t$.) with different choices of a. 1156
Figure 21.2.2 Example trajectories of MA(1) models (upper) and MA(2) models (lower). 1163
Figure 21.2.3 Representative simulated trajectories for AR(1) process with coefficient 1, which forms a unit-root process, and with coefficient -1. 1172
Figure 21.2.4 The ACF and PACF corrlogram for a white noise process. 1179
Figure 21.2.5 The ACF and PACF corrlogram for an AR(1) process with coefficient 0.8. 1179
Figure 21.2.6 The ACF and PACF corrlogram for an MA(1) process. 1180
Figure 21.2.7 The ACF and PACF corrlogram for an ARMA(1,1) process. 1180
Figure 21.2.8 Diagnosis plot of residuals for AR(2) model estimation. 1189
Figure 21.2.9 Diagnosis plot of residuals for AR(1) model fitted to time series generated by AR(2) ground truth model. 1190
Figure 21.4.1 Stock index SP500 daily return between 2014 and 2019. 1203
Figure 21.4.2 Simulated representative trajectories from ARCH(1) model with coefficients $a = 0.9$ and $a = 0.5$. 1205
Figure 22.1.1 Scheme of a supervised learning task. Training samples are fed into a learning system to obtain an optimized model, which will be further used in a prediction system for regression and classification tasks. 1225
Figure 22.1.2 Input feature data type examples. 1225
Figure 22.2.1 A simple regression problem illustrating underfitting and overfitting. Solid lines are models, and points are samples. 1229
Figure 22.2.2 The commonly observed phenomenon of overfitting and underfitting in machine learning. 1230
Figure 22.2.3 The performance of different types of models as training proceeds. 1233

Figure 22.3.1 Regression loss functions: MSE Loss, MAE Loss, Huber loss ($\delta = 0.1, 1, 3$), and Log-Cosh Loss. 1237
Figure 22.3.2 Common classification loss functions. 1239
Figure 22.3.3 Scheme for ROC curves diagram. A and B demote ROC curves of different model. 1244
Figure 22.4.1 Scheme for cross-validation error calculation procedure. 1247
Figure 22.4.2 Hyperparameter search via turning regularization parameter λ. At large λ, heavy regularization causes underfitting; at small λ, insufficient regularization causes overfitting. 1249
Figure 22.5.1 Left: A sample of nine real-world time series reveals a diverse range of temporal patterns [4, 5]. Right: Examples of different classes of methods for quantifying the different types of structure, such as those seen in time series on the left: (i) distribution (the distribution of values in the time series, regardless of their sequential ordering); (ii) autocorrelation properties (how values of a time series are correlated to themselves through time); (iii) stationarity (how statistical properties change across a recording); (iv) entropy (measures of complexity or predictability of the time series quantified using information theory); and (v) nonlinear time-series analysis (methods that quantify nonlinear properties of the dynamics).[9] 1258
Figure 23.1.1 Correlation among features and the label MEDV. 1271
Figure 23.1.2 Pair plot among features and the label. 1272
Figure 23.2.1 Comparison different penalization: Lasso $L1$, elastic net, and Ridge $L2$. Orange regions are admissible set for parameter β. Contours are objective function value as a function of parameter β. Black solid circles are the minimizers $\hat{\beta}$ when there are no penalties, and red solid circles are the minimizers when penalties are applied. 1281
Figure 23.2.2 Penalized regression path in a toy regression problem. 1282
Figure 23.3.1 Linear regression with non-linear high order terms. The samples are generated via $y = 2x_1 + x_2 - 0.8x_1x_2 + 0.5x_1^2 + \epsilon$, where ϵ is noise. 1285
Figure 23.3.2 Linear model enhancement flowchart. 1285
Figure 24.1.1 Logistic regression for classification on the Iris data set. 1290
Figure 24.1.2 Pair plot analysis results on South Africa heart disease problem. 1298
Figure 24.1.3 L1 regularization path for South Africa heart disease problem. 1299
Figure 24.1.4 Logistic regression result with L1 penalty. 1301
Figure 24.1.5 Balanced accuracy score vs. inverse regularization strength in credit card fraud detection problem. 1302
Figure 24.1.6 Logistic regression coefficients corresponding to each class. 1303

Figure 24.2.1 Geometry of decision boundary in linear Gaussian discriminant model. 1307
Figure 24.2.2 Comparison of Gaussian LDA and Gaussian QDA on binary classification. Decision boundary of LDA is simply a line in 2D input space and unable to discriminate difficult cases. Gaussian discrimination can have richer decision boundary geometry. LDA using polynomial features is a special case of GDA. 1310
Figure 24.2.3 The decision boundary geometry of LDA and GDA can be understood via their decision functions 1311
Figure 24.3.1 The linear discriminant w that maximizes the separability for 2D sample points belonging to two classes. 1313
Figure 24.3.2 Fisher linear discriminate will fail to achieve class separability for complex data structures. 1317
Figure 24.4.1 Scheme of a hyperplane. 1322
Figure 24.4.2 Binary classification using the Perceptron learning algorithm. The hyperplane learned separates the two clusters. 1324
Figure 24.5.1 Left: existence of multiple separating hyperplanes in 2D binary classification problem. Right: hyperplanes with maximum margin. 1326
Figure 24.5.2 SVM classification with different regularization strength. Small C tends to emphasize the margin and ignore the outliers in the training data, while large C may tend to overfit the training data. 1329
Figure 24.5.3 SVM classification using Gaussian kernel. The original problem cannot be separated by linear kernel. 1334
Figure 24.5.4 Comparison of classification loss functions. 1336
Figure 25.2.1 Histogram of the features group by class label (fraud vs. genuine). 1351
Figure 25.2.2 Feature density similarity and predictive performance of model 1352
Figure 26.2.1 Binary classification via KNN algorithm with different choices $K = 1, 3, 5, 7$. Scattered points are training examples classified into two different classes (red and blue). Colored regions are corresponding decision boundaries. 1365
Figure 27.2.1 Demonstration of decision trees. 1373
Figure 27.2.2 Different types of impurity measure. Entropy function, Gini function and classification error function. 1376
Figure 27.2.3 Different splitting strategy when variables taking more than two discrete values. 1377
Figure 27.2.4 The visualization of the decision tree classifier for Iris data set. The tree grows until all examples are classified correctly. The splitting criterion is Gini impurity. 1382

Figure 27.2.5 The visualization of the decision tree classifier for Iris data set. The tree grows until examples in each node is smaller than 10. The splitting criterion is Gini impurity. 1383
Figure 27.2.6 The visualization of the decision tree classifier for Iris data set. The tree grows until examples in each node is smaller than 10. The splitting criterion is entropy and information gain. 1383
Figure 27.3.1 Demonstration of a tree and input space partitioning. 1386
Figure 27.3.2 2D input space partitions cannot be represented by a regression tree. 1386
Figure 27.3.3 Regression tree demonstration in a toy example. 1388
Figure 27.3.4 Variable importance from regression tree in the Boston Housing Pricing problem. 1389
Figure 28.1.1 The correctness probability of a majority vote is greater than the correctness probability of individual votes when individual accuracy probability is greater than 0.5. 1394
Figure 28.3.1 Illustration of adaptive boosting where sample weights are adjusted iteratively based on the classification error. 1401
Figure 29.1.1 Demonstration of SVD for matrices of two different shapes. The dashed lines highlight the compact form SVD. 1423
Figure 29.1.2 Principal components for 2D samples. 1427
Figure 29.2.1 Singular value spectrum of LSA on 20-news-group text data. 1442
Figure 29.2.2 A simplified illustration of the latent factor approach, which characterizes both users and movies using two axes—male versus female and serious versus escapist. [9] 1447
Figure 29.3.1 Triangle and Tetrahydron reconstructed from distance matrix by MDS method. 1454
Figure 29.3.2 Application of MDS, based on Euclidean distance, to Swiss Roll data set cannot fully reveal of the global structure. 1455
Figure 29.3.3 Isomap analysis of MNIST dataset. 1466
Figure 29.3.4 Isomap analysis of digit '5' in MNIST dataset 1467
Figure 29.4.1 Demonstration of k-means clustering on a data set with two blobs. 1469
Figure 29.4.2 K-means performance can be affected by a number of factors, including incorrect number of clusters/blobs, non-spherical clusters/blobs, clusters/blobs with unequal variance, and bad initial cluster centers. 1471
Figure 29.4.3 Clustering comparison between Kmeans and Kmeans++. 1472
Figure 29.4.4 DBSCAN demo with different ϵ. 1474
Figure 29.4.5 Spectral clustering demo. 1476
Figure 29.4.6 Clustering comparison between K-means and GMM. 1480
Figure 29.4.7 K-means application to image segmentation. 1481

Figure 30.1.1 Scheme of an artificial neuron. 1487
Figure 30.1.2 Common activation functions in artificial neural networks. 1488
Figure 30.1.3 Scheme for an artificial neural network. 1489
Figure 30.1.4 A four-layer feed-forward neural network. 1489
Figure 30.1.5 A three-layer feed-forward neural network with three output units. 1490
Figure 30.1.6 A four-layer feed-forward neural network. 1492
Figure 30.2.1 An example saddle point at $(0,0,0)$, which locally minimizes the x direction but maximizes the y direction.. 1499
Figure 30.2.2 SGD without momentum and with momentum. SGD with momentum can accumulate gradient/velocity in horizontal direction and move faster towards the minimum located at the center. 1503
Figure 30.3.1 Dropout technique for a simple feedforward neural networks. The original network (left) and the neural network after some neurons being dropped out (right). 1511
Figure 30.4.1 Neural network architecture for polynomial regression. 1513
Figure 30.4.2 Polynomial regression with degree d = 1, 3, 6, 10. 1514
Figure 30.4.3 Visualization of first layer weight for a one-layer linear multi-class classification neural network 1515
Figure 30.4.4 Example images from the Fashion MNIST dataset. 1516
Figure 30.4.5 The confusion matrix from fashion MNIST classification results. 1517
Figure 30.4.6 Classification results for a set of randomly selected samples. 1518
Figure 30.4.7 (a) Embedding layer maps large, sparse one-hot vectors to short, dense vectors. (b) Example of low dimensional embeddings that capture semantic meanings. 1519
Figure 30.4.8 (a) The Skip-gram architecture that predicts surrounding words given the central word. (b) The CBOW architecture that predicts the central word given its surrounding context words. The one-hot vector has size V; the dense vector has length $D \ll V$. Also note that no nonlinearity activation is applied between input and hidden layer. 1520
Figure 30.4.9 A feed-forward neural network architecture for sentiment analysis. 1524
Figure 30.5.1 Comparison of receptive fields in fully-connected layer and local-connected layer in CNN. Credit 1528
Figure 30.5.2 Demo for one kernel 'convoluting' with an input image. 1529
Figure 30.5.3 Pooling layer demo. 1530
Figure 30.5.4 A typical CNN architecture for image classification tasks. 1531
Figure 30.5.5 Scheme for LeNet [24] 1531
Figure 30.5.6 Architecture of AlexNet. 1532

Figure 30.5.7 A typical VGG architecture: VGG-19 scheme. 1532
Figure 30.5.8 The depth of the configurations increases from the left (A) to the right (E), as more layers are added (the added layers are shown in bold). The convolutional layer parameters are denoted as "conv-receptive field size-number of channels" [26] 1533
Figure 30.5.9 Training error (left) and testing error (right) on CIFAR-10 with 20-layer and 56-layer vanilla CNN networks. The deeper network has both higher training error and testing error.[27] 1534
Figure 30.5.10 Scheme for a residual block. 1534
Figure 30.5.11 Scheme of a 18 layer ResNet 1535
Figure 30.6.1 Example images from CIFAR10 image dataset. 1536
Figure 30.6.2 Visualization of convolution layer. 1538
Figure 30.6.3 Grad-CAM method applied to understand image classification. Middle and right are class-discriminative localization map superimposed onto the original image. 1539
Figure 30.6.4 A CNN based autoencoder. An autoencoder consists of an encoder that transforms high-dimensional image into a low-dimensional code and a decoder that unfolds the code to reconstruct the image. 1541
Figure 30.6.5 Comparison of reconstruction performance on random samples from MNIST data set. Top row is the original data. Middle row is autoencoder result based on a 49 dimensional code. Bottom row is PCA result based on a 50 dimensional code. 1541
Figure 30.6.6 Denoising autoencoders applied to remove the noise in the MNIST dataset. 1542
Figure 30.6.7 Demonstration of neural style transfer with Van Gogh painting style. 1544
Figure 30.6.8 Demonstration of neural style transfer with Picasso painting style. 1545
Figure 30.6.9 Application of CNN in deep reinforcement learning in Q learning approach and Actor-Critic approach. Two streams of sensory inputs are fed to the neural network, including a pixel image of the robot's neighborhood fed into a convolutional layer and the target's position fed into a fully connected layer. 1547
Figure 30.6.10 Demonstration of a CNN filter applying to a sentence to produce a one-dimensional feature vector. 1548
Figure 30.6.11 CNN for sentence classification proposed in [43]. 1549
Figure 30.7.1 Scheme of recurrent units in a neural network (left). Recurrent neural network can be unrolled (right) 1551
Figure 30.7.2 Scheme for backpropogation through time in a simple RNN. Red arrows are backpropogation directions. 1552

Figure 30.7.3 Scheme of an LSTM cell. Modified from [45, p. 149]. 1554
Figure 30.7.4 Scheme of a GRU cell.Modified from [45, p. 152]. 1557
Figure 30.7.5 Different types of units in RNNs: (a) Vanilla RNN cell. (b) LSTM cell. (c) GRU cell. Credit 1558
Figure 30.7.6 Typical RNN connection to the output layer. 1559
Figure 30.7.7 Scheme for stacked RNN. 1560
Figure 30.7.8 Scheme for bidirectional RNN. 1560
Figure 30.8.1 RNN architecture for time series prediction . (a) In the training phase, RNN are updated by minimizing the next step prediction error. (b) In the prediction phase, trained RNN is used to sequentially predict next step state value based on preceding predicted state value. 1562
Figure 30.8.2 RNN one-step forward and multiple forward prediction performance for Sine time series. 1563
Figure 30.8.3 RNN architecture for time series prediction with covariates. (a) In the training phase, RNN are updated by minimizing the next step prediction error. (b) In the prediction phase, trained RNN is used to sequentially predict next step state value based on preceding predicted state value. Note that covariate time series are assumed available for all time steps. 1564
Figure 30.8.4 DeepAR model architecture for time series prediction. Outputs are the parameters characterizing the condition distribution of x_{t+1} conditioned on histories of x_t and z_t. (a) In the training phase, RNN are updated by minimizing the negative log likelihood function. (b) In the prediction phase, a predicted $\hat{x}_{t+1}$ are sampled from predicted conditional distribution and then used to predict next step conditional distribution. 1565
Figure 30.8.5 A RNN architecture for MNIST image recognition. 1567
Figure 30.8.6 RNN architecture for sentiment analysis. 1568
Figure 30.8.7 A RNN for character-level word classification. 1569
Figure 30.8.8 A RNN for character-level language model. During the training session, one-hot coded characters are directly fed into RNN and predict the next character in the word. 1570
Figure 30.8.9 A RNN for character-level language model. During the word generation session, the network starts with a user input character and continues the generation process with predicted character from the previous step. 1571
Figure 30.9.1 Seq2seq modeling for language transformation. The input and output sequences might have different lengths, and not in synchrony. 1573

Figure 30.9.2 The Encoder-decoder architecture for seq2seq language modeling. The input sequence is fed into the encoder RNN and terminated by an explicit <EOS> symbol. Then the decoder RNN starts with the context vector and the final prediction of the encoder to generate an output sequence until an explicit <EOS> symbol is produced. 1574
Figure 30.9.3 The Encoder-decoder architecture with attention mechanism for seq2seq modeling. During the encoding phase, all hidden states, rather than the final one, are saved to construct different context vectors via linear combination for the decoding stage. During the decoding phase, relevant context vectors are constructed and fed into the each hidden states in the decoder. 1576
Figure 30.9.4 A bidirectional RNN encoder system with attention mechanism. [51] 1577
Figure 30.10.1 Scheme for a canonical GAN. The discriminator is trained to distinguish between real and fake image, while the generator is trained to generate realistic image to 'fool' the discriminator. The generator usually uses a decoder-like neural network structure that generate a high-dimensional data from a sample point in the low-dimensional latent space. 1579
Figure 30.10.2 Generated image samples from a GAN consisting of feed-forward networks. 1581
Figure 30.10.3 DCGAN generator network architecture. A 100 dimensional uniform noise is passing through a series of fractionally-strided convolutions then is converted into a final image. Notably, no fully connected or pooling layers are used [56] 1584
Figure 30.10.4 Understanding DCGAN. Each row represents the image generated as we interpolate a random point z in the latent space. Images show smooth transitions from one bedroom and another bedroom.[56] 1584
Figure 30.10.5 Scheme for a conditional GAN. The discriminator is trained to distinguish between real and fake image given external label information, while the generator is trained to generate realistic image to 'fool' the discriminator given external label information. The generator usually uses a decoder-like neural network structure that generate a high-dimensional data from a sample point in the low-dimensional latent space. 1586
Figure 32.1.1 Policy iteration involves iteratively carrying out policy evaluation and policy improvement procedures. 1614

Figure 32.2.1 One core component in reinforcement learning is agent environment interaction. The agent takes actions based on observations on the environment and a decision-making module that maps observations to action. The environment model updates system state and provides rewards according to the action 1622
Figure 32.2.2 Scheme of the Atari game *breakout*. 1623
Figure 32.2.3 Policy evaluation and policy improvement framework in the context reinforcement learning. 1624
Figure 32.3.1 Neural network parameterization for a Gaussian policy (a) and (b) a generic stochastic policy. 1652
Figure 32.4.1 A typical feed-forward neural network used in NFQ to approximate the Q function. 1659
Figure 32.4.2 The network architecture for canonical deep Q learning. The network takes a state or an observation, denoted by s, as the input, and outputs multiple values corresponding $Q(s,a)$. The number of outputs 1661
Figure 32.4.3 A typical single stream Q-network (top) in deep Q learning and a dueling Q-network (bottom). The dueling network has two streams to separately estimate (scalar) state-value and the advantage function for each action; the green output module synthesize the Q value from two streams. Both networks output Q-values for each action. [10]. 1664
Figure 32.4.4 In a DQRN, recurrent layers are usually placed on the last layer before output. Unlike canonical DQN, we need to feed sequence of observation into the network and finally output Q values. Above scheme only unfolds to two steps.[11] 1665
Figure 32.4.5 An example architecture that implements the asynchronous reinforcement learning paradigm. Multiple agents interact with multiple instances of environments in parallel. Agents collect experiences to train a globally shared network that learns control policies. 1666
Figure 32.4.6 A comparison between a typical deep Q learning network (left) and a typical universal value function approximator network (right). 1668
Figure 32.4.7 A typical deep neural network architecture for DDPG reinforcement learning. The actor network outputs control policy; the critic network outputs estimate of Q function. Through back-prorogation, the critic network improves estimation accuracy and the actor network improves policy. 1670
Figure 32.5.1 Illustration of planning curriculum on a swiss roll manifold. Red targets can generating along the path connecting from an intended start point to the target goal position. 1687

Figure 32.5.2 One representative trajectory on the curved surface via a control policy learned via curriculum learning on a low-dimensional manifold. 1688

LIST OF TABLES

Table 13.7.1 Test on mean with known variance σ^2 708

Table 13.7.2 Test on mean with unknown variance σ^2 710

Table 13.7.3 Test on variance 710

Table 13.7.4 Test on variance comparison between two samples 711

Table 14.2.1 Eigenvectors and eigenvalues for swap rate daily change 739

Table 14.5.1 statistics on Fama-French 3 factors from July 1963 to Dec. 1991. 796

Table 14.5.2 AAPL stock return modeled by the Fama-French 3 factor model. 798

Table 20.2.1 Summary of Markov chain state property[3, p. 140] 1113

Table 21.2.1 Summary of PACF and ACF for AR, MA, and ARMA processes. 1179

Table 23.1.1 Linear regression results. 1273

Table 24.1.1 Logistic regression results on South Africa heart disease problem. 1299

Table 29.2.1 Most frequent words in the top 8 topics 1443

Table 29.2.2 Rating matrix or utility matrix, where each row is a user's ratings for different movies. SW1, SW2 are Star wars episodes; HP1 and HP2 are Harry Potter episodes; TW is Twilight; BM is Batman. 1445

Table 32.2.1 Estimating cumulative rewards $G_t^{(n)}$ of different steps n as the target for value function V. $G^{(1)}$ corresponds to temporal-difference TD(0) and $G^{(\infty)}$ corresponds to Monte-Carlo estimation. If the process terminates at K and $K < n$, then we use $G_t^{(n)} = G_t^{(K)}$. Trajectories are generated under policy π. 1634

Table A.9.1 Closed Newton-Cotes Formula 1711

CONTENTS

i mathematical foundations

1 SETS, SEQUENCES, AND SERIES 2
- 1.1 Sets 4
  - 1.1.1 Definitions and basic properties 4
  - 1.1.2 DeMorgan's Law 5
  - 1.1.3 Set equivalence and partition 5
  - 1.1.4 Countability 6
- 1.2 Functions 8
  - 1.2.1 Basic concepts 8
  - 1.2.2 Inverse image vs. inverse function 8
  - 1.2.3 Set operations in function mapping 9
  - 1.2.4 Parameter change of function 9
- 1.3 Real numbers 10
  - 1.3.1 Rational numbers 10
  - 1.3.2 Dense subset 10
  - 1.3.3 Axiom of completeness 11
- 1.4 Sequence in $\mathbb{R}$ 14
  - 1.4.1 Basics 14
  - 1.4.2 Cauchy criterion 16
  - 1.4.3 Sequence characterization of a dense subset 17
- 1.5 Monotone sequence 19
  - 1.5.1 Fundamentals 19
  - 1.5.2 Applications 19
- 1.6 Subsequence and limits 23
  - 1.6.1 Subsequence 23
  - 1.6.2 Bolzano-Weierstrass theorem 23
  - 1.6.3 Subsequence limits 24
- 1.7 Infinite series 27
  - 1.7.1 Fundamental results 27
  - 1.7.2 Tests for convergence 28
  - 1.7.3 Inequalities and l_2 series 30
    - 1.7.3.1 Holder's and Minkowski's inequality 30
    - 1.7.3.2 Cauchy-Schwarz inequality 31
  - 1.7.4 Alternating series 32

1.8 Notes on bibliography 34

2 METRIC SPACE 36

2.1 Metric space 38

2.1.1 Definitions 38

2.1.2 metric space vs. normed (vector) space vs. Banach space 40

2.2 Sequences in metric space 41

2.3 Closed sets & open sets in metric space 43

2.3.1 Closed set 43

2.3.2 Open sets 43

2.3.3 Further characterization and properties 44

2.3.4 Open and closed sets in $\mathbb{R}^n$ 46

2.4 Compact sets 48

2.4.1 Basic concepts 48

2.4.1.1 closed set vs. compact set 49

2.4.2 Compact sets in $\mathbb{R}^N$ 49

2.4.3 The Hine-Borel Theorem and boundedness of continuous function 50

2.5 Completeness of metric space 51

2.5.1 Sequence and completeness 51

2.5.2 Completeness of $\mathbb{R}^n$ 51

2.6 Topology space 53

2.6.1 Definitions 53

2.6.2 Continuous function, Homeomorphism in topological space 54

2.6.3 Subspaces of topological space 54

2.7 Notes on bibliography 56

3 ADVANCED CALCULUS 58

3.1 Continuous functions 61

3.1.1 Continuous function on $\mathbb{R}$ 61

3.1.1.1 Basics 61

3.1.1.2 Continuity and inverse 64

3.1.2 Continuous function in metric space 65

3.1.3 Boundedness and extreme value theorems 66

3.1.4 More on extreme values 68

3.1.5 Curves and surfaces 68

3.1.5.1 Curvature 71

3.1.5.2 Surfaces 71

3.2 Uniform continuity 74

3.2.1 Uniform continuity on real line 74

3.2.1.1 Concepts 74

3.2.1.2 Lipschitz continuity 76

3.2.2 Uniform continuity on metric space 79

3.2.3 Locally and globally Lipschitz continuous 80
3.3 Differentiation 82
3.3.1 Differential function concept 82
3.3.2 Differential rules 83
3.3.3 Mean value theorem 85
3.4 Function sequence and series 88
3.4.1 Pointwise convergence, uniform convergence 88
3.4.2 Properties of uniform convergence 89
3.4.2.1 Uniform convergence preserve continuity 89
3.4.2.2 Exchange limits and integration 90
3.4.2.3 Exchange limits and differential 90
3.4.2.4 Linearity of uniform convergence 90
3.5 Power series 92
3.5.1 Fundamentals 92
3.5.2 Term-by-term operation 94
3.5.3 Power series and analytic function 94
3.5.4 Approximation by polynomials 95
3.6 Taylor polynomial and Taylor series 97
3.6.1 Taylor polynomial and approximation 97
3.6.2 Taylor series and Taylor's theorem 99
3.6.3 Common Taylor series 101
3.6.4 Useful approximations 103
3.7 Riemann Integral Theory 105
3.7.1 Construction of Riemann integral 105
3.7.2 Riemann integrability 106
3.7.2.1 Basics 106
3.7.2.2 Lebesgue characterization of integrability 107
3.7.2.3 limits and integrability 107
3.7.2.4 Algebraic properties 108
3.7.3 First Fundamental Theorem of Calculus 109
3.7.4 Second Fundamental Theorem of Calculus 109
3.7.4.1 Fundamentals 109
3.7.4.2 Differentiating definite integrals 112
3.7.4.3 Application to differential equation 113
3.7.5 Essential theorems 114
3.7.6 Integration rules 115
3.7.7 Improper Riemann integrals 115
3.8 Basic measure theory 118
3.8.1 Measurable space 118
3.8.1.1 σ algebra 118
3.8.1.2 Measurable space and positive measure 119

3.8.1.3 Borel algebra and Lebesgue measure 119
3.8.2 Measurable functions and properties 121
3.8.2.1 Measurable function and measurability 121
3.8.2.2 Properties 122
3.8.3 Convergence of measurable functions 124
3.8.4 Almost everywhere convergence 124
3.9 Lebesgue integral 126
3.9.1 Simple function and its Lebesgue integral 126
3.9.2 Lebesgue integral of measurable functions 128
3.9.2.1 Integral of non-negative functions 128
3.9.2.2 Integral of general functions 130
3.9.3 Riemann vs. Lebesgue integrals 131
3.9.4 Convergence theorems 131
3.9.4.1 Applications 133
3.10 Notes on bibliography 136
4 LINEAR ALGEBRA AND MATRIX ANALYSIS 138
4.1 Theory for system of linear equations 143
4.1.1 Overview 143
4.1.2 Homogeneous systems 143
4.1.3 Non-homogeneous systems 144
4.1.4 Overdetermined vs. underdetermined systems 145
4.1.5 Solution methods 146
4.1.6 Error bounds in numerical solutions 151
4.1.6.1 Condition number 151
4.1.6.2 Error bounds 151
4.2 Vector space theory 153
4.2.1 Vector space 153
4.2.2 Subspace 154
4.2.3 Sum and direct sum 155
4.2.4 Basis and dimensions 157
4.2.5 Complex vector space vs. real vector space 159
4.3 Linear maps & linear operators 161
4.3.1 Basic concepts of linear maps 161
4.3.2 Fundamental theorem of linear maps 162
4.3.3 Isomorphism 164
4.3.4 Coordinate map properties 166
4.3.5 Change of basis and similarity 167
4.3.5.1 Change of basis for coordinate vector 167
4.3.5.2 Change of basis for linear maps 167
4.3.6 Linear maps and matrices 167
4.3.6.1 Similarity 169

4.4 Fundamental theorems of ranks and linear algebra 170
4.4.1 Basics of ranks 170
4.4.2 Fundamental theorem of ranks 171
4.4.3 Fundamental theorem of linear algebra 172
4.5 Complementary subspaces and projections 174
4.5.1 General complementary subspaces 174
4.5.2 Orthogonal complementary spaces and projections 176
4.5.3 Decomposition of orthogonal projectors 180
4.6 Orthonormal basis and projections 183
4.6.1 Gram-Schmidt Procedure 183
4.6.2 Orthogonal-triangular decomposition 183
4.6.3 Orthonormal basis for linear operators 184
4.6.4 Riesz representation theorem 185
4.7 Eigenvectors and eigenvalues of Matrices: general theory 186
4.7.1 Existence and properties of eigenvalues 186
4.7.2 Properties of eigenvectors 188
4.7.3 Right and left eigenvectors 189
4.7.4 Diagonalizable matrices 190
4.8 Eigenvalue and eigenvectors of matrices: case studies 193
4.8.1 Real diagonalizable matrix 193
4.8.2 Real symmetric matrix 194
4.8.2.1 Spectral properties 194
4.8.2.2 Rayleigh quotients 196
4.8.2.3 Pointcare inequality 199
4.8.3 Hermitian matrix 200
4.8.4 Matrix congruence 202
4.8.5 Complex symmetric matrix 203
4.8.6 Unitary, orthonormal & rotation matrix 203
4.9 Singular Value Decomposition theory 205
4.9.1 SVD fundamentals 205
4.9.2 SVD and matrix norm 207
4.9.3 SVD vs. eigendecomposition 208
4.9.4 SVD low rank approximation 209
4.9.4.1 Frobenius norm low rank approximation 209
4.9.4.2 Two-norm low rank approximation 211
4.10 Generalized eigenvectors and Jordan normal forms 213
4.10.1 Generalized eigenvectors 213
4.10.2 Upper triangle matrix and nilpotent matrix 216
4.10.3 Jordan normal forms 218
4.11 Matrix factorization 222
4.11.1 Orthogonal-triangular decomposition 222

4.11.2 LU decomposition 223
4.11.3 Cholesky decomposition 223
4.12 Positive definite matrices and quadratic forms 225
4.12.1 Quadratic forms 225
4.12.2 Real symmetric non-negative definite matrix 226
4.12.2.1 Characterization 226
4.12.2.2 Decomposition and transformation 229
4.12.2.3 Matrix square root 230
4.12.2.4 Maximization of quadratic forms 231
4.12.2.5 Gramian matrix 233
4.12.3 Completing the square 234
4.13 Matrix norm and spectral estimation 235
4.13.1 Basics 235
4.13.2 Singularity from matrix norm and spectral radius 236
4.13.3 Gerschgorin theorem 237
4.13.4 Irreducible matrix and stronger results 238
4.14 Pseudoinverse of matrix 239
4.14.1 Pseudoinverse for full rank system 239
4.14.2 Pseudoinverse for general matrix 241
4.14.3 Application in linear systems 243
4.15 Multilinear forms 246
4.15.1 Bilinear forms 246
4.15.2 Multilinear forms 247
4.16 Determinant 250
4.16.1 Basic properties 250
4.16.2 Vandermonde matrix and determinant 256
4.17 Numerical iteration analysis 258
4.17.1 Numerical linear equation solution 258
4.17.1.1 Goals and general principles 258
4.17.1.2 Jacobi algorithm 258
4.17.1.3 Gauss Seidel algorithm 259
4.17.2 Power method for eigen-decomposition 259
4.18 Appendix: supplemental results for polynomials 262
4.18.1 Basics 262
4.18.2 Factorization of polynomial over $\mathbb{C}$ 263
4.18.3 Factorization of polynomial over $\mathbb{R}$ 264
4.19 Notes on bibliography 266
5 BASIC FUNCTIONAL ANALYSIS 268
5.1 Normed vector space 270
5.1.1 Basic properties 270
5.1.2 Equivalence of norms 272

5.2 Contraction mapping and fixed point theorems 274
5.2.1 Complete normed space (Banach space) 274
5.2.2 Contraction mapping 275
5.2.3 Banach fixed point theorem 276
5.2.4 Applications in root finding 277
5.2.5 Application to numerical linear equations 277
5.2.6 Applications to integral and differential equations 278
5.3 Inner product space and Hilbert space 281
5.3.1 Inner product space (pre-Hilbert space) and Hilbert space 281
5.3.1.1 Foundations 281
5.3.2 Hilbert spaces 283
5.3.2.1 Basics 283
5.3.3 Orthogonal decomposition of Hilbert spaces 284
5.3.3.1 Orthogonality 284
5.3.4 Projection and orthogonal decomposition 285
5.4 Approximations in Hilbert space 288
5.4.1 Approximation via projection 288
5.4.2 Application examples 289
5.4.2.1 Orthogonal projection and normal equations in $\mathbb{R}^n$ 289
5.4.2.2 Approximation by continuous polynomials 291
5.4.2.3 Legendre polynomial via Gram-Schmidt process 292
5.5 Orthonormal systems 293
5.5.1 Basic definitions 293
5.5.2 Gram-Schmidt process 293
5.5.3 Properties of orthonormal systems 293
5.5.4 Orthonormal expansion in Hilbert space 295
5.5.5 Complete orthonormal system 296
5.5.5.1 Weierstrass approximation theorem for polynomials 298
5.5.5.2 Examples of complete orthonormal function set 298
5.6 Theory for trigonometric Fourier Series 300
5.6.1 Basic definitions 300
5.6.2 Completeness of Fourier series 302
5.6.3 Complex representation 303
5.7 Fourier transform 305
5.7.1 Definitions and basic concepts 305
5.7.2 Convolution theorem 307
5.7.3 Fourier transform and Fourier series 308
5.7.4 Discrete Fourier transform 309
5.7.4.1 Properties 309
5.8 Notes on bibliography 312

ii mathematical optimization methods

6 UNCONSTRAINED NONLINEAR OPTIMIZATION 315
6.1 Optimality conditions 317
6.1.1 Optimality concepts 317
6.1.2 Necessary and sufficient conditions 319
6.1.3 Special case: unconstrained quadratic programming 322
6.2 Line search method 324
6.2.1 A generic algorithm 324
6.2.2 Theory and computation of descent directions 325
6.2.2.1 Gradient descent direction and properties 325
6.2.2.2 Curvature-modified descent direction 326
6.2.2.3 Quasi-Newton method 328
6.2.2.4 Subspace optimization in quadratic forms 330
6.2.3 Theory and computation of step length 331
6.2.3.1 Overview 331
6.2.3.2 Lipschitz bounded convex functions 331
6.2.3.3 Backtracking-Armijo step side search 334
6.2.3.4 Wolfe condition 336
6.2.4 Complete algorithms 337
6.3 Trust region method 339
6.3.1 Motivation and the framework 339
6.3.2 Cauchy point method 340
6.3.3 Exact solution method 342
6.3.4 Approximate method 342
6.4 Conjugate gradient method 345
6.4.1 Motivating problems 345
6.4.2 Theory conjugate direction 346
6.4.3 Linear conjugate gradient algorithm 347
6.5 Least square problems 350
6.5.1 Linear least square theory and algorithm 350
6.5.1.1 Linear least square problems 350
6.5.1.2 SVD methods 351
6.5.1.3 Extension to L^p norm optimization 351
6.5.2 nonlinear least square problem 352
6.5.3 Line search Gauss-Newton method 353
6.5.4 Trust region method 355
6.5.5 Application: roots for nonlinear equation 355
6.6 Notes on bibliography 357
7 CONSTRAINED NONLINEAR OPTIMIZATION 359
7.1 Quadratic optimization I: equality constraints 361
7.1.1 Problem formulation 361

7.1.2 Optimality condition 361
7.1.2.1 General case 361
7.1.2.2 Positive semi-definitive quadratic programming 364
7.1.3 Solving KKT systems 365
7.1.3.1 Factorization approach 365
7.1.3.2 Range space approach 366
7.1.4 Linear least square with linear constraints 366
7.1.4.1 Least norm problem 366
7.1.5 Application: Markovitz Portfolio Optimization Model 368
7.2 Quadratic optimization II: inequality constraints 371
7.2.1 Problem formulation 371
7.2.2 Optimality conditions 371
7.2.2.1 Pure inequality case 371
7.2.2.2 General constrained optimization 373
7.2.2.3 Positive semi-definitive quadratic programming 374
7.2.3 Primal active-set method 375
7.2.4 Gradient projection method 380
7.2.5 Dual convex quadratic programming 381
7.3 General equality constrained optimization 383
7.3.1 Feasible path and optimality 383
7.3.2 Constraint qualification and Lagrange theory 384
7.3.3 Second order condition 387
7.4 General inequality constrained optimization 391
7.4.1 Feasible path and optimality 391
7.4.2 Constraint qualifications and KKT conditions 392
7.4.3 Second order conditions 396
7.5 Envelope theorem and sensitive analysis 400
7.6 Notes on bibliography 403
8 LINEAR OPTIMIZATION 405
8.1 Equality constrained linear programming 406
8.2 Inequality constrained linear programming 408
8.2.1 Linear optimization with inequality constraints 408
8.2.2 Geometry of linear programming 408
8.2.3 Optimality property and condition 410
8.2.4 Standard form of linear programming 411
8.2.5 Application examples 412
8.3 Linear programming geometry and simplex algorithm 413
8.3.1 Geometrical approach to linear programming 413
8.3.1.1 Overview 413
8.3.1.2 Vertex and optimality 413
8.3.1.3 Descent direction at a vertex 417

8.3.1.4 Stepping along a descent direction 418
8.3.2 The simplex algorithm 419
8.4 Interior point method 420
8.4.1 Optimality condition 420
8.4.2 Newton step and perturbed system 422
8.4.3 Algorithms 424
8.5 Notes on bibliography 426
9 CONVEX ANALYSIS AND CONVEX OPTIMIZATION 428
9.1 Affine sets 430
9.1.1 Basic concepts 430
9.1.2 Affine independence and dimensions 432
9.2 Convex sets and properties 436
9.2.1 Concepts of convex sets 436
9.2.2 Projection theorems 438
9.2.3 Separation theorems 439
9.2.3.1 Separating hyperplane theorem 439
9.2.3.2 Farka's lemma 441
9.3 Convex functions 445
9.3.1 Basic concepts 445
9.3.2 Connection to convex set 447
9.3.3 Strongly convex functions 447
9.3.4 Operations preserve convexity 448
9.3.5 Convexity and derivatives 449
9.3.6 Subgradient 451
9.4 Duality theory 453
9.5 Convex optimization and optimality conditions 457
9.5.1 Local optimality vs. global optimality 457
9.5.2 Unconstrained optimization optimality conditions 458
9.5.3 Constrained optimization optimality conditions 458
9.6 Subgradient methods 463
9.6.1 A generic algorithm for unconstrained problem 463
9.6.2 Convergence under Lipschitz smoothness 465
9.6.3 Projected gradient methods 468
9.6.3.1 Foundations 468
9.6.3.2 Algorithms 470
9.6.4 Proximal gradient methods 471
9.6.4.1 Foundations 471
9.6.4.2 Algorithms 472
9.6.4.3 Case study: sparsity regularization problem 473
9.7 Notes on bibliography 475
10 BASIC GAME THEORY 477

10.1 Static normal form game 478
10.1.1 Normal form game concepts 478
10.1.2 Pure strategy and equilibrium 478
10.1.2.1 Solution concepts 478
10.1.3 Mixed strategy and equilibrium 482
10.1.4 Pareto optimality 484
10.2 Zero-sum matrix game 485
10.2.1 Fundamentals 485
10.2.2 Optimal strategy and Nash equilibrium 486
10.2.3 Saddle points as solutions 488
10.2.4 Maxmin strategies and Nash equilibrium 489
10.2.5 Linear programming approach to optimal strategy 492
10.3 Notes on bibliography 496
iii classical statistical methods
11 PROBABILITY THEORY 499
11.1 σ algebra 501
11.1.1 σ algebra concepts 501
11.1.2 Generation of sigma algebra 501
11.1.3 Partition of sample space 502
11.1.4 Filtration & information 502
11.1.5 Borel σ algebra 503
11.1.6 Measurable set and measurable space 504
11.2 Probability space 507
11.2.1 Event, sample point and sample space 507
11.2.2 Probability space 507
11.2.3 Properties of probability measure 509
11.2.4 Conditional probability 510
11.2.4.1 Basics 510
11.2.4.2 Bayes' theorem 511
11.2.4.3 Independence of events and sigma algebra 512
11.3 Measurable map and random variable 515
11.3.1 Random variable 515
11.3.2 σ algebra of random variables 516
11.3.3 Independence of random variables 517
11.4 Distributions of random variables 519
11.4.1 Basic concepts 519
11.4.1.1 Probability mass function 519
11.4.1.2 Distributions on $\mathbb{R}^n$ 519
11.4.1.3 Probability density function 520
11.4.1.4 Conditional distributions 521

11.4.1.5 Bayes law 522
11.4.2 Independence 523
11.4.3 Conditional independence 525
11.4.4 Transformations 525
11.4.4.1 Transformation for univariate distribution 525
11.4.4.2 Location-scale transformation 526
11.4.4.3 Transformation for multivariate distribution 527
11.5 Expectation, variance, and covariance 531
11.5.1 Expectation 531
11.5.2 Expectation in the Lebesgue framework 532
11.5.3 Properties of expectation 534
11.5.4 Variance and covariance 534
11.5.5 Conditional variance 535
11.5.6 Delta method 536
11.6 Moment generating functions and characteristic functions 538
11.6.1 Moment generating function 538
11.6.2 Characteristic function 541
11.6.3 Joint moment generating functions for random vectors 542
11.6.4 Cumulants 543
11.7 Conditional expectation 545
11.7.1 General intuitions 545
11.7.2 Formal definitions 545
11.7.3 Different versions of conditional expectation 547
11.7.3.1 Conditioning on an event 547
11.7.3.2 Conditioning on a discrete random variable as a new random variable 547
11.7.3.3 Condition on random variable vs. event vs σ algebra 548
11.7.4 Properties 548
11.7.4.1 Linearity 548
11.7.4.2 Taking out what is known 549
11.7.4.3 Law of total expectation 549
11.7.4.4 Law of iterated expectations 551
11.7.4.5 Conditioning on independent random variable/σ algebra 551
11.7.4.6 Least Square minimizing property 552
11.8 The Hilbert space of random variables 553
11.8.1 Definitions 553
11.8.2 Subspaces, projections, and approximations 553
11.8.3 Connection to conditional expectation 558
11.9 Probability inequalities 561
11.9.1 Chebychev inequalities 561

11.9.2 Jensen's inequality 562
11.9.3 Holder's, Minkowski, and Cauchy-Schwarz inequalities 563
11.9.4 Popoviciu's inequality for variance 565
11.10 Convergence of random variables 567
11.10.1 Different levels of equivalence among random variables 567
11.10.2 Convergence almost surely 567
11.10.3 Convergence in probability 568
11.10.4 Mean square convergence 570
11.10.5 Convergence in distribution 570
11.11 Law of Large Number and Central Limit theorem 573
11.11.1 Law of Large Numbers 573
11.11.2 Central limit theorem 575
11.12 Finite sampling models 578
11.12.1 Counting principles 578
11.12.2 Matching problem 581
11.12.3 Birthday problem 583
11.12.4 Coupon collection problem 584
11.12.5 Balls into bins model 585
11.13 Order statistics 588
11.14 Information theory 592
11.14.1 Concept of entropy 592
11.14.2 Entropy maximizing distributions 593
11.14.3 KL divergence 597
11.14.4 Conditional entropy and mutual information 598
11.14.5 Cross-entropy 599
11.15 Notes on bibliography 601
12 STATISTICAL DISTRIBUTIONS 603
12.1 Common distributions and properties 604
12.1.1 Overview 604
12.1.2 Bernoulli distribution 604
12.1.3 Poisson distribution 604
12.1.4 Geometric distribution 606
12.1.5 Binomial distribution 607
12.1.6 Normal distribution 609
12.1.7 Half-normal distribution 612
12.1.8 Laplace distribution 612
12.1.9 Multivariate Gaussian/normal distribution 613
12.1.9.1 Basic definitions 613
12.1.9.2 Affine transformation and its consequences 615
12.1.9.3 Marginal and conditional distribution 616
12.1.9.4 Box Muller transformation 618

12.1.10 Lognormal distribution 619
12.1.10.1 Univariate lognormal distribution 619
12.1.10.2 Extension to univariate lognormal distribution 620
12.1.10.3 Multivariate lognormal distribution 622
12.1.11 Exponential distribution 623
12.1.12 Gamma distribution 624
12.1.13 Hypergeometric distribution 626
12.1.14 Beta distribution 626
12.1.15 Multinomial distribution 629
12.1.16 Dirichlet distribution 630
12.1.17 χ^2-distribution 631
12.1.17.1 Basic properties 631
12.1.17.2 Noncentral chi-squared distribution 633
12.1.18 Wishart distribution 633
12.1.19 t-distribution 634
12.1.19.1 Standard t distribution 634
12.1.19.2 classical t distribution 635
12.1.19.3 Multivariate t distribution 635
12.1.20 F-distribution 636
12.1.21 Empirical distributions 637
12.1.22 Heavy-tailed distributions 638
12.1.22.1 Basic characterization 638
12.1.22.2 Pareto and power distribution 638
12.1.22.3 Student t distribution family 639
12.1.22.4 Gaussian mixture distributions 640
12.2 Characterizing distributions 642
12.2.1 Skewness and kurtosis 642
12.2.2 Percentiles and quantiles 644
12.2.2.1 Basics 644
12.2.2.2 Cornish-Fisher expansion 646
12.3 Moment matching approximation methods 648
12.4 Gaussian quadratic forms 650
12.4.0.1 Quadratic forms and chi-square distribution 650
12.4.0.2 Applications 653
12.5 Notes on bibliography 656
13 STATISTICAL ESTIMATION THEORY 657
13.1 Parameter estimators 660
13.1.1 Overview 660
13.1.2 Statistic and Estimator 661
13.1.2.1 Statistic 661
13.1.2.2 Estimator properties 662

13.1.2.3 Variance-bias decomposition 664
13.1.2.4 Consistence 666
13.1.2.5 Efficiency 668
13.1.2.6 Robust statistics 669
13.1.3 Method of moments 670
13.1.4 Maximum likelihood estimation 671
13.1.4.1 Basic concepts 671
13.1.4.2 MLE examples 673
13.1.4.3 Bias and consistence of MLE 676
13.2 Information and efficiency 679
13.2.1 Fisher information 679
13.2.2 Cramer-Rao lower bound 683
13.2.2.1 Preliminary: information inequality 683
13.2.2.2 Cramer-Rao lower bound: univariate case 684
13.2.2.3 Cramer-Rao lower bound: multivariate case 685
13.2.3 Efficient estimators 687
13.2.4 Asymptotic normality and efficiency of MLE 688
13.3 Sufficiency and data reduction 689
13.3.1 Sufficient estimators 689
13.3.2 Factorization theorem 690
13.4 Bayesian estimation theory 693
13.4.1 Overview 693
13.4.2 Basics 693
13.5 Bootstrap method 696
13.6 Hypothesis testing theory 698
13.6.1 Basics 698
13.6.2 Characterizing errors and power 701
13.6.3 Power of a statistical test 702
13.6.4 Common statistical tests 704
13.6.4.1 Chi-square goodness-of-fit test 704
13.6.4.2 Chi-square test for statistical independence 706
13.6.4.3 Kolmogorov-Smirnov goodness-of-fit test 707
13.7 Hypothesis testing on normal distributions 708
13.7.1 Normality test 708
13.7.2 Sample mean with known variance 708
13.7.3 Sample mean with unknown variance 710
13.7.4 Variance test 710
13.7.5 Variance comparison test 711
13.7.6 Person correlation t test 711
13.7.7 Two sample tests 712
13.7.7.1 Two-sample z test 712

13.7.7.2 Two-sample t test 712
13.7.7.3 Paired Data 713
13.7.8 Interval estimation for normal distribution 713
13.8 Notes on bibliography 715
14 MULTIVARIATE STATISTICAL METHODS 716
14.1 Multivariate data and distribution 718
14.1.1 Sample statistics 718
14.1.2 Multivariate Gaussian distribution 719
14.1.3 Estimation methods 721
14.1.3.1 Maximum likelihood estimation 721
14.1.3.2 Weighted estimation 723
14.2 Principal component analysis (PCA) 725
14.2.1 Statistical fundamentals of PCA 725
14.2.1.1 PCA for random vectors 725
14.2.1.2 Sample principal components 726
14.2.2 Geometric fundamentals of PCA 729
14.2.2.1 Optimization approach 729
14.2.2.2 Properties 731
14.2.3 Probabilistic PCA 732
14.2.4 Applications 734
14.2.4.1 Eigenfaces and eigendigits 734
14.2.4.2 Interest rate curve dynamics modeling 736
14.3 Canonical correlation analysis 740
14.3.1 Basics 740
14.3.2 Sparse CCA 742
14.4 Copulas and dependence modeling 744
14.4.1 Definitions and properties 744
14.4.2 Copulas and distributions 747
14.4.2.1 Fundamentals 747
14.4.2.2 Survival copula 754
14.4.2.3 Partial differential and conditional distribution 755
14.4.3 Common copula functions 759
14.4.3.1 Gaussian copula 759
14.4.3.2 t copula 764
14.4.3.3 Common copula functions: other copula 764
14.4.4 Dependence and copula 765
14.4.4.1 Linear correlations 765
14.4.4.2 Rank correlations 767
14.4.4.3 Tail dependence 773
14.4.5 Estimating copula function 775
14.4.5.1 Empirical copula method 775

14.4.5.2 Maximum likelihood method 776
14.4.6 Applications of copula 777
14.4.6.1 Generating correlated uniform random number 777
14.4.6.2 Generating general correlated random number 779
14.4.6.3 Multivariate distribution approximation with Gaussian copula 783
14.5 Covariance structure and factor analysis 784
14.5.1 The orthogonal factor model 784
14.5.1.1 Motivation and factor models 784
14.5.1.2 Covariance structure implied by factor model 784
14.5.2 Parameter estimation 786
14.5.2.1 Data collection and preparation 786
14.5.2.2 PCA method 787
14.5.2.3 Maximum likelihood method 788
14.5.3 Factor score estimation 788
14.5.4 Application I: Joint default modeling 789
14.5.4.1 Single factor model 789
14.5.4.2 Multiple factor model 792
14.5.5 Application II: factor models for stock return 793
14.5.5.1 Overview 793
14.5.5.2 The Fama-French 3 factor model 795
14.6 Graphical models 799
14.6.1 Fundamentals 799
14.7 Notes on Bibliography 805
15 LINEAR REGRESSION ANALYSIS 806
15.1 Linear regression analysis: basics 808
15.1.1 Linear regression models 808
15.1.2 Ordinary least square (OLS): fundamentals 811
15.1.2.1 Review on orthogonal projections 811
15.1.2.2 OLS results 812
15.1.2.3 OLS results with demeaned data 817
15.1.2.4 Gauss-Markov theorem 820
15.1.2.5 Variance decomposition 821
15.1.2.6 Residual and variance estimation 824
15.1.3 Ordinary least square (OLS): Additional topics 825
15.1.3.1 Orthogonal input and successive regression 825
15.1.3.2 Frisch-Waugh-Lovell(FWL) theorem and partial regression 827
15.1.3.3 Forecasting analysis with normality assumption 828
15.1.4 Hypothesis testing and analysis of variance 830
15.1.4.1 Distribution of coefficients 831

15.1.4.2 t test and normality test of single coefficients 833
15.1.4.3 F lack-of-fit test 835
15.1.4.4 χ^2 test for variance 837
15.1.5 Maximum likelihood method with normality assumption 838
15.1.6 Asymptotic properties of least square solutions 840
15.1.6.1 Asymptotic properties of standard OLS 840
15.1.6.2 Asymptotic efficiency of standard OLS 842
15.1.7 Partial and multiple correlation 842
15.1.7.1 Multiple correlation coefficient, R^2 842
15.1.7.2 Partial correlation coefficient 845
15.1.8 Generalized linear regression (GLR) 846
15.1.8.1 Linear regression with structural error 846
15.1.8.2 Generalized least square solution 847
15.1.8.3 Gauss-Markov theorem for GLR 849
15.1.8.4 Feasible GLS 850
15.1.9 Linear structure in joint distributions 850
15.2 Model specification and selection 853
15.2.1 Model order mis-specification 853
15.2.1.1 Omission of relevant regressors 853
15.2.1.2 Inclusion of irrelevant regressors 854
15.2.2 Model selection methods 856
15.2.2.1 Adjusted R square method 856
15.2.2.2 F test method 856
15.2.2.3 Information criterion methods 858
15.2.2.4 Bayesian information criterion (BIC) 859
15.2.3 Test for structure change 860
15.3 Linear regression analysis: diagnostics & solutions 862
15.3.1 Multi-collinearity 862
15.3.1.1 Detection and characterization 862
15.3.1.2 Regressor linear regression and variance inflation factor 862
15.3.1.3 Principal component linear regression (PCLR) 865
15.3.2 Rank deficiency and rigid regression 865
15.3.3 Heteroskedasticity 867
15.3.3.1 Test for heteroskedasticity 867
15.3.3.2 Heteroskedasticity robust estimator 868
15.3.3.3 Feasible weighted least square 868
15.3.4 Residual normality test 870
15.3.4.1 Jarque-Bera test 870
15.3.4.2 D'Agostino's K^2 test 870
15.3.5 Autocorrelation of errors 871

15.3.5.1 Motivation and general remarks 871
15.3.5.2 Test of autocorrelation of errors 872
15.3.5.3 Models with known autocorrelation 874
15.3.5.4 Transformation to generalized linear regression 875
15.3.6 Outliers analysis and robust linear regression 877
15.3.6.1 Outliers and influential points 877
15.3.6.2 Outlier impact analysis 878
15.3.6.3 Robust M-estimation linear regression 881
15.3.7 Visual diagnosis 884
15.4 Linear regression case studies 887
15.4.1 Standard linear regression 887
15.4.2 Boston Housing example 889
15.5 Multivariate multiple linear regression (MMLR) 892
15.5.1 Canonical MMLR 892
15.5.1.1 Motivation and model 892
15.5.1.2 Ordinary least square solution 893
15.5.2 Reduced rank regression 894
15.6 Notes on Bibliography 899
16 MONTE CARLO METHODS 900
16.1 Generating random variables 902
16.1.1 Inverse transform method 902
16.1.2 Box-Muller method for standard normal random variable 904
16.1.3 Acceptance-rejection method 904
16.1.4 Composition approach 905
16.1.5 Generate dependent continuous random variables 908
16.1.5.1 Multivariate normal and lognormal distribution 908
16.1.5.2 Multivariate student t distribution 908
16.1.5.3 General joint distribution 909
16.1.6 Generate discrete random variables 909
16.1.6.1 Generate single discrete random variables 909
16.1.6.2 Generate correlated discrete random variables 910
16.2 Monte Carlo integration 912
16.2.1 Naive approach 912
16.2.2 Importance sampling 913
16.3 Markov chain Monte Carlo 916
16.3.1 Basics 916
16.3.1.1 Markov chain Monte Carlo (MCMC) 916
16.3.2 Metropolis-Hasting algorithm 917
16.3.3 Gibbs sampling 919
16.4 Monte Carlo for random processes 920
16.4.1 Simulating stochastic differential equations 920

16.4.1.1 Simulating Brownian motion 920
16.4.1.2 Simulating linear arithmetic SDE 920
16.4.1.3 Simulating linear geometric SDE 921
16.4.1.4 Simulation mean-reversion(OU) process 921
16.4.2 Stochastic interpolation 922
16.4.2.1 Interpolating Gaussian processes 922
16.4.2.2 Interpolating one Dimensional Brownian motions 923
16.4.2.3 Interpolating multi-dimensional Brownian motions 925
16.5 Monte Carlo variance reduction 928
16.5.1 Antithetic sampling 928
16.5.1.1 Basic principles 928
16.5.1.2 Methods and analysis 929
16.5.2 Control variates 931
16.5.2.1 Basic principles 931
16.5.2.2 Multiple control variates 933
16.6 Notes on bibliography 934

iv dynamics modeling methods

17 MODELS AND ESTIMATION IN LINEAR SYSTEMS 936
17.1 Difference equation 937
17.1.1 Introduction 937
17.1.2 Solution structure of linear difference equations 938
17.1.3 Solution to non-homogeneous equation 940
17.1.4 Linear equations with constant coefficients 941
17.1.4.1 Basic case 941
17.1.4.2 General case 944
17.2 Differential equations 947
17.2.1 Linear differential equations 947
17.2.1.1 Concepts 947
17.2.1.2 Wronskian and linear independence 948
17.2.1.3 General solution theory 951
17.2.1.4 Existence & uniqueness of solution 954
17.2.2 Linear homogeneous differential equations with constant coefficients 955
17.2.2.1 The key identity 955
17.2.2.2 The case of real roots 957
17.2.2.3 The case of complex roots 958
17.2.2.4 The complete solution set 958
17.2.3 Solution to non-homogeneous ODEs 961
17.2.3.1 General principles 961
17.2.3.2 Key identity approach 962

17.2.4 First order linear differential equation 968
17.3 Linear system 970
17.3.1 Solution space for linear homogeneous system 970
17.3.2 Linear independence and the Wronskian 972
17.3.3 The fundamental system and solution method 974
17.3.4 The non-homogeneous linear equation 975
17.3.5 Conversion of linear differential/difference equation to linear systems 979
17.3.6 Solution method for discrete system 980
17.4 Linear system with constant coefficients 981
17.4.1 General solutions 981
17.4.2 System eigenvector method: continuous-time system 981
17.4.2.1 Diagonalizable system 981
17.4.2.2 two-by-two non-diagonalizable system 988
17.4.2.3 Non-diagonalizable system 989
17.4.3 Equilibrium point 991
17.4.3.1 Discrete-time system 991
17.4.3.2 Continuous-time system 992
17.4.4 Stability 993
17.4.5 Complex eigenvalues/eigenvectors 995
17.4.6 Boundedness of linear systems 995
17.4.7 One dimensional Nonlinear dynamical system analysis 996
17.5 Least square estimation of constant vectors 998
17.5.1 linear static estimation from single measurement with no prior information 998
17.5.2 linear static estimation from single measurement with prior information 999
17.5.3 Batch and recursive least square estimation with multiple measurements 1000
17.5.4 Nonlinear least square estimation 1003
17.6 Kalman filer 1004
17.6.1 Preliminary: error propagation in linear systems 1004
17.6.1.1 Discrete-time system 1004
17.6.1.2 Continuous-time system 1004
17.6.2 Batch estimation 1005
17.6.3 From batch estimation to Kalman filter 1006
17.6.4 Extended Kalman filter for nonlinear system 1007
17.7 Notes on bibliography 1009
18 STOCHASTIC PROCESS 1010
18.1 Stochastic process 1012
18.1.1 Basic definition and concepts 1012

18.1.2 Stationarity 1014
18.2 Gaussian process 1017
18.2.1 Basic Gaussian process 1017
18.2.2 Stationarity 1018
18.3 Brownian motion (Wiener process) 1019
18.3.1 Definition and elementary properties 1019
18.3.2 Multi-dimensional Brownian motion 1021
18.3.3 Asymptotic behaviors 1022
18.3.4 The reflection principle 1023
18.3.5 Quadratic variation 1024
18.3.6 Discrete-time approximations and simulation 1026
18.4 Brownian motion variants 1027
18.4.1 Gaussian process generated by Brownian motion 1027
18.4.2 Brownian bridge 1028
18.4.2.1 Constructions 1028
18.4.2.2 Applications 1032
18.4.3 Geometric Brownian motion 1032
18.5 Poisson process 1034
18.5.1 Basics 1034
18.5.2 Arrival and Inter-arrival Times 1035
18.6 Martingale theory 1037
18.6.1 Preliminaries: Filtration and adapted process 1037
18.6.1.1 Basic concepts in filtration 1037
18.6.1.2 Filtration for Brownian motion 1039
18.6.2 Basics of martingales 1039
18.6.3 Martingale transformation 1042
18.7 Stopping time 1043
18.7.1 Stopping time examples 1043
18.7.1.1 First passage time 1043
18.7.1.2 Trivial stopping time 1043
18.7.1.3 Counter example: last exit time 1044
18.7.2 Wald's equation 1044
18.7.3 Optional stopping 1045
18.7.4 martingale method for first hitting time 1045
18.8 Notes on bibliography 1046
19 STOCHASTIC CALCULUS 1047
19.1 Ito stochastic integral 1048
19.1.1 Motivation 1048
19.1.2 Construction of Ito integral 1048
19.1.2.1 Ito integral of a simple process 1048
19.1.2.2 Ito integral of a general process 1051

19.1.3 Ito integral with deterministic integrands (Wiener integral) 1055
19.1.3.1 Basics 1055
19.1.3.2 Integration by parts 1058
19.2 Stochastic differential equations 1061
19.2.1 Ito Stochastic differential equations 1061
19.2.2 Ito's lemma 1062
19.2.3 Useful results of Ito's lemma 1065
19.2.3.1 Product rule and quotient rule 1065
19.2.3.2 Logarithm and exponential 1066
19.2.3.3 Ito integral by parts 1066
19.2.3.4 Differentiate integrals of Ito process 1067
19.3 Linear SDE 1069
19.3.1 State-independent linear arithmetic SDE 1069
19.3.2 State-independent linear geometric SDE 1069
19.3.3 Multiple dimension extension 1071
19.3.4 Exact SDE 1073
19.3.5 Calculation mean and variance from SDE 1074
19.3.6 Integrals of Ito SDE 1075
19.4 Ornstein-Uhlenbeck(OU) process 1080
19.4.1 OU process 1080
19.4.1.1 Constant coefficient OU process 1080
19.4.1.2 Time-dependent coefficient OU process 1084
19.4.1.3 Integral of OU process 1086
19.4.2 Exponential OU process 1089
19.4.3 Parameter estimation for OU process 1091
19.4.4 Multiple factor extension 1091
19.5 Notes on bibliography 1094
20 MARKOV CHAIN AND RANDOM WALK 1095
20.1 Discrete-time Markov chain 1097
20.1.1 The model 1097
20.1.2 Evolution of discrete chain 1099
20.2 Classification of states 1101
20.2.1 accessibility and communicating classes 1101
20.2.2 Transient and recurrent states and classes 1103
20.2.2.1 Transient and recurrent states 1103
20.2.2.2 From states to classes 1107
20.2.2.3 Qualitative classification of recurrent and transient classes 1108
20.2.3 Periodicity 1109
20.2.4 Positive and null recurrent 1111
20.2.5 Summary 1113

20.3 Absorption analysis 1114
20.3.1 Matrix structure for adsorption analysis 1114
20.3.2 Absorbing Markov chains 1116
20.3.3 Hitting and return analysis 1118
20.3.4 Examples 1120
20.3.4.1 Consecutive coin toss game 1120
20.4 Limiting behavior & distributions 1122
20.4.1 Preliminary: eigenvalue proproties of stochastic matrices 1122
20.4.1.1 Preliminary: Frobenius-Perron matrix theory 1122
20.4.1.2 More general situations 1124
20.4.2 Limiting theorem 1126
20.4.2.1 Limiting distribution 1126
20.4.2.2 Extensions via Long run return analysis 1130
20.4.3 Application: PageRank algorithm 1132
20.5 Detailed balance and spectral properties 1134
20.6 Random walk 1136
20.6.1 Basic concepts and properties 1136
20.6.2 Persistent random walk 1136
20.6.3 Asymptotic properties 1138
20.6.4 Gambler's ruin problems 1138
20.7 Notes on bibliography 1143
21 TIME SERIES ANALYSIS 1144
21.1 Overview of time series analysis 1145
21.1.1 Introduction to time series 1145
21.1.2 Stationarity 1146
21.1.2.1 Stationarity concept 1146
21.1.2.2 Rolling analysis 1148
21.1.3 Remove trend and seasonality 1149
21.2 Linear stationary process theory 1152
21.2.1 Preliminaries: the lag operator and polynomial 1152
21.2.2 Linear process 1153
21.2.3 Autoregressive (AR) process 1155
21.2.3.1 Basics 1155
21.2.3.2 Stationarity and invertibility condition 1158
21.2.3.3 Forecasting 1159
21.2.4 Moving average (MA) process 1162
21.2.4.1 Basics 1162
21.2.4.2 Stationarity and invertibility 1165
21.2.4.3 Forecasting 1166
21.2.5 ARMA process 1169
21.2.5.1 Basic properties 1169

21.2.6 Unit root AR process 1171
21.2.6.1 Unit root process 1171
21.2.6.2 Trend stationarity vs. unit root process 1173
21.2.6.3 Unit root test 1173
21.2.6.4 Forecasting 1174
21.2.7 Correlation analysis 1174
21.2.7.1 Autocorrelation statistical analysis 1174
21.2.7.2 Partial autocorrelation function theory 1175
21.2.7.3 Correlogram analysis example 1178
21.2.8 Model analysis and calibration 1180
21.2.8.1 Order selection 1180
21.2.8.2 Yule-Walker equations and related methods 1181
21.2.8.3 Linear regression approach 1184
21.2.8.4 Maximum likelihood estimation 1186
21.2.8.5 Example: a toy example 1187
21.2.9 Wold Representation theorem 1190
21.3 Extensions to multivariate time series 1193
21.3.1 Introduction 1193
21.3.2 Vector autoregressive models 1194
21.3.2.1 VAR(1) model 1194
21.3.2.2 VAR(2) model 1196
21.3.2.3 VAR(p) model 1198
21.3.3 Vector moving-average model 1200
21.4 Autoregressive conditional heteroscedastic model 1203
21.4.1 ARCH models 1203
21.4.1.1 The motivation and the model 1203
21.4.1.2 Statistical properties 1205
21.4.1.3 Variance forecasting 1211
21.4.1.4 Detect ARCH effect 1214
21.4.1.5 Parameter estimation 1215
21.4.2 GARCH models 1215
21.4.2.1 The model 1215
21.4.2.2 Connecting GARCH to ARCH 1218
21.4.2.3 Variance forecasting 1218
21.5 Notes on Bibliography 1221

v statistical learning methods

22 SUPERVISED LEARNING PRINCIPLES 1223
22.1 The supervised learning problem 1224
22.1.1 Concepts 1224
22.1.2 Framework 1226

22.2 Variance bias trade-off 1228
- 22.2.1 Underfitting and Overfitting 1228
- 22.2.2 Variance and bias trade-off 1230
- 22.2.3 Examples 1233
  - 22.2.3.1 Linear regression 1233
- 22.2.4 No free lunch theorem 1234

22.3 Model loss and evaluation 1236
- 22.3.1 Common loss functions 1236
- 22.3.2 Model evaluation metrics 1240
  - 22.3.2.1 Regression metrics 1240
  - 22.3.2.2 Classification metrics 1241
  - 22.3.2.3 ROC and PRC metrics 1243
  - 22.3.2.4 Metrics for imbalanced data 1245

22.4 Model selection methods 1246
- 22.4.1 The training-validation-testing idea 1246
- 22.4.2 Cross-validation 1246

22.5 Data and feature engineering 1251
- 22.5.1 Data preprocessing 1251
  - 22.5.1.1 Data standardization 1251
  - 22.5.1.2 Data normalization 1252
  - 22.5.1.3 Handle categorical data 1252
  - 22.5.1.4 Handle missing values 1253
  - 22.5.1.5 Dimensional reduction 1253
  - 22.5.1.6 Centering kernel matrix 1253
- 22.5.2 Feature engineering I: basic routines 1254
  - 22.5.2.1 Nonlinear transformation 1254
  - 22.5.2.2 Polynomial features 1254
  - 22.5.2.3 Binning 1254
- 22.5.3 Feature engineering II: feature selection 1255
  - 22.5.3.1 Filtering methods 1255
  - 22.5.3.2 Recursive elimination methods 1256
  - 22.5.3.3 Regularization methods 1256
- 22.5.4 Feature engineering III: feature extraction 1256
  - 22.5.4.1 Text analytics 1256
  - 22.5.4.2 Image 1257
  - 22.5.4.3 Time series 1258
- 22.5.5 Imbalanced data 1259
  - 22.5.5.1 Motivations 1259
  - 22.5.5.2 Data resampling: undersampling 1259
  - 22.5.5.3 Data resampling: upsampling 1259
  - 22.5.5.4 Choice of loss functions, algorithms, and metrics 1260

22.6 Kernel methods 1261
22.6.1 Basic concepts of kernels and feature maps 1261
22.6.2 Mercer's theorem 1261
22.6.3 Common kernels 1263
22.6.4 Kernel trick and elementary algorithms using kernels 1265
22.6.5 Elementary algorithms 1265
22.7 Note on bibliography 1267
23 LINEAR MODELS FOR REGRESSION 1268
23.1 Standard linear regression 1269
23.1.1 Ordinary linear regression 1269
23.1.2 Application examples 1270
23.1.2.1 Boston housing prices 1270
23.2 Penalized linear regression 1274
23.2.1 Ridge regression 1274
23.2.1.1 Basics 1274
23.2.1.2 Dual form of ridge regression 1277
23.2.2 Lasso regression 1277
23.2.3 Elastic net 1280
23.2.4 Shrinkage Comparison 1280
23.2.5 Effective degree of freedom 1283
23.3 Basis function extension 1284
23.4 Note on bibliography 1286
24 LINEAR MODELS FOR CLASSIFICATION 1287
24.1 Logistic regression 1289
24.1.1 Logistic regression model 1289
24.1.2 Parameter estimation via maximum likelihood estimation 1290
24.1.3 Logistic regression with regularization 1294
24.1.4 Feature augmentation strategies 1295
24.1.5 Multinomial logistic regression 1296
24.1.6 Application examples 1297
24.1.6.1 South Africa heart disease 1297
24.1.6.2 Credit card fraud detection 1300
24.1.6.3 MNIST 1302
24.2 Gaussian discriminate analysis 1304
24.2.1 Linear Gaussian discriminant model 1304
24.2.1.1 The model 1304
24.2.1.2 Model parameter estimation 1305
24.2.1.3 Geometry of decision boundary 1305
24.2.2 Quadratic Gaussian discriminant model 1307
24.2.2.1 The model 1307
24.2.2.2 Model parameter estimation 1309

24.2.3 Application examples 1309
24.2.3.1 A toy example 1309
24.3 Fisher Linear discriminate analysis (Fisher LDA) 1312
24.3.1 One dimensional linear discriminant 1312
24.3.1.1 Basics 1312
24.3.1.2 Application in classification 1314
24.3.1.3 Possible issues 1316
24.3.2 Multi-dimensional linear discriminate 1317
24.3.2.1 Basics 1317
24.3.2.2 Application in classification 1318
24.3.3 Supervised dimensional reduction via Fisher LDA 1320
24.4 Separating hyperplane and Perceptron learning algorithm 1322
24.4.1 Basic geometry of hyperplanes 1322
24.4.2 The Perceptron learning algorithm 1323
24.5 Support vector machine classifier 1325
24.5.1 Motivation and formulation 1325
24.5.2 Optimality condition and dual form 1326
24.5.3 Soft margin SVM 1328
24.5.3.1 Basics 1328
24.5.3.2 Optimality condition for soft margin SVM 1329
24.5.3.3 Algorithm 1331
24.5.4 SVM with kernels 1333
24.5.5 A unified perspective from loss functions 1334
24.6 Note on bibliography 1337
25 GENERATIVE MODELS 1338
25.1 Naive Bayes classifier (NBC) 1342
25.1.1 Overview 1342
25.1.2 Binomial NBC 1342
25.1.3 Multinomial NBC 1344
25.1.4 Gaussian NBC 1347
25.1.5 Discussion 1349
25.2 Application 1350
25.2.1 Classifying documents using bag of words 1350
25.2.2 Credit card fraud prediction 1350
25.3 Supporting mathematical results 1353
25.3.1 Beta-binomial model 1353
25.3.1.1 The model 1353
25.3.1.2 Parameter inference 1354
25.3.2 Dirichlet-multinomial model 1356
25.3.2.1 The model 1356
25.3.2.2 Parameter inference 1359

26 K NEAREST NEIGHBORS 1360
- 26.1 Principles 1361
  - 26.1.1 The algorithm 1361
  - 26.1.2 Metrics and features 1362
- 26.2 Application examples 1364

27 TREE METHODS 1366
- 27.1 Preliminaries: entropy concepts 1367
  - 27.1.1 Concept of entropy 1367
  - 27.1.2 Conditional entropy and mutual information 1368
- 27.2 Classification tree 1372
  - 27.2.1 Basic concepts of decision tree learning 1372
  - 27.2.2 A generic tree-growth algorithm 1373
  - 27.2.3 Splitting criterion 1374
  - 27.2.4 Tree pruning 1378
  - 27.2.5 Practical algorithms 1378
  - 27.2.6 Examples 1381
    - 27.2.6.1 Tree structures in Iris data classification 1381
- 27.3 Regression tree 1384
  - 27.3.1 Basics 1384
  - 27.3.2 Practical algorithms 1387
  - 27.3.3 Examples 1387
    - 27.3.3.1 A toy example 1387
    - 27.3.3.2 Boston Housing prices 1388

28 ENSEMBLE AND BOOSTING METHODS 1390
- 28.1 Motivation and overview 1393
- 28.2 Bagging Methods 1395
  - 28.2.1 A basic bagging method 1395
  - 28.2.2 Tree bagging 1396
  - 28.2.3 Random Forest 1398
- 28.3 Adaboost 1401
  - 28.3.1 Adaboost classifier 1401
  - 28.3.2 Adaboost regressor 1405
  - 28.3.3 Additive model framework 1406
    - 28.3.3.1 Generic additive model algorithm 1406
    - 28.3.3.2 Adaboost as a special additive model 1407
- 28.4 Gradient boosting machines 1409
  - 28.4.1 Fundamental 1409
  - 28.4.2 Gradient boosting tree 1410
- 28.5 XGBoost 1415
- 28.6 Notes on Bibliography 1419

29 UNSUPERVISED STATISTICAL LEARNING 1420
29.1 Singular value decomposition (SVD) and matrix factorization 1421
29.1.1 SVD theory 1421
29.1.1.1 SVD fundamentals 1421
29.1.1.2 SVD and matrix norm 1423
29.1.1.3 SVD low rank approximation 1424
29.1.2 Principal component analysis (PCA) 1426
29.1.2.1 Statistical perspective of PCA 1426
29.1.2.2 Geometric fundamentals of PCA 1429
29.1.2.3 Robust PCA with outliers 1431
29.1.3 Sparse coding and dictionary learning 1433
29.1.3.1 Sparse coding 1433
29.1.3.2 Dictionary learning 1434
29.1.3.3 Online dictionary learning 1436
29.1.4 Non-negative matrix factorization 1438
29.2 Advanced applications of matrix factorization methods 1440
29.2.1 Latent sementic analysis 1440
29.2.2 Collaborative filtering in recommender systems 1443
29.2.3 Co-occurrence based word embedding 1448
29.3 Manifold learning 1450
29.3.1 Overview 1450
29.3.2 Preliminary: multidimensional scaling (MDS) 1450
29.3.2.1 Motivation 1450
29.3.2.2 Solution to classical MDS 1451
29.3.3 Isomap 1455
29.3.4 Kernel PCA 1456
29.3.5 Laplacian eigenmap 1458
29.3.5.1 Preliminary: graph Laplacian 1458
29.3.5.2 Laplacian eigenmap 1460
29.3.6 Diffusion map 1463
29.3.7 Application examples 1466
29.3.7.1 MNIST 1466
29.4 Clustering 1468
29.4.1 Overview 1468
29.4.2 K-means 1468
29.4.2.1 Canonical K-means 1468
29.4.2.2 K means++ 1471
29.4.2.3 Kernel K means 1472
29.4.3 Density-based spatial clustering of applications with noise (DBSCAN) 1473
29.4.4 Spectral clustering 1475

29.4.5 Gaussian mixture models (GMM) 1476
29.4.5.1 Preliminaries: Expectation Maximization (EM) algorithm 1476
29.4.5.2 The GMM model and algorithm 1478
29.4.6 Application examples 1480
29.4.6.1 Image segmentation 1480
29.5 Notes on Bibliography 1482
30 NEURAL NETWORK AND DEEP LEARNING 1483
30.1 Neural network foundations 1485
30.1.1 From machine learning to deep learning 1485
30.1.2 Neurons and neural networks 1486
30.1.2.1 Artificial neurons 1486
30.1.2.2 Artificial neural networks 1488
30.1.3 Universal approximation 1491
30.1.4 Training via backpropagation 1492
30.2 Optimization algorithms 1498
30.2.1 Motivation 1498
30.2.2 Full Batch gradient descent 1499
30.2.3 Minibatch stochastic gradient descent 1500
30.2.4 Adaptive gradient method 1501
30.2.4.1 Adaptive gradient (AdaGrad) 1501
30.2.4.2 RMSProp & AdaDelta 1501
30.2.5 Momentum method 1503
30.2.6 Combined together: adaptive momentum (Adam) 1504
30.3 Training and regularization techniques 1506
30.3.1 Choices of activation functions 1506
30.3.2 Weight initialization 1506
30.3.2.1 Motivation 1506
30.3.2.2 Xvaier initialization 1507
30.3.2.3 He initialization 1508
30.3.3 Data normalization 1508
30.3.3.1 Initial data standardization 1508
30.3.3.2 Batch normalization 1509
30.3.4 Regularization 1510
30.3.4.1 L_p regularization 1510
30.3.4.2 Weight decay 1510
30.3.4.3 Early stopping 1511
30.3.4.4 Dropout 1511
30.3.4.5 Data augmentation 1512
30.3.4.6 Label smoothing 1512
30.4 Feed-forward neural network examples 1513

30.4.1 Linear regression and classification 1513
30.4.2 Image classification 1515
30.4.3 Word embedding 1518
30.4.4 Sentiment analysis 1522
30.4.5 Approximating numerical partial differential equations 1524
30.5 Convolutional neural networks (CNN) 1528
30.5.1 Foundations 1528
30.5.2 CNN classical architectures 1531
30.5.2.1 LeNet 1531
30.5.2.2 AlexNet 1531
30.5.2.3 VGG 1532
30.5.2.4 ResNet 1533
30.6 CNN application examples 1536
30.6.1 Image classification 1536
30.6.2 Visualizing CNN 1537
30.6.2.1 Visualizing filters 1537
30.6.2.2 Visualizing classification activation map 1538
30.6.3 Autoencoders and denoising 1540
30.6.3.1 Autoencoders 1540
30.6.3.2 Denoising autoencoder 1541
30.6.4 Neural style transfer 1542
30.6.5 Visual based deep reinforcement learning 1545
30.6.6 Sentence classification 1547
30.7 Recurrent neural networks (RNN) 1550
30.7.1 Recurrent units 1550
30.7.1.1 Simple recurrent unit (SRU) 1550
30.7.1.2 Simple RNN and its approximation capability 1551
30.7.1.3 Backpropogation through time (BPTT) 1551
30.7.2 Recurrent unit variants 1553
30.7.2.1 Long short term memory (LSTM) 1553
30.7.2.2 Gated Recurrent Unit (GRU) 1556
30.7.3 Common RNN architectures 1557
30.8 RNN application examples 1561
30.8.1 Time series prediction 1561
30.8.1.1 Simple RNN prediction 1561
30.8.1.2 Deep autoregressive (DeepAR) model 1564
30.8.1.3 Deep factor model 1566
30.8.2 MNIST classification with sequential observation 1567
30.8.3 Sentiment classification 1567
30.8.4 Character-level language modeling 1568
30.8.4.1 Word classification 1568

30.8.4.2 Text generation 1569
30.9 Sequence-to-sequence modeling 1572
30.9.1 Encoder decoder model 1572
30.9.2 Attention mechanism 1574
30.10 Generative adversarial network (GAN) 1578
30.10.1 Canonical GAN 1578
30.10.1.1 Basics 1578
30.10.1.2 An example 1580
30.10.1.3 Understand training difficulties in GAN 1581
30.10.1.4 Deep Convolutional GAN (DCGAN) 1583
30.10.2 Conditional GAN 1585
30.10.3 Wasserstein GAN (WGAN) 1587
30.11 Notes on Bibliography 1591

vi optimal control and reinforcement learning methods

31 CLASSICAL OPTIMAL CONTROL THEORY 1593
31.1 Basic problem 1594
31.2 Controllability & observability 1595
31.3 Dynamic programming principle 1596
31.3.1 Principle of optimality 1596
31.3.2 The Hamilton-Jacobi-Bellman equation (finite horizon) 1596
31.3.3 The Hamilton-Jacobi-Bellman equation (infinite horizon) 1597
31.4 Deterministic linear quadratic control 1600
31.4.1 Linear quadratic control (finite horizon) 1600
31.4.2 Linear quadratic control(infinite horizon) 1601
31.5 Continuous-time stochastic optimal control 1603
31.5.1 HJB equation for general nonlinear systems 1603
31.5.2 Linear Gaussian quadratic system 1604
31.6 Stochastic dynamic programming 1605
31.6.1 Discrete-time Stochastic dynamic programming: finite horizon 1605
31.6.2 Discrete-time stochastic dynamic programming: infinite horizon 1607
31.6.2.1 Fundamentals 1607
31.6.2.2 Convergence analysis 1608
31.7 Notes on bibliography 1610
32 REINFORCEMENT LEARNING 1611
32.1 Preliminaries 1612
32.1.1 Notations 1612
32.1.2 Finite state Markov decision process 1612
32.1.3 Policy iteration and value iteration 1614

32.1.3.1 Policy iteration 1614
32.1.3.2 Value iteration 1618
32.2 Reinforcement learning theory 1622
32.2.1 Overview 1622
32.2.2 State-action Value function (Q function) 1624
32.2.3 Monte-Carlo method 1626
32.2.3.1 On-policy value estimation 1626
32.2.3.2 Off-policy value estimation 1628
32.2.3.3 MC-based reinforcement learning control 1628
32.2.4 TD(0) learning 1629
32.2.4.1 TD(0) for value estimation 1629
32.2.4.2 On-policy reinforcement learning control 1630
32.2.4.3 Off-policy reinforcement learning control 1631
32.2.5 TD(n) learning 1633
32.2.5.1 Motivation and concepts 1633
32.2.5.2 TD(n) for value estimation 1634
32.2.5.3 TD(n) for reinforcement learning control 1636
32.2.6 Standing challenges in reinforcement learning 1636
32.2.6.1 Curse of dimensionality 1636
32.2.6.2 Sample efficiency 1637
32.2.6.3 Exploration-exploitation dilemma 1637
32.2.6.4 Deadly triad 1637
32.3 Policy gradient learning 1638
32.3.1 Stochastic policy gradient fundamentals 1638
32.3.1.1 Preliminaries: deriative and expectation 1638
32.3.1.2 Theoretical framework based on finite-horizon trajectories 1639
32.3.1.3 Theoretical framework based on distributions* 1642
32.3.1.4 Estimate policy gradient and basic algorithms 1646
32.3.1.5 Bootstrap and Actor-Critic methods 1648
32.3.1.6 Common stochastic policies and their representations 1650
32.3.2 Advanced methods for policy gradient estimation 1652
32.3.2.1 Stochastic policy gradient with baseline 1652
32.3.2.2 Generalized advantage estimation 1655
32.3.2.3 Summary of stochastic gradient descent forms 1656
32.3.3 Deterministic policy gradient 1657
32.4 Algorithms zoo 1659
32.4.1 Neural Fitted Q Iteration (NFQ) 1659
32.4.2 Canonical deep Q learning 1660
32.4.3 DQN variants 1662

32.4.3.1 Overview 1662
32.4.3.2 Double Q learning 1663
32.4.3.3 Dueling network 1663
32.4.3.4 Deep Recurrent Q network (DRQN) 1664
32.4.3.5 Asynchronous Methods 1664
32.4.4 Universal value function approximator 1666
32.4.5 Deep deterministic policy gradient (DDPG) algorithm 1669
32.4.6 Twin-delayed deep deterministic policy gradient (TD3) 1671
32.4.7 Trust Region Policy Optimization (TRPO) 1674
32.4.7.1 TRPO 1674
32.4.7.2 Evaluating Hessian of KL-divergence 1676
32.4.8 Proximal Policy Optimization (PPO) 1677
32.4.9 Soft Actor-Critic(SAC) 1679
32.4.9.1 Entropy regulated reinforcement learning 1679
32.4.9.2 The SAC algorithm 1680
32.4.10 Evolution strategies 1681
32.5 Advanced training strategies 1684
32.5.1 Priority experience replay 1684
32.5.2 Hindsight experience generation 1685
32.5.3 Reverse goal generation 1686
32.5.4 Reverse goal generation on low-dimensional manifolds 1687
32.5.4.1 Key idea 1687
32.5.4.2 Example: navigation on a curved surface 1688
32.6 Notes on bibliography 1689

vii appendix

A SUPPLEMENTAL MATHEMATICAL FACTS 1691
A.1 Basic logic for proof 1692
A.2 Some common limits 1693
A.3 Common series summation 1695
A.4 Some common spaces 1696
A.4.1 Notations on continuously differentiable functions 1697
A.5 Different modes of continuity 1698
A.5.1 continuity vs. uniform continuity 1699
A.6 Exchanges of limits 1700
A.6.1 Overall remark 1700
A.6.2 exchange limits with infinite summations 1700
A.6.3 Exchange limits with integration and differentiation 1700
A.6.4 Exchange differentiation with integration 1701
A.6.5 Exchange limit and function evaluations 1702
A.7 Useful inequalities 1703

A.7.1 Gronwall's inequality 1703
A.7.2 Inequality for norms 1703
A.7.3 Young's inequality for product 1704
A.8 Useful properties of matrix 1705
A.8.1 Matrix derivatives 1705
A.8.2 Matrix inversion lemma 1705
A.8.3 Block matrix 1706
A.8.4 Matrix trace 1707
A.8.5 Matrix elementary operator 1708
A.8.6 Matrix determinant 1710
A.9 Numerical integration 1711
A.9.1 Gaussian quadrature 1712
A.10 Vector calculus 1714
A.11 Numerical linear algebra computation complexity 1715
A.12 Distributions 1716
A.13 Common integrals 1717
A.14 Nonlinear root finding 1718
A.14.1 Bisection method 1718
A.14.2 Newton method 1718
A.14.3 Secant method 1718
A.15 Interpolation 1720
A.15.1 cubic interpolation 1720
Alphabetical Index 1721

Part I

MATHEMATICAL FOUNDATIONS