$\label{lem:machine-learning-cheat-sheet} soulmachine@gmail.com$

Machine Learning Cheat Sheet

Classical equations, diagrams and tricks in machine learning

December 1, 2022

©2013 soulmachine

 $\label{thm:continuous} Except where otherwise noted, This document is licensed under a Creative Commons Attribution-ShareAlike 3.0 Unported (CC BY-SA3.0) license$

(http://creativecommons.org/licenses/by/3.0/).

Preface

This cheat sheet is a condensed version of machine learning manual, which contains many classical equations and diagrams on machine learning, and aims to help you quickly recall knowledge and ideas in machine learning.

This cheat sheet has two significant advantages:

- 1. Clearer symbols. Mathematical formulas use quite a lot of confusing symbols. For example, *X* can be a set, a random variable, or a matrix. This is very confusing and makes it very difficult for readers to understand the meaning of math formulas. This cheat sheet tries to standardize the usage of symbols, and all symbols are clearly pre-defined, see section §.
- 2. Less thinking jumps. In many machine learning books, authors omit some intermediary steps of a mathematical proof process, which may save some space but causes difficulty for readers to understand this formula and readers get lost in the middle way of the derivation process. This cheat sheet tries to keep important intermediary steps as where as possible.

Contents

| Notation | | | V | | 2.7 | | Carlo approximation | 12 | |
|----------|-----|--------|------------------------------------|----|-----|-------|---------------------|---------------------------------------|----|
| | | | | | 2.8 | | ation theory | 12 | |
| | | | Хİ | | | 2.8.1 | Entropy | 12 | |
| | | | | | | | 2.8.2 | KL divergence | 12 |
| 1 | | | | 1 | | | 2.8.3 | Mutual information | 13 |
| | 1.1 | | of machine learning | 1 | | | | | |
| | 1.2 | | elements of a machine learning | | 3 | | | nodels for discrete data | 15 |
| | | | <u> </u> | 1 | | 3.1 | | ative classifier | 15 |
| | | 1.2.1 | Representation | 1 | | 3.2 | | an concept learning | 15 |
| | | 1.2.2 | Evaluation | 1 | | | 3.2.1 | Likelihood | 15 |
| | | 1.2.3 | Optimization | 2 | | | 3.2.2 | Prior | 15 |
| | 1.3 | | pasic concepts | 2 | | | 3.2.3 | Posterior | 15 |
| | | 1.3.1 | Parametric vs non-parametric | _ | | | 3.2.4 | Posterior predictive distribution. | 15 |
| | | 1.0.0 | models | 2 | | 3.3 | | ta-binomial model | 16 |
| | | 1.3.2 | A simple non-parametric | 2 | | | 3.3.1 | Likelihood | 16 |
| | | 1.0.0 | classifier: K-nearest neighbours. | 2 | | | 3.3.2 | Prior | 16 |
| | | 1.3.3 | Overfitting | 2 | | | 3.3.3 | Posterior | 16 |
| | | 1.3.4 | Cross validation | 2 | | | 3.3.4 | Posterior predictive distribution. | 16 |
| | | 1.3.5 | Model selection | 2 | | 3.4 | | richlet-multinomial model | 17 |
| • | D1. | -1.914 | | 2 | | | 3.4.1 | Likelihood | 17 |
| 2 | | | entries - Proportions | 3 | | | 3.4.2 | Prior | 17 |
| | 2.1 | | ntists vs. Bayesians | 3 | | | 3.4.3 | Posterior | 17 |
| | 2.2 | | review of probability theory | 3 | | | 3.4.4 | Posterior predictive distribution. | 18 |
| | | 2.2.1 | Basic concepts | 3 | | 3.5 | | Bayes classifiers | 18 |
| | | 2.2.2 | Mutivariate random variables | 3 | | | 3.5.1 | Optimization | 18 |
| | | 2.2.3 | Bayes rule | 4 | | | 3.5.2 | Using the model for prediction . | 19 |
| | | 2.2.4 | Independence and conditional | | | | 3.5.3 | The log-sum-exp trick | 19 |
| | | | independence | 4 | | | 3.5.4 | Feature selection using mutual | |
| | | 2.2.5 | Quantiles | 4 | | | | information | 19 |
| | | 2.2.6 | Mean and variance | 4 | | | 3.5.5 | Classifying documents using | |
| | 2.3 | | common discrete distributions | 4 | | | | bag of words | 19 |
| | | 2.3.1 | The Bernoulli and binomial | _ | | _ | | | |
| | | 2.2.2 | distributions | 5 | 4 | | | dels | 21 |
| | | 2.3.2 | The multinoulli and | _ | | 4.1 | | | 21 |
| | | 2.2.2 | multinomial distributions | 5 | | | 4.1.1 | MLE for a MVN | 21 |
| | | 2.3.3 | The Poisson distribution | 5 | | | 4.1.2 | Maximum entropy derivation | |
| | - 4 | 2.3.4 | The empirical distribution | 5 | | | | of the Gaussian * | 21 |
| | 2.4 | | common continuous distributions | 5 | | 4.2 | | an discriminant analysis | 22 |
| | | 2.4.1 | Gaussian (normal) distribution | 5 | | | 4.2.1 | Quadratic discriminant analysis | |
| | | 2.4.2 | Student's t-distribution | 6 | | | | (QDA) | 22 |
| | | 2.4.3 | The Laplace distribution | 6 | | | 4.2.2 | Linear discriminant analysis | |
| | | 2.4.4 | The gamma distribution | 7 | | | | (LDA) | 22 |
| | | 2.4.5 | The beta distribution | 7 | | | 4.2.3 | Two-class LDA | 23 |
| | | 2.4.6 | Pareto distribution | 7 | | | 4.2.4 | MLE for discriminant analysis | 24 |
| | 2.5 | | robability distributions | 8 | | | 4.2.5 | Strategies for preventing | |
| | | 2.5.1 | Covariance and correlation | 8 | | | | overfitting | 24 |
| | | 2.5.2 | Multivariate Gaussian distribution | 9 | | | 4.2.6 | Regularized LDA * | 24 |
| | | 2.5.3 | Multivariate Student's | | | | 4.2.7 | Diagonal LDA | 24 |
| | | | t-distribution | 9 | | | 4.2.8 | Nearest shrunken centroids | |
| | | 2.5.4 | Dirichlet distribution | 9 | | | | classifier * | 24 |
| | 2.6 | | ormations of random variables | 10 | | 4.3 | | ace in jointly Gaussian distributions | 24 |
| | | 2.6.1 | Linear transformations | 10 | | | 4.3.1 | Statement of the result | 25 |
| | | 2.6.2 | General transformations | 10 | | | 4.3.2 | Examples | 25 |
| | | 2.6.3 | Central limit theorem | 10 | | 4.4 | Linear | Gaussian systems | 25 |

vi Preface

| | | 4.4.1 | Statement of the result | 25 | | | 7.4.3 | Connection with PCA * | 39 |
|---|--|---|---|--|----|---|---|---|--|
| | 4.5 | Digress | sion: The Wishart distribution * | 25 | | | 7.4.4 | Regularization effects of big data | 39 |
| | 4.6 | | ng the parameters of an MVN | 25 | | 7.5 | | an linear regression | 39 |
| | 1.0 | 4.6.1 | Posterior distribution of μ | 25 | | 7.5 | Dayesic | un inicai regression | 3) |
| | | 4.6.2 | Posterior distribution of Σ^* | 25 | 8 | Logic | tic Door | ession | 41 |
| | | 4.6.3 | | 23 | 0 | _ | _ | | 41 |
| | | 4.0.3 | Posterior distribution of μ and | 25 | | 8.1 | - | entation | |
| | | 1.6.1 | Σ^* | 25 | | 8.2 | _ | zation | 41 |
| | | 4.6.4 | Sensor fusion with unknown | | | | 8.2.1 | MLE | 41 |
| | | | precisions * | 25 | | | 8.2.2 | MAP | 41 |
| _ | - | | | 2= | | 8.3 | Multino | omial logistic regression | 41 |
| 5 | • | | istics | 27 | | | 8.3.1 | Representation | 41 |
| | 5.1 | | iction | 27 | | | 8.3.2 | MLE | 42 |
| | 5.2 | | arizing posterior distributions | 27 | | | 8.3.3 | MAP | 42 |
| | | 5.2.1 | MAP estimation | 27 | | 8.4 | Bayesia | an logistic regression | 42 |
| | | 5.2.2 | Credible intervals | 28 | | | 8.4.1 | Laplace approximation | 42 |
| | | 5.2.3 | Inference for a difference in | | | | 8.4.2 | Derivation of the BIC | 42 |
| | | | proportions | 28 | | | 8.4.3 | Gaussian approximation for | |
| | 5.3 | Bayesia | an model selection | 29 | | | 01.10 | logistic regression | 42 |
| | | 5.3.1 | Bayesian Occam's razor | 29 | | | 8.4.4 | Approximating the posterior | |
| | | 5.3.2 | Computing the marginal | | | | 0.7.7 | predictive | 42 |
| | | | likelihood (evidence) | 30 | | | 8.4.5 | Residual analysis (outlier | 72 |
| | | 5.3.3 | Bayes factors | 31 | | | 0.4.5 | | 42 |
| | 5.4 | Priors | • | 31 | | 0.5 | 0.1 | detection) * | |
| | | 5.4.1 | Uninformative priors | 31 | | 8.5 | | learning and stochastic optimization | |
| | | 5.4.2 | Robust priors | 31 | | 0.6 | 8.5.1 | The perceptron algorithm | 42 |
| | | 5.4.3 | Mixtures of conjugate priors | 31 | | 8.6 | | tive vs discriminative classifiers | 44 |
| | 5.5 | | chical Bayes | 32 | | | 8.6.1 | Pros and cons of each approach. | 44 |
| | 5.6 | | cal Bayes | 32 | | | 8.6.2 | Dealing with missing data | 44 |
| | 5.7 | | | 32 | | | 8.6.3 | Fisher's linear discriminant | |
| | 3.7 | | an decision theory | 32 | | | | analysis (FLDA) * | 45 |
| | | 5.7.1 | Bayes estimators for common | 22 | | | | | |
| | | 570 | loss functions | 32 | 9 | Gene | ralized l | inear models and the | |
| | | 5.7.2 | The false positive vs false | | | | | | 47 |
| | | | | 22 | | expo | nential fa | mily | 4/ |
| | | | negative tradeoff | 33 | | expo 9.1 | | conential family | 47 |
| 6 | Frag | uantist s | negative tradeoff | | | | | | |
| 6 | | | negative tradeoff | 35 | | | The exp | ponential family | 47 |
| 6 | Freq 6.1 | Sampli | negative tradeoff tatistics ng distribution of an estimator | 35 35 | | | The exp 9.1.1 | Definition | 47 47 |
| 6 | | Sampli 6.1.1 | negative tradeoff tatistics | 35 | | | The exp 9.1.1 9.1.2 | Donential family Definition Examples Log partition function | 47 47 47 |
| 6 | | Sampli | negative tradeoff | 35 35 35 | | | The exp 9.1.1 9.1.2 9.1.3 9.1.4 | Definition | 47 47 47 48 48 |
| 6 | 6.1 | Sampli 6.1.1 6.1.2 | negative tradeoff | 35 35 35 35 | | | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 | Definition | 47 47 47 48 |
| 6 | 6.1 | Sampli 6.1.1 6.1.2 Freque | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory | 35 35 35 35 35 | | | The exp 9.1.1 9.1.2 9.1.3 9.1.4 | Definition | 47 47 47 48 48 49 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desirab | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory Dele properties of estimators | 35 35 35 35 35 35 | | 9.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 | Definition | 47 47 48 48 49 |
| 6 | 6.1 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ole properties of estimators cal risk minimization | 35 35 35 35 35 35 35 | | | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 | Definition | 47 47 48 48 49 49 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ple properties of estimators cal risk minimization Regularized risk minimization | 35 35 35 35 35 35 35 35 | | 9.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 General 9.2.1 | Definition | 47 47 48 48 49 49 49 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ble properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization | 35 35 35 35 35 35 35 | | 9.19.29.3 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 General 9.2.1 Probit r | Definition | 47 47 48 48 49 49 49 49 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ple properties of estimators cal risk minimization Regularized risk minimization | 35 35 35 35 35 35 35 35 35 | | 9.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 General 9.2.1 Probit r | Definition | 47 47 48 48 49 49 49 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ole properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation | 35 35 35 35 35 35 35 35 | 10 | 9.1 9.2 9.3 9.4 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-ta | Definition | 47 47 48 48 49 49 49 49 49 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ole properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross | 35 35 35 35 35 35 35 35 35 | 10 | 9.1 9.2 9.3 9.4 Direct | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-teted grap | Definition | 47 47 48 48 49 49 49 49 51 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ole properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation | 35 35 35 35 35 35 35 35 35 | 10 | 9.1 9.2 9.3 9.4 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-ta | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family *lized linear models (GLMs) Basics egression ask learning chical models (Bayes nets) | 47 47 48 48 49 49 49 49 51 51 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ble properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * | 35 35 35 35 35 35 35 35 35 35 | 10 | 9.1 9.2 9.3 9.4 Direct | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-tated grap Introdu 10.1.1 | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family *lized linear models (GLMs) Basics egression ask learning Chical models (Bayes nets) ction Chain rule | 47 47 48 48 49 49 49 49 51 51 |
| 6 | 6.1 6.2 6.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ble properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions | 35 35 35 35 35 35 35 35 35 35 | 10 | 9.1 9.2 9.3 9.4 Direct | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-tated grap Introdu 10.1.1 10.1.2 | Definition | 47 47 48 48 49 49 49 49 51 51 51 |
| 6 | 6.2 6.3 6.4 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ble properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * | 35 35 35 35 35 35 35 35 35 35 35 35 35 | 10 | 9.1 9.2 9.3 9.4 Direct | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-tated grap Introdu 10.1.1 | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family *lized linear models (GLMs) Basics egression ask learning Chical models (Bayes nets) ction Chain rule | 47 47 48 48 49 49 49 49 51 51 |
| 7 | 6.2 6.3 6.4 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ble properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions | 35 35 35 35 35 35 35 35 35 35 35 35 35 | 10 | 9.1 9.2 9.3 9.4 Direct | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-tated grap Introdu 10.1.1 10.1.2 | Definition | 47 47 48 48 49 49 49 49 51 51 51 |
| | 6.2 6.3 6.4 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * Intist decision theory Die properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions ogies of frequentist statistics * | 35 35 35 35 35 35 35 35 35 35 35 35 35 | 10 | 9.1 9.2 9.3 9.4 Direct | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 General 9.2.1 Probit r Multi-tated grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 | Definition | 47 47 48 48 49 49 49 49 51 51 51 51 |
| | 6.1 6.2 6.3 6.4 6.5 Line: 7.1 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE* ntist decision theory ole properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions ogies of frequentist statistics * | 35 35 35 35 35 35 35 35 35 35 35 35 35 3 | 10 | 9.1 9.2 9.3 9.4 Direc 10.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 General 9.2.1 Probit r Multi-tated grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 | Definition | 47 47 48 48 49 49 49 49 51 51 51 51 51 |
| | 6.2 6.3 6.4 6.5 Line 7.1 7.2 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo ar Regre Introdu Represe | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE* ntist decision theory ple properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions ogies of frequentist statistics * ssion ection entation. | 35 35 35 35 35 35 35 35 35 35 35 35 37 37 37 | 10 | 9.1 9.2 9.3 9.4 Direc 10.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 General 9.2.1 Probit r Multi-tal eted grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 Example | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family * .lized linear models (GLMs) Basics egression ask learning chical models (Bayes nets) ction Chain rule Conditional independence Graphical models Directed graphical model | 47 47 48 48 49 49 49 49 51 51 51 51 51 |
| | 6.1 6.2 6.3 6.4 6.5 Line: 7.1 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo ar Regre Introdu Repress MLE. | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ple properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions origies of frequentist statistics * ssion ection entation. | 35 35 35 35 35 35 35 35 35 35 35 37 37 37 37 | 10 | 9.1 9.2 9.3 9.4 Direc 10.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-ta ted grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 Example 10.2.1 | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family *lized linear models (GLMs) Basics egression ask learning Chical models (Bayes nets) ction Chain rule Conditional independence Graphical models Directed graphical model les Naive Bayes classifiers | 47 47 48 48 49 49 49 49 51 51 51 51 51 51 |
| | 6.2 6.3 6.4 6.5 Line 7.1 7.2 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo ar Regre Introdu Repress MLE. 7.3.1 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE* ntist decision theory ole properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions ogies of frequentist statistics * ssion oction entation OLS | 35 35 35 35 35 35 35 35 35 35 35 37 37 37 37 37 | 10 | 9.1 9.2 9.3 9.4 Direct 10.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-ta ted grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 Examp 10.2.1 10.2.2 | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family * lized linear models (GLMs) Basics regression ask learning Chical models (Bayes nets) ction Chain rule Conditional independence Graphical models Directed graphical model les Naive Bayes classifiers Markov and hidden Markov models | 47 47 48 48 49 49 49 49 51 51 51 51 51 51 51 |
| | 6.2 6.3 6.4 6.5 Line 7.1 7.2 7.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo ar Regre Introdu Repres MLE . 7.3.1 7.3.2 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * Intist decision theory Die properties of estimators Cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions Degies of frequentist statistics * ssion OLS SGD | 35 35 35 35 35 35 35 35 35 35 35 37 37 37 37 37 37 38 | 10 | 9.1 9.2 9.3 9.4 Direct 10.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 General 9.2.1 Probit r Multi-tated grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 Example 10.2.1 Inference | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family *lized linear models (GLMs). Basics regression ask learning Chical models (Bayes nets) ction Chain rule Conditional independence Graphical models Directed graphical model les Naive Bayes classifiers Markov and hidden Markov models ce | 47 47 48 48 49 49 49 49 51 51 51 51 51 51 52 52 |
| | 6.2 6.3 6.4 6.5 Line 7.1 7.2 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo ar Regre Introdu Repres MLE . 7.3.1 7.3.2 Ridge I | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ole properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions ogies of frequentist statistics * ssion entation OLS SGD regression(MAP) | 35 35 35 35 35 35 35 35 35 35 35 37 37 37 37 37 38 38 | 10 | 9.1 9.2 9.3 9.4 Direct 10.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-ta ted grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 Examp 10.2.1 10.2.2 Inference | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family * dized linear models (GLMs) Basics regression ask learning Chical models (Bayes nets) ction Chain rule Conditional independence Graphical models Directed graphical model les Naive Bayes classifiers Markov and hidden Markov models ce | 47 47 48 48 49 49 49 49 49 51 51 51 51 51 51 52 52 52 |
| | 6.2 6.3 6.4 6.5 Line 7.1 7.2 7.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo ar Regre Introdu Repres MLE . 7.3.1 7.3.2 Ridge i 7.4.1 | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE* ntist decision theory ole properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions ogies of frequentist statistics * ssion entation OLS SGD regression(MAP) Basic idea | 35 35 35 35 35 35 35 35 35 35 35 37 37 37 37 37 37 38 | 10 | 9.1 9.2 9.3 9.4 Direct 10.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 General 9.2.1 Probit r Multi-ta ted grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 Example 10.2.1 10.2.2 Inference Learnin 10.4.1 | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family * .lized linear models (GLMs) Basics egression ask learning Chain rule Conditional independence Graphical models Directed graphical model les Naive Bayes classifiers Markov and hidden Markov models Ce Learning from complete data | 47 47 48 48 49 49 49 49 51 51 51 51 51 51 52 52 |
| | 6.2 6.3 6.4 6.5 Line 7.1 7.2 7.3 | Sampli 6.1.1 6.1.2 Freque Desiral Empiri 6.4.1 6.4.2 6.4.3 6.4.4 6.4.5 Patholo ar Regre Introdu Repres MLE . 7.3.1 7.3.2 Ridge I | negative tradeoff tatistics ng distribution of an estimator Bootstrap Large sample theory for the MLE * ntist decision theory ole properties of estimators cal risk minimization Regularized risk minimization Structural risk minimization Estimating the risk using cross validation Upper bounding the risk using statistical learning theory * Surrogate loss functions ogies of frequentist statistics * ssion entation OLS SGD regression(MAP) | 35 35 35 35 35 35 35 35 35 35 35 37 37 37 37 37 38 38 | 10 | 9.1 9.2 9.3 9.4 Direct 10.1 | The exp 9.1.1 9.1.2 9.1.3 9.1.4 9.1.5 9.1.6 Genera 9.2.1 Probit r Multi-ta ted grap Introdu 10.1.1 10.1.2 10.1.3 10.1.4 Examp 10.2.1 10.2.2 Inference | Definition Examples Log partition function MLE for the exponential family Bayes for the exponential family Maximum entropy derivation of the exponential family * dized linear models (GLMs) Basics regression ask learning Chical models (Bayes nets) ction Chain rule Conditional independence Graphical models Directed graphical model les Naive Bayes classifiers Markov and hidden Markov models ce | 47 47 48 48 49 49 49 49 49 51 51 51 51 51 51 52 52 52 |

Preface vii

| | 10.5 | Conditional independence properties of | | | | 12.2.1 | Classical PCA | 65 |
|----|-------|--|----------|----|-------|------------------|---|----------|
| | | DGMs | 52 | | | 12.2.2 | Singular value decomposition | |
| | | 10.5.1 d-separation and the Bayes | | | | | (SVD) | 66 |
| | | Ball algorithm (global Markov | | | | 12.2.3 | Probabilistic PCA | 67 |
| | | properties) | 52 | | | 12.2.4 | EM algorithm for PCA | 67 |
| | | 10.5.2 Other Markov properties of | 52 | | 12.3 | | g the number of latent dimensions | 68 |
| | | DGMs | 53 | | | 12.3.1 12.3.2 | Model selection for FA/PPCA Model selection for PCA | 68 68 |
| | | conditionals | 53 | | 12.4 | | categorical data | 68 |
| | | 10.5.4 Multinoulli Learning | 53 | | 12.5 | | paired and multi-view data | 68 |
| | 10.6 | Influence (decision) diagrams * | 53 | | 12.5 | 12.5.1 | Supervised PCA (latent factor | 00 |
| | | | | | | | regression) | 68 |
| 11 | Mixtu | re models and the EM algorithm | 55 | | | 12.5.2 | Discriminative supervised PCA. | 68 |
| | 11.1 | Latent variable models | 55 | | | 12.5.3 | Canonical correlation analysis | 68 |
| | 11.2 | Mixture models | 55 | | 12.6 | Indepen | dent Component Analysis (ICA). | 68 |
| | | 11.2.1 Mixtures of Gaussians | 55 | | | 12.6.1 | Maximum likelihood estimation | 69 |
| | | 11.2.2 Mixtures of multinoullis | 55 | | | 12.6.2 | The FastICA algorithm | 69 |
| | | 11.2.3 Using mixture models for | 56 | | | 12.6.3 | Using EM | 69 |
| | | clustering | 56 | | | 12.6.4 | Other estimation principles * | 69 |
| | 11.3 | Parameter estimation for mixture models. | 57 | 13 | Spare | sa linaar 1 | models | 71 |
| | 11.5 | 11.3.1 Unidentifiability | 57 | 13 | Spars | se iiiicai i | models | / 1 |
| | | 11.3.2 Computing a MAP estimate is | Ο, | 14 | Kern | els | | 73 |
| | | non-convex | 57 | | 14.1 | Introduc | etion | 73 |
| | 11.4 | The EM algorithm | 57 | | 14.2 | Kernel f | unctions | 73 |
| | | 11.4.1 Introduction | 57 | | | 14.2.1 | RBF kernels | 73 |
| | | 11.4.2 Basic idea | 57 | | | 14.2.2 | TF-IDF kernels | 73 |
| | | 11.4.3 EM for GMMs | 58 | | | 14.2.3 | Mercer (positive definite) kernels | 73 |
| | | 11.4.4 EM for K-means | 59 | | | 14.2.4 | Linear kernels | 74 |
| | | 11.4.5 EM for mixture of experts | 60 | | | 14.2.5 | Matern kernels | 74 |
| | | 11.4.6 EM for DGMs with hidden | (0 | | | 14.2.6 | String kernels | 74 |
| | | variables | 60 | | | 14.2.7 14.2.8 | Pyramid match kernels Kernels derived from | 74 |
| | | 11.4.7 EM for the Student distribution * 11.4.8 EM for probit regression * | 60 60 | | | 14.2.0 | probabilistic generative models . | 74 |
| | | 11.4.9 Derivation of the <i>Q</i> function | 60 | | 14.3 | Using ke | ernels inside GLMs | 75 |
| | | 11.4.10 Convergence of the EM | 00 | | 1 1 | 14.3.1 | Kernel machines | 75 |
| | | Algorithm * | 60 | | | 14.3.2 | L1VMs, RVMs, and other | |
| | | 11.4.11 Generalization of EM | | | | | sparse vector machines | 76 |
| | | Algorithm * | 61 | | 14.4 | The kerr | nel trick | 76 |
| | | 11.4.12 Online EM | 62 | | | 14.4.1 | Kernelized KNN | 76 |
| | | 11.4.13 Other EM variants * | 62 | | | 14.4.2 | Kernelized K-medoids clustering | 76 |
| | 11.5 | Model selection for latent variable models | 62 | | | 14.4.3 | Kernelized ridge regression | 76 |
| | | 11.5.1 Model selection for | | | | 14.4.4 | Kernel PCA | 76 |
| | | probabilistic models | 62 | | 14.5 | | vector machines (SVMs) | 77 |
| | | 11.5.2 Model selection for | (2) | | | 14.5.1 | SVMs for classification | 77 |
| | 11.6 | non-probabilistic methods | 62 62 | | | 14.5.2 14.5.3 | SVMs for regression | 78 78 |
| | 11.0 | Fitting models with missing data 11.6.1 EM for the MLE of an MVN | 02 | | | 14.5.4 | A probabilistic interpretation | 70 |
| | | with missing data | 62 | | | 14.5.4 | of SVMs | 78 |
| | | with inissing data | 02 | | | 14.5.5 | Summary of key points | 79 |
| 12 | Laten | at linear models | 63 | | 14.6 | | ison of discriminative kernel | |
| | 12.1 | Factor analysis | 63 | | | | · | 79 |
| | | 12.1.1 FA is a low rank | | | 14.7 | | for building generative models | 79 |
| | | parameterization of an MVN | 63 | | | | | |
| | | 12.1.2 Inference of the latent factors | 63 | 15 | | _ | esses | 81 |
| | | 12.1.3 Unidentifiability | 63 | | 15.1 | | etion | 81 |
| | | 12.1.4 Mixtures of factor analysers | 64 | | 15.2 | | regression | 81 |
| | | 12.1.5 EM for factor analysis models | 64 | | 15.3 | | et GLMs | 81 |
| | | 12.1.6 Fitting FA models with missing | 65 | | 15.4 | | ion with other methods | 81 |
| | 12.2 | data | 65 65 | | 15.5 | | nt variable model | 81 81 |
| | 12.2 | Principal components analysis (PCA) | UJ | | 15.6 | Approxi | mation methods for large datasets | 01 |

viii Preface

| 16 | Adaptive basis function models | 83 | | 24.5 | Auxiliary variable MCMC * | 99 |
|-----------|---|----|-----------|----------|--|-----|
| | 16.1 AdaBoost | 83 | | | | |
| | 16.1.1 Representation | 83 | 25 | Cluste | ring | 101 |
| | 16.1.2 Evaluation | 83 | | | | |
| | 16.1.3 Optimization | 83 | 26 | Graph | ical model structure learning 1 | 103 |
| | 16.1.4 The upper bound of the training | | | . | | |
| | error of AdaBoost | 83 | 27 | | t variable models for discrete data | |
| | | | | | Introduction | |
| 17 | Hidden markov Model | 85 | | 27.2 | Distributed state LVMs for discrete data . 1 | 105 |
| | 17.1 Introduction | 85 | ••• | | | |
| | 17.2 Markov models | 85 | 28 | Deep I | earning 1 | 107 |
| 18 | State space models | 87 | A | Optim | ization methods 1 | 109 |
| 10 | State space models | 07 | | _ | Convexity | |
| 19 | Undirected graphical models (Markov | | | A.2 | Gradient descent | |
| | random fields) | 89 | | | A.2.1 Stochastic gradient descent 1 | |
| | | | | | A.2.2 Batch gradient descent | |
| 20 | Exact inference for graphical models | 91 | | | A.2.3 Line search | |
| | | | | | A.2.4 Momentum term | |
| 21 | Variational inference | 93 | | | Lagrange duality | |
| 22 | More variational inference | 95 | | | A.3.1 Primal form | |
| 44 | Wiore variational inference | 93 | | | A.3.2 Dual form | 110 |
| 23 | Monte Carlo inference | 97 | | A.4 | Newton's method | 110 |
| | | | | A.5 | Quasi-Newton method | 110 |
| 24 | Markov chain Monte Carlo (MCMC)inference | 99 | | | A.5.1 DFP | 110 |
| | 24.1 Introduction | 99 | | | A.5.2 BFGS | 110 |
| | 24.2 Metropolis Hastings algorithm | 99 | | | A.5.3 Broyden | |
| | 24.3 Gibbs sampling | 99 | | | • | |
| | 24.4 Speed and accuracy of MCMC | 99 | Glo | ssary . | | 111 |
| | | | | | | |

List of Contributors

Wei Zhang

PhD candidate at the Institute of Software, Chinese Academy of Sciences (ISCAS), Beijing, P.R.CHINA, e-mail: zh3feng@gmail.com, has written chapters of Naive Bayes and SVM.

Fei Pan

Master at Beijing University of Technology, Beijing, P.R.CHINA, e-mail: example@gmail.com, has written chapters of KMeans, AdaBoost.

Yong Li

PhD candidate at the Institute of Automation of the Chinese Academy of Sciences (CASIA), Beijing, P.R.CHINA, e-mail: liyong3forever@gmail.com, has written chapters of Logistic Regression.

Jiankou Li

PhD candidate at the Institute of Software, Chinese Academy of Sciences (ISCAS), Beijing, P.R.CHINA, e-mail: lijiankoucoco@163.com, has written chapters of BayesNet.