Machine Learning: A Probabilistic Perspective

Machine Learning A Probabilistic Perspective

Kevin P. Murphy

The MIT Press Cambridge, Massachusetts London, England

© 2012 Massachusetts Institute of Technology

All rights reserved. No part of this book may be reproduced in any form by any electronic or mechanical means (including photocopying, recording, or information storage and retrieval) without permission in writing from the publisher.

For information about special quantity discounts, please email special_sales@mitpress.mit.edu

This book was set in the $\mathbb{M}_{E\!X}$ programming language by the author. Printed and bound in the United States of America.

Library of Congress Cataloging-in-Publication Information

Murphy, Kevin P.
Machine learning : a probabilistic perspective / Kevin P. Murphy.
p. cm. — (Adaptive computation and machine learning series)
Includes bibliographical references and index.
ISBN 978-0-262-01802-9 (hardcover : alk. paper)
1. Machine learning. 2. Probabilities. I. Title.
Q325.5.M87 2012
006.3'1—dc23
2012004558

10 9 8 7 6 5 4 3 2 1

This book is dedicated to Alessandro, Michael and Stefano, and to the memory of Gerard Joseph Murphy.

Contents

1 Introduction

2

1

1.1	Machine	learning: what and why? 1
	1.1.1	Types of machine learning 2
1.2	Supervis	ed learning 2
	1.2.1	Classification 3
	1.2.2	Regression 8
1.3	Unsuper	vised learning 9
	1.3.1	Discovering clusters 10
	1.3.2	Discovering latent factors 11
	1.3.3	Discovering graph structure 12
	1.3.4	Matrix completion 13
1.4	Some ba	sic concepts in machine learning 15
	1.4.1	Parametric vs non-parametric models 15
	1.4.2	A simple non-parametric classifier: K-nearest neighbors
	1.4.3	The curse of dimensionality 17
	1.4.4	Parametric models for classification and regression 18
	1.4.5	Linear regression 19
	1.4.6	Logistic regression 20
	1.4.7	Overfitting 22
	1.4.8	Model selection 22
	1.4.9	No free lunch theorem 24
Proba	ıbility	25
2.1	Introduc	tion 25
2.2	A brief r	eview of probability theory 26
	2.2.1	Discrete random variables 26
	2.2.2	Fundamental rules 26
	2.2.3	Bayes rule 27

16

- 2.2.4 Independence and conditional independence 28
- 2.2.5 Continuous random variables 30
- 2.2.6 Quantiles 31

52

		2.2.7	Mean and variance 31
	2.3	Some co	mmon discrete distributions 32
		2.3.1	The binomial and Bernoulli distributions 32
		2.3.2	The multinomial and multinoulli distributions 33
		2.3.3	The Poisson distribution 35
		2.3.4	The empirical distribution 35
	2.4	Some co	mmon continuous distributions 36
		2.4.1	Gaussian (normal) distribution 36
		2.4.2	Degenerate pdf 37
		2.4.3	The Student t distribution 37
		2.4.4	The Laplace distribution 39
		2.4.5	The gamma distribution 39
		2.4.6	The beta distribution 40
		2.4.7	Pareto distribution 41
	2.5	Joint pro	bability distributions 42
		2.5.1	Covariance and correlation 42
		2.5.2	The multivariate Gaussian 44
		2.5.3	Multivariate Student t distribution 44
		2.5.4	Dirichlet distribution 45
	2.6	Transform	nations of random variables 47
		2.6.1	Linear transformations 47
		2.6.2	General transformations 48
		2.6.3	Central limit theorem 49
	2.7	Monte C	arlo approximation 50
		2.7.1	Example: change of variables, the MC way 51
		2.7.2	Example: estimating π by Monte Carlo integration
		2.7.3	Accuracy of Monte Carlo approximation 52
	2.8	Informat	ion theory 54
		2.8.1	Entropy 54
		2.8.2	KL divergence 55
		2.8.3	Mutual information 57
3	Gonor	ative mo	dels for discrete data 63
Ū	31	Introduct	tion 63
	3.2	Bayesian	concent learning 63
	5.2	3.2.1	Likelihood 65
		322	Prior 65
		323	Posterior 66
		324	Posterior predictive distribution 69
		3.2.5	A more complex prior 70
	3.3	The Beta	-Binomial model 70
		3.3.1	Likelihood 71
		3.3.2	Prior 72
		3.3.3	Posterior 73
		3.3.4	Posterior predictive distribution 75

- 3.4 The Dirichlet-multinomial model 76
 - 3.4.1 Likelihood 77
 - 3.4.2 Prior 77
 - 3.4.3 Posterior 77
 - 3.4.4 Posterior predictive 79
- 3.5 Naive Bayes classifiers 80
 - 3.5.1 Model fitting 81
 - 3.5.2 Using the model for prediction 83
 - 3.5.3 The log-sum-exp trick 84
 - 3.5.4 Feature selection using mutual information 84
 - 3.5.5 Classifying documents using bag of words 85

4 Gaussian models 95

- 4.1 Introduction 95
 - 4.1.1 Notation 95
 - 4.1.2 Basics 95
 - 4.1.3 MLE for an MVN 97
 - 4.1.4 Maximum entropy derivation of the Gaussian * 99
- 4.2 Gaussian Discriminant analysis 99
 - 4.2.1 Quadratic discriminant analysis (QDA) 100
 - 4.2.2 Linear discriminant analysis (LDA) 101
 - 4.2.3 Two-class LDA 102
 - 4.2.4 MLE for discriminant analysis 104
 - 4.2.5 Strategies for preventing overfitting 104
 - 4.2.6 Regularized LDA * 105
 - 4.2.7 Diagonal LDA 106
 - 4.2.8 Nearest shrunken centroids classifier * 107
- 4.3 Inference in jointly Gaussian distributions 108
 - 4.3.1 Statement of the result 109
 - 4.3.2 Examples 109
 - 4.3.3 Information form 113
 - 4.3.4 Proof of the result * 114
- 4.4 Linear Gaussian systems 117
 - 4.4.1 Statement of the result 117
 - 4.4.2 Examples 118
 - 4.4.3 Proof of the result * 122
- 4.5 Digression: The Wishart distribution * 123
 - 4.5.1 Inverse Wishart distribution 124
 - 4.5.2 Visualizing the Wishart distribution * 125
- 4.6 Inferring the parameters of an MVN 125
 - 4.6.1 Posterior distribution of μ 126
 - 4.6.2 Posterior distribution of Σ * 126
 - 4.6.3 Posterior distribution of μ and Σ * 130
 - 4.6.4 Sensor fusion with unknown precisions * 136

5 Bayesian statistics 147

- 5.1 Introduction 147
- 5.2 Summarizing posterior distributions 147
 - 5.2.1 MAP estimation 147
 - 5.2.2 Credible intervals 150
 - 5.2.3 Inference for a difference in proportions 152
- 5.3 Bayesian model selection 154
 - 5.3.1 Bayesian Occam's razor 154
 - 5.3.2 Computing the marginal likelihood (evidence) 156
 - 5.3.3 Bayes factors 161
 - 5.3.4 Jeffreys-Lindley paradox * 162
- 5.4 Priors 163
 - 5.4.1 Uninformative priors 163
 - 5.4.2 Jeffreys priors * 164
 - 5.4.3 Robust priors 166
 - 5.4.4 Mixtures of conjugate priors 166
- 5.5 Hierarchical Bayes 169
 - 5.5.1 Example: modeling related cancer rates 169
- 5.6 Empirical Bayes 170
 - 5.6.1 Example: Beta-Binomial model 171
 - 5.6.2 Example: Gaussian-Gaussian model 171
- 5.7 Bayesian decision theory 174
 - 5.7.1 Bayes estimators for common loss functions 175
 - 5.7.2 The false positive vs false negative tradeoff 178
 - 5.7.3 Other topics * 182

6 Frequentist statistics 189

- 6.1 Introduction 189
- 6.2 Sampling distribution of an estimator 189
 - 6.2.1 Bootstrap 190
 - 6.2.2 Large sample theory for the MLE * 191
- 6.3 Frequentist decision theory 192
 - 6.3.1 Bayes risk 193
 - 6.3.2 Minimax risk 194
 - 6.3.3 Admissible estimators 195
- 6.4 Desirable properties of estimators 198
 - 6.4.1 Consistent estimators 198
 - 6.4.2 Unbiased estimators 198
 - 6.4.3 Minimum variance estimators 199
 - 6.4.4 The bias-variance tradeoff 200
- 6.5 Empirical risk minimization 202
 - 6.5.1 Regularized risk minimization 203
 - 6.5.2 Structural risk minimization 204
 - 6.5.3 Estimating the risk using cross validation 204
 - 6.5.4 Upper bounding the risk using statistical learning theory * 207

- 6.5.5 Surrogate loss functions 208
- 6.6 Pathologies of frequentist statistics * 209
 - 6.6.1 Counter-intuitive behavior of confidence intervals 210
 - p-values considered harmful 211
 - 6.6.3 The likelihood principle 212
 - 6.6.4 Why isn't everyone a Bayesian? 213

7 Linear regression 215

6.6.2

- 7.1 Introduction 215
- 7.2 Model specification 215
- 7.3 Maximum likelihood estimation (least squares) 215
 - 7.3.1 Derivation of the MLE 217
 - 7.3.2 Geometric interpretation 218
 - 7.3.3 Convexity 219
- 7.4 Robust linear regression * 221
- 7.5 Ridge regression 223
 - 7.5.1 Basic idea 223
 - 7.5.2 Numerically stable computation * 225
 - 7.5.3 Connection with PCA * 226
 - 7.5.4 Regularization effects of big data 228

7.6 Bayesian linear regression 229

- 7.6.1 Computing the posterior 230
- 7.6.2 Computing the posterior predictive 231
- 7.6.3 Bayesian inference when σ^2 is unknown * 232
- 7.6.4 EB for linear regression (evidence procedure) 236

8 Logistic regression 243

- 8.1 Introduction 243
- 8.2 Model specification 243
- 8.3 Model fitting 243
 - 8.3.1 MLE 244
 - 8.3.2 Steepest descent 245
 - 8.3.3 Newton's method 247
 - 8.3.4 Iteratively reweighted least squares (IRLS) 248
 - 8.3.5 Quasi-Newton (variable metric) methods 249
 - 8.3.6 ℓ_2 regularization 250
 - 8.3.7 Multi-class logistic regression 250

8.4 Bayesian logistic regression 252

- 8.4.1 Gaussian/ Laplace approximation in general 252
- 8.4.2 Derivation of the BIC 253
- 8.4.3 Gaussian approximation for logistic regression 254
- 8.4.4 Approximating the posterior predictive 255
- 8.4.5 Residual analysis (outlier detection) * 258

8.5 Online learning and stochastic optimization 259

8.5.1 Online learning and regret minimization 259

	8.5.2 8.5.3 8.5.4 8.5.5	Stochastic optimization and risk minimization260The LMS algorithm263The perceptron algorithm263A Bayesian view264
8.6	Generat: 8.6.1 8.6.2 8.6.3	ive vs discriminative classifiers 265 Pros and cons of each approach 265 Dealing with missing data 266 Fisher's linear discriminant analysis (FLDA) * 269
9 Ger	neralized li	near models and the exponential family 277
9.1 9.2	Introduc The exp 9.2.1 9.2.2	ction 277 onential family 277 Definition 278 Examples 278
	9.2.3 9.2.4 9.2.5 9.2.6	Log partition function280MLE for the exponential family282Bayes for the exponential family *283Maximum entropy derivation of the exponential family *285
9.3	Generali 9.3.1 9.3.2 9.3.3	ized linear models (GLMs) 286 Basics 286 ML and MAP estimation 288 Bayesian inference 289
9.4	Probit re 9.4.1 9.4.2 9.4.3 9.4.4	egression 289 ML/ MAP estimation using gradient-based optimization 290 Latent variable interpretation 290 Ordinal probit regression * 291 Multinomial probit models * 291
9.5	Multi-ta 9.5.1 9.5.2 9.5.3 9.5.4 9.5.5	sk learning and mixed effect GLMs * 293 Basic model 293 Example: semi-parametric GLMMs for medical data 294 Example: discrete choice modeling 294 Other kinds of prior 295 Computational issues 295
9.6	Learning 9.6.1 9.6.2 9.6.3 9.6.4	g to rank * 295 The pointwise approach 296 The pairwise approach 297 The listwise approach 297 Loss functions for ranking 298
10 Dii	rected grap	hical models (Bayes nets) 301
10.1	Introduce 10.1.1 10.1.2 10.1.3 10.1.4	ction 301 Chain rule 301 Conditional independence 302 Graphical models 302 Graph terminology 303

		10.1.5	Directed graphical models 304
	10.2	Exampl	es 305
		10.2.1	Naive Bayes classifiers 305
		10.2.2	Markov and hidden Markov models 306
		10.2.3	Medical diagnosis 307
		10.2.4	Genetic linkage analysis * 309
		10.2.5	Directed Gaussian graphical models * 312
	10.3	Inferen	ce 313
	10.4	Learnin	ng 314
		10.4.1	Plate notation 314
		10.4.2	Learning from complete data 316
		10.4.3	Learning with missing and/or latent variables 317
	10.5	Conditi	onal independence properties of DGMs 318
		10.5.1	d-separation and the Bayes Ball algorithm (global Markov
			properties) 318
		10.5.2	Other Markov properties of DGMs 321
		10.5.3	Markov blanket and full conditionals 321
	10.6	Influen	ce (decision) diagrams * 322
11	Mixti	ire mod	els and the FM algorithm 331
11	11 1	Latopt	variable modele 321
	11.1 11.2	Mixture	variable filodels 551
	11.2	11 2 1	Mixtures of Courseigner 333
		11.2.1	Mixture of multinoullic 334
		11.2.2	Using mixture models for clustering 334
		11.2.3	Mixtures of experts 336
	11 3	Parame	ter estimation for mixture models 339
	11.5	1131	Unidentifiability 340
		11.3.2	Computing a MAP estimate is non-convex 341
	11.4	The EN	1 algorithm 342
	1111	11.4.1	Basic idea 343
		11.4.2	EM for GMMs 344
		11.4.3	EM for mixture of experts 351
		11.4.4	EM for DGMs with hidden variables 352
		11.4.5	EM for the Student distribution * 353
		11.4.6	EM for probit regression * 356
		11.4.7	Theoretical basis for EM * 357
		11.4.8	Online EM 359
		11.4.9	Other EM variants * 361
	11.5	Model	selection for latent variable models 363
		11.5.1	Model selection for probabilistic models 364
		11.5.2	Model selection for non-probabilistic methods 364
	11.6	Fitting	models with missing data 366
		11.6.1	EM for the MLE of an MVN with missing data 367

12 Latent linear models 375 12.1 Factor analysis 375 12.1.1 FA is a low rank parameterization of an MVN 375 12.1.2 Inference of the latent factors 376 12.1.3 Unidentifiability 377 12.1.4 Mixtures of factor analysers 379 12.1.5 EM for factor analysis models 380 12.1.6 Fitting FA models with missing data 381 12.2 Principal components analysis (PCA) 381 12.2.1 Classical PCA: statement of the theorem 381 12.2.2 Proof * 383 12.2.3 Singular value decomposition (SVD) 386 12.2.4 Probabilistic PCA 389 12.2.5 EM algorithm for PCA 390 12.3 Choosing the number of latent dimensions 392 12.3.1 Model selection for FA/ PPCA 392 12.3.2 Model selection for PCA 393 12.4 PCA for categorical data 396 12.5 PCA for paired and multi-view data 398 Supervised PCA (latent factor regression) 12.5.1 399 12.5.2 Partial least squares 400 12.5.3 Canonical correlation analysis 401 12.6 Independent Component Analysis (ICA) 401 12.6.1 Maximum likelihood estimation 404 12.6.2 The FastICA algorithm 405 12.6.3 Using EM 408 12.6.4 Other estimation principles * 409 13 Sparse linear models 415 13.1 Introduction 415 13.2 Bayesian variable selection 416 13.2.1 The spike and slab model 418 From the Bernoulli-Gaussian model to ℓ_0 regularization 13.2.2 419 13.2.3 Algorithms 420 13.3 ℓ_1 regularization: basics 423 13.3.1 Why does ℓ_1 regularization yield sparse solutions? 424 13.3.2 Optimality conditions for lasso 425 13.3.3 Comparison of least squares, lasso, ridge and subset selection 429 13.3.4 Regularization path 430 13.3.5 Model selection 433 13.3.6 Bayesian inference for linear models with Laplace priors 434 ℓ_1 regularization: algorithms 13.4 435 13.4.1 Coordinate descent 435 13.4.2 LARS and other homotopy methods 435 13.4.3 Proximal and gradient projection methods 436

- 13.4.4 EM for lasso 441
- 13.5 ℓ_1 regularization: extensions 443
 - 13.5.1 Group Lasso 443
 - 13.5.2 Fused lasso 448
 - 13.5.3 Elastic net (ridge and lasso combined) 449
- 13.6 Non-convex regularizers 451
 - 13.6.1 Bridge regression 452
 - 13.6.2 Hierarchical adaptive lasso 452
 - 13.6.3 Other hierarchical priors 456
- 13.7 Automatic relevance determination (ARD)/ sparse Bayesian learning (SBL) 457
 - 13.7.1 ARD for linear regression 457
 - 13.7.2 Whence sparsity? 459
 - 13.7.3 Connection to MAP estimation 459
 - 13.7.4 Algorithms for ARD * 460
 - 13.7.5 ARD for logistic regression 462
- 13.8 Sparse coding * 462
 - 13.8.1 Learning a sparse coding dictionary 463
 - 13.8.2 Results of dictionary learning from image patches 464
 - 13.8.3 Compressed sensing 466
 - 13.8.4 Image inpainting and denoising 466

14 Kernels 473

- 14.1 Introduction 473
- 14.2 Kernel functions 473
 - 14.2.1 RBF kernels 474
 - 14.2.2 Kernels for comparing documents 474
 - 14.2.3 Mercer (positive definite) kernels 475
 - 14.2.4 Linear kernels 476
 - 14.2.5 Matern kernels 476
 - 14.2.6 String kernels 477
 - 14.2.7 Pyramid match kernels 478
 - 14.2.8 Kernels derived from probabilistic generative models 479
- 14.3 Using kernels inside GLMs 480
 - 14.3.1 Kernel machines 480
 - 14.3.2 LIVMs, RVMs, and other sparse kernel machines 481
- 14.4 The kernel trick 482
 - 14.4.1 Kernelized nearest neighbor classification 483
 - 14.4.2 Kernelized K-medoids clustering 483
 - 14.4.3 Kernelized ridge regression 486
 - 14.4.4 Kernel PCA 487

14.5 Support vector machines (SVMs) 490

- 14.5.1 SVMs for regression 491
- 14.5.2 SVMs for classification 492
- 14.5.3 Choosing C 498
- 14.5.4 Summary of key points 498

545

		14.5.5	A probabilistic interpretation of SVMs 499
	14.6	Compari	son of discriminative kernel methods 499
	14.7	Kernels f	for building generative models 501
		14.7.1	Smoothing kernels 501
		14.7.2	Kernel density estimation (KDE) 502
		14.7.3	From KDE to KNN 504
		14.7.4	Kernel regression 504
		14.7.5	Locally weighted regression 506
15	Gaus	sian nroc	esses 509
10	15.1	Introduc	tion 509
	15.1 15.2	CPs for 1	regression 510
	13.2	15 2 1	Predictions using noise free observations 511
		15.2.1	Predictions using noise observations 512
		15.2.2	Effect of the kernel perameters 513
		15.2.5	Estimating the kernel parameters 515
		15.2.4	Computational and numerical issues * 519
		15.2.5	Computational and numerical issues 510
	15.0	13.2.0	t CI Ma 510
	10.5	GPS mee	Pinewy algorithmation 510
		10.0.1	Multi alage alageifaction 519
		10.0.2	CDa for Daisson regression 522
	15.4	13.3.3 Commont	GPS for Poisson regression 525
	15.4	Connect	Linger we dele service del CDs 526
		15.4.1	Linear models compared to GPS 526
		15.4.2	Linear smoothers compared to GPs 527
		15.4.3	SVMs compared to GPs 528
		15.4.4	LIVM and RVMs compared to GPs 528
		15.4.5	Neural networks compared to GPs 529
		15.4.6	Smootning splines compared to GPS * 530
	15 5	15.4.7	RKHS methods compared to GPs * 532
	15.5	GP laten	t variable model 534
	15.6	Approxir	nation methods for large datasets 536
16	Adap	tive basis	function models 537
	10.1		$\begin{array}{cccc} \text{tion} & 537 \\ \text{comparison} & 520 \\ \text{comparison} & 52$
	16.2		Basis 520
		10.2.1	Dasics 550
		10.2.2	Browing a tree 540
		16.2.3	Pruning a tree 543
		10.2.4	Pros and cons of trees 544
		10.2.5	CADT
	10.0	10.2.0	CART compared to nierarchical mixture of experts *
	16.3	Generali	zed additive models 546
		16.3.1	Backfitting 546

16.3.2 Computational efficiency 547

		16.3.3 Multivariate adaptive regression splines (MARS) 547
	16.4	Boosting 548
		16.4.1 Forward stagewise additive modeling 549
		16.4.2 L2boosting 552
		16.4.3 AdaBoost 552
		16.4.4 LogitBoost 554
		16.4.5 Boosting as functional gradient descent 554
		16.4.6 Sparse boosting 556
		16.4.7 Multivariate adaptive regression trees (MART) 556
		16.4.8 Why does boosting work so well? 557
		16.4.9 A Bayesian view 557
	16.5	Feedforward neural networks (multilayer perceptrons) 558
		16.5.1 Convolutional neural networks 559
		16.5.2 Other kinds of neural networks 562
		16.5.3 A brief history of the field 563
		16.5.4 The backpropagation algorithm 564
		16.5.5 Identifiability 566
		10.5.6 Regularization 566
	16.6	10.5.7 Bayesian inference 570
	10.0	Lisenible learning 574
		16.6.2 Error correcting output codes 575
		16.6.3 Ensemble learning is not equivalent to Bayes model averaging 575
	167	Ensemble rearining is not equivalent to bayes model averaging 575
	10.1	16.7.1 Low-dimensional features 576
		16.7.2 High-dimensional features 577
	16.8	Interpreting black-box models 579
17	Mark	ov and hidden Markov Models 583
	17.1	Introduction 583
	17.2	Markov models 583
		1/.2.1 Transition matrix 583
		17.2.2 Application: Language modeling 585
		17.2.3 Stationary distribution of a Markov chain * 590
	17.0	17.2.4 Application: Google's Pagerank algorithm for web page ranking * 594
	17.3	Hidden Markov models 597
	174	Information in HMMs 600
	17.4	17.41 Trans of information problems for temporal models 600
		17.4.2 The forwards algorithm 603
		17.4.3 The forwards backwards algorithm 604
		17.4.4 The Viterbi algorithm 606
		17.4.5 Forwards filtering, backwards sampling 610
	17.5	Learning for HMMs 611
	11.0	17.5.1 Training with fully observed data 611

- 17.5.2 EM for HMMs (the Baum-Welch algorithm) 612
- 17.5.3 Bayesian methods for "fitting" HMMs * 614
- 17.5.4 Discriminative training 614
- 17.5.5 Model selection 615
- 17.6 Generalizations of HMMs 615
 - 17.6.1 Variable duration (semi-Markov) HMMs 616
 - 17.6.2 Hierarchical HMMs 618
 - 17.6.3 Input-output HMMs 619
 - 17.6.4 Auto-regressive and buried HMMs 620
 - 17.6.5 Factorial HMM 621
 - 17.6.6 Coupled HMM and the influence model 622
 - 17.6.7 Dynamic Bayesian networks (DBNs) 622

18 State space models 625

- 18.1 Introduction 625
- 18.2 Applications of SSMs 626
 - SSMs for object tracking 18.2.1 626
 - 18.2.2 Robotic SLAM 627
 - 18.2.3 Online parameter learning using recursive least squares 630
 - SSM for time series forecasting * 18.2.4 631
- 18.3 Inference in LG-SSM 634
 - 18.3.1 The Kalman filtering algorithm 634
 - 18.3.2 The Kalman smoothing algorithm 637
- Learning for LG-SSM 18.4 640
 - 18.4.1 Identifiability and numerical stability 640
 - 18.4.2 Training with fully observed data 641
 - 18.4.3 EM for LG-SSM
 - 18.4.4 Subspace methods 641
 - Bayesian methods for "fitting" LG-SSMs 18.4.5 641
- Approximate online inference for non-linear, non-Gaussian SSMs 18.5 641

641

- 18.5.1 Extended Kalman filter (EKF) 642
- 18.5.2 Unscented Kalman filter (UKF) 644
- Assumed density filtering (ADF) 18.5.3 646
- 18.6 Hybrid discrete/ continuous SSMs 649
 - 650 18.6.1 Inference
 - Application: Data association and multi target tracking 18.6.2 652
 - 18.6.3 Application: fault diagnosis 653
 - 18.6.4 Application: econometric forecasting 654

19 Undirected graphical models (Markov random fields) 655

- 19.1 Introduction 655
- Conditional independence properties of UGMs 655 19.2
 - 19.2.1 Key properties
 - 655 19.2.2 An undirected alternative to d-separation 657
 - 19.2.3 Comparing directed and undirected graphical models 658

	19.3	Parameterization of MRFs 659
		19.3.1 The Hammersley-Clifford theorem 659
	10.4	19.3.2 Representing potential functions 661
	19.4	Examples of MRFs 662
		13.4.1 Ising model 002
		19.4.3 Potts model 665
		1944 Gaussian MRFs 666
		19.4.5 Markov logic networks * 668
	19.5	Learning 670
		19.5.1 Training maxent models using gradient methods 670
		19.5.2 Training partially observed maxent models 671
		19.5.3 Approximate methods for computing the MLEs of MRFs 672
		19.5.4 Pseudo likelihood 672
		19.5.5 Stochastic Maximum Likelihood 673
		19.5.6 Feature induction for maxent models * 674
		19.5.7 Iterative proportional fitting (IPF) * 675
	19.6	Conditional random fields (CRFs) 678
	10.7	19.6.1 Chain-structured CRFs, MEMMs and the label-bias problem 678
	19.7	Applications of CRFs 680
		19.7.1 Handwinning recognition 600
		19.7.2 Nouri prinase churching 001
		19.7.4 CRFs for protein side-chain prediction 682
		19.7.5 Stereo vision 683
	19.8	CRF training 685
	19.9	Max margin methods for structured output classifiers * 686
20	Exact	inference for graphical models 689
	20.1	Introduction 689
	20.2	Belief propagation for trees 689
		20.2.1 Serial protocol 689
		20.2.2 Parallel protocol 691
		20.2.3 Gaussian BP * 692
	20.2	20.2.4 Other BP variants 694
	20.3	20.3.1 The generalized distributive law * 699
		20.3.2 Computational complexity of VE 699
		20.3.3 A weakness of VE 702
	20.4	The junction tree algorithm * 702
		20.4.1 Creating a junction tree 702
		20.4.2 Message passing on a junction tree 704
		20.4.3 Computational complexity of JTA 707

- 20.4.4 JTA generalizations * 708
- 20.5 Computational intractability of exact inference in the worst case 708

		20.5.1	Approximate inference 709
21	Varia	tional in	ference 713
	21.1	Introduc	tion 713
	21.2	Variation	nal inference 714
		21.2.1	Alternative interpretations of the variational objective 715
		21.2.2	Forward or reverse KL? * 715
	21.3	The mea	in field method 717
		21.3.1	Derivation of the mean field update equations 718
		21.3.2	Example: Mean field for the Ising model 719
	21.4	Structure	ed mean field * 721
		21.4.1	Example: factorial HMM 722
	21.5	Variation	nal Bayes 724
		21.5.1	Example: VB for a univariate Gaussian 724
		21.5.2	Example: VB for linear regression 728
	21.6	Variation	nal Bayes EM 731
		21.6.1	Example: VBEM for mixtures of Gaussians * 732
	21.7	Variation	nal message passing and VIBES 738
	21.8	Local va	riational bounds * 738
		21.8.1	Motivating applications 738
		21.8.2	Bohning's quadratic bound to the log-sum-exp function 740
		21.8.3	Bounds for the sigmoid function 742
		21.8.4	Other bounds and approximations to the log-sum-exp function * 744
		21.8.5	Variational inference based on upper bounds 745
22	More	variation	nal inference 749
	22.1	Introduc	tion 749
	22.2	Loopy be	elief propagation: algorithmic issues 749
		22.2.1	A brief history 749
		22.2.2	LBP on pairwise models 750
		22.2.3	LBP on a factor graph 751
		22.2.4	Convergence 753
		22.2.5	Accuracy of LBP 756
	00.0	22.2.6	Other speedup tricks for BP * 757
	22.3	Loopy be	elief propagation: theoretical issues * 758
		22.3.1	UGMs represented in exponential family form 758
		22.3.2	Exact inference as a variational antimization problem 760
		22.3.3	Exact interence as a variational optimization problem 760
		22.3.4	LBD as a variational optimization problem 761
		22.3.3	Loopy RD vs mean field 765
	22.4	Extensio	ns of boliof propagation * 765
	<i>LL</i> .T	22 4 1	Generalized helief propagation 765
		22.4.2	Convex helief propagation 767
	22.5	Expectat	ion propagation 769
	0	<u>r</u> 00144	I I O

- 22.5.1 EP as a variational inference problem 770
- 22.5.2 Optimizing the EP objective using moment matching 771
- 22.5.3 EP for the clutter problem 773
- 22.5.4 LBP is a special case of EP 774
- 22.5.5 Ranking players using TrueSkill 775
- 22.5.6 Other applications 781
- 22.6 MAP state estimation 781
 - 22.6.1 Linear programming relaxation 781
 - 22.6.2 Max-product belief propagation 782
 - 22.6.3 Graphcuts 783
 - 22.6.4 Experimental comparison of graphcuts and BP 786
 - 22.6.5 Dual decomposition 788

23 Monte Carlo inference 795

- 23.1 Introduction 795
- 23.2 Sampling from standard distributions 795
 - 23.2.1 Using the cdf 795
 - 23.2.2 Sampling from a Gaussian (Box-Muller method) 797
- 23.3 Rejection sampling 797
 - 23.3.1 Basic idea 797
 - 23.3.2 Example 798
 - 23.3.3 Application to Bayesian statistics 799
 - 23.3.4 Adaptive rejection sampling 799
 - 23.3.5 Rejection sampling in high dimensions 800
- 23.4 Importance sampling 800
 - 23.4.1 Basic idea 800
 - 23.4.2 Handling unnormalized distributions 801
 - 23.4.3 Importance sampling for a DGM: Likelihood weighting 802
 - 23.4.4 Sampling importance resampling (SIR) 802
- 23.5 Particle filtering 803
 - 23.5.1 Sequential importance sampling 804
 - 23.5.2 The degeneracy problem 805
 - 23.5.3 The resampling step 805
 - 23.5.4 The proposal distribution 807
 - 23.5.5 Application: Robot localization 808
 - 23.5.6 Application: Visual object tracking 808
 - 23.5.7 Application: time series forecasting 811
- 23.6 Rao-Blackwellised particle filtering (RBPF) 811
 - 23.6.1 RBPF for switching LG-SSMs 811
 - 23.6.2 Application: Tracking a maneuvering target 812
 - 23.6.3 Application: Fast SLAM 814

24 Markov Chain Monte Carlo (MCMC) inference 817

- 24.1 Introduction 817
- 24.2 Gibbs sampling 818

820

		24.2.1	Basic idea 818
		24.2.2	Example: Gibbs sampling for the Ising model 818
		24.2.3	Example: Gibbs sampling for inferring the parameters of a GMM
		24.2.4	Collapsed Gibbs sampling * 821
		24.2.5	Gibbs sampling for hierarchical GLMs 824
		24.2.6	BUGS and IAGS 826
		24.2.7	The Imputation Posterior (IP) algorithm 827
		24.2.8	Blocking Gibbs sampling 827
	24.3	Metropo	lis Hastings algorithm 828
	- 110	24.3.1	Basic idea 828
		24.3.2	Gibbs sampling is a special case of MH 829
		24.3.3	Proposal distributions 830
		24.3.4	Adaptive MCMC 833
		24.3.5	Initialization and mode hopping 834
		24.3.6	Why MH works * 834
		24.3.7	Reversible jump (trans-dimensional) MCMC * 835
	24.4	Speed ar	nd accuracy of MCMC 836
		24.4.1	The burn-in phase 836
		24.4.2	Mixing rates of Markov chains * 837
		24.4.3	Practical convergence diagnostics 838
		24.4.4	Accuracy of MCMC 840
		24.4.5	How many chains? 842
	24.5	Auxiliary	variable MCMC * 843
		24.5.1	Auxiliary variable sampling for logistic regression 843
		24.5.2	Slice sampling 844
		24.5.3	Swendsen Wang 846
		24.5.4	Hybrid/ Hamiltonian MCMC * 848
	24.6	Annealin	g methods 848
		24.6.1	Simulated annealing 849
		24.6.2	Annealed importance sampling 851
	047	24.6.3	Parallel tempering 851
	24.7	Approxim	The send data worth ad
		24.7.1	Harmonia maan astimata 952
		24.1.2	Annoaled importance compliag 952
		24.7.3	Annealeu Importance sampling 655
25	Cluste	ering	855
	25.1	Introduc	tion 855
		25.1.1	Measuring (dis)similarity 855
		25.1.2	Evaluating the output of clustering methods * 856
	25.2	Dirichlet	process mixture models 859
		25.2.1	From finite to infinite mixture models 859
		25.2.2	The Dirichlet process 862
		25.2.3	Applying Dirichlet processes to mixture modeling 865
		25.2.4	Fitting a DP mixture model 866

	25.3	Affinity propagation 867
	25.4	Spectral clustering 870
		25.4.1 Graph Laplacian 871
		25.4.2 Normalized graph Laplacian 872
		25.4.3 Example 873
	25.5	Hierarchical clustering 873
		25.5.1 Agglomerative clustering 875
		25.5.2 Divisive clustering 878
		25.5.3 Choosing the number of clusters 879
		25.5.4 Bayesian hierarchical clustering 879
	25.6	Clustering datapoints and features 881
		25.6.1 Biclustering 883
		25.6.2 Multi-view clustering 883
26	Graph	ical model structure learning 887
	26.1	Introduction 887
	26.2	Quick and dirty ways to learn graph structure 888
		26.2.1 Relevance networks 888
		26.2.2 Dependency networks 889
	26.3	Learning tree structures 890
		26.3.1 Directed or undirected tree? 891
		26.3.2 Chow-Liu algorithm for finding the ML tree structure 892
		26.3.3 Finding the MAP forest 892
	26.4	Learning DAC structures 894
	20.4	26.4.1 Evact structural inference 894
		26.4.2 Scaling up to larger graphs 900
	26.5	Learning DAG structure with latent variables 902
	20.0	26.5.1 Approximating the marginal likelihood when we have missing data 902
		26.5.2 Structural EM 905
		26.5.3 Discovering hidden variables 905
		26.5.4 Case study: Google's Rephil 908
		26.5.5 Structural equation models * 909
	26.6	Learning causal DAGs 911
		26.6.1 Causal interpretation of DAGs 911
		26.6.2 Using causal DAGs to resolve Simpson's paradox 912
		26.6.3 Learning causal DAG structures 915
	26.7	Learning undirected Gaussian graphical models 918
		26.7.1 MLE for a GRF 918
		26.7.2 Graphical lasso 919
		26.7.3 Bayesian interence for GRF structure 921
	00.0	26.7.4 Handling non-Gaussian data * 923
	26.8	Learning undirected discrete graphical models 923
		26.8.2 This imposes of MKFs/ UKFs 923
		20.0.2 I HIII JUNCTION TREES 924

27	Laten	t variable models for discrete data 927
	27.1	Introduction 927
	27.2	Distributed state LVMs for discrete data 928
		27.2.1 Mixture models 928
		27.2.2 Exponential family PCA 929
		27.2.3 LDA and mPCA 930
		27.2.4 GaP model and non-negative matrix factorization 931
	27.3	Latent Dirichlet allocation (LDA) 932
		27.3.1 Basics 932
		27.3.2 Unsupervised discovery of topics 935
		27.3.3 Quantitatively evaluating LDA as a language model 935
		27.3.4 Fitting using (collapsed) Gibbs sampling 937
		27.3.5 Example 938
		27.3.6 Fitting using batch variational inference 939
		27.3.7 Fitting using online variational inference 941
		27.3.8 Determining the number of topics 942
	27.4	Extensions of LDA 943
		27.4.1 Correlated topic model 943
		27.4.2 Dynamic topic model 944
		27.4.3 LDA-HMM 945
		27.4.4 Supervised LDA 949
	27.5	LVMs for graph-structured data 952
		27.5.1 Stochastic block model 953
		27.5.2 Mixed membership stochastic block model 955
	07.0	27.5.3 Relational topic model 956
	27.6	LVIVIS FOR relational data 957
		27.6.1 Infinite relational model 956
	27.7	27.0.2 Probabilistic matrix factorization for conaborative intering 501 Postricted Boltzmann machines (DBMs) 965
	21.1	27.7.1 Variation of RRMs 967
		2772 Learning RBMs 969
		27.7.3 Applications of RBMs 973
28	Deep	learning 977
	28.1	Introduction 977
	28.2	Deep generative models 978
		28.2.1 Deep sigmoid networks 978
		28.2.2 Deep Boltzmann machines 979
		28.2.3 Deep belief networks 980
	28.3	Training deep networks 981
		28.3.1 Greedy layer-wise learning of DBNs 981
		28.3.2 Fitting deep neural nets 983
		28.3.5 Fitting deep auto-encoders 983
	20.4	20.3.4 Stacked denoising auto-encoders 984
	2ŏ.4	Applications of deep networks 984

- 28.4.1Handwritten digit classification using DBNs984
- 28.4.2 Data visualization using deep auto-encoders 986
- 28.4.3 Information retrieval using deep autoencoders (semantic hashing) 986
- 28.4.4 Learning audio features using 1d convolutional DBNs 987
- 28.4.5 Learning image features using 2d convolutional DBNs 988
- 28.5 Discussion 989

Bibliography 991

Index to code 1021 Index to keywords 1025

Preface

Introduction

With the ever increasing amounts of data in electronic form, the need for automated methods for data analysis continues to grow. The goal of machine learning is to develop methods that can automatically detect patterns in data, and then to use the uncovered patterns to predict future data or other outcomes of interest. Machine learning is thus closely related to the fields of statistics and data mining, but differs slightly in terms of its emphasis and terminology. This book provides a detailed introduction to the field, and includes worked examples drawn from application domains such as biology, text processing, computer vision, and robotics.

Target audience

This book is suitable for upper-level undergraduate students and beginning graduate students in computer science, statistics, electrical engineering, econometrics, or any one else who has the appropriate mathematical background. Specifically, the reader is assumed to already be familiar with basic multivariate calculus, probability, linear algebra, and computer programming. Prior exposure to statistics is helpful but not necessary.

A probabilistic approach

This books adopts the view that the best way to make machines that can learn from data is to use the tools of probability theory, which has been the mainstay of statistics and engineering for centuries. Probability theory can be applied to any problem involving uncertainty. In machine learning, uncertainty comes in many forms: what is the best prediction (or decision) given some data? what is the best model given some data? what measurement should I perform next? etc.

The systematic application of probabilistic reasoning to all inferential problems, including inferring parameters of statistical models, is sometimes called a Bayesian approach. However, this term tends to elicit very strong reactions (either positive or negative, depending on who you ask), so we prefer the more neutral term "probabilistic approach". Besides, we will often use techniques such as maximum likelihood estimation, which are not Bayesian methods, but certainly fall within the probabilistic paradigm.

Rather than describing a cookbook of different heuristic methods, this book stresses a principled model-based approach to machine learning. For any given model, a variety of algorithms can often be applied. Conversely, any given algorithm can often be applied to a variety of models. This kind of modularity, where we distinguish model from algorithm, is good pedagogy and good engineering.

We will often use the language of graphical models to specify our models in a concise and intuitive way. In addition to aiding comprehension, the graph structure aids in developing efficient algorithms, as we will see. However, this book is not primarily about graphical models; it is about probabilistic modeling in general.

A practical approach

Nearly all of the methods described in this book have been implemented in a MATLAB software package called **PMTK**, which stands for probabilistic modeling toolkit. This is freely available from pmtk3.googlecode.com (the digit 3 refers to the third edition of the toolkit, which is the one used in this version of the book). There are also a variety of supporting files, written by other people, available at pmtksupport.googlecode.com.

MATLAB is a high-level, interactive scripting language ideally suited to numerical computation and data visualization, and can be purchased from www.mathworks.com. (Additional toolboxes, such as the Statistics toolbox, can be purchased, too; we have tried to minimize our dependence on this toolbox, but it is nevertheless very useful to have.) There is also a free version of Matlab called **Octave**, available at http://www.gnu.org/software/octave/, which supports most of the functionality of MATLAB (see the PMTK website for a comparison).

PMTK was used to generate many of the figures in this book; the source code for these figures is included on the PMTK website, allowing the reader to easily see the effects of changing the data or algorithm or parameter settings. The book refers to files by name, e.g., naiveBayesFit. In order to find the corresponding file, you can use two methods: within Matlab you can type which naiveBayesFit and it will return the full path to the file; or, if you do not have Matlab but want to read the source code anyway, you can use your favorite search engine, which should return the corresponding file from the pmtk3.googlecode.com website.

Details on *how to use* PMTK can be found on the PMTK website, which will be udpated over time. Details on the *underlying theory* behind these methods can be found in this book.

Acknowledgments

A book this large is obviously a team effort. I would especially like to thank the following people: my wife Margaret, for keeping the home fires burning as I toiled away in my office for the last six years; Matt Dunham, who created many of the figures in this book, and who wrote much of the code in PMTK; Baback Moghaddam, who gave extremely detailed feedback on every page of an earlier draft of the book; Chris Williams, who also gave very detailed feedback; Cody Severinski and Wei-Lwun Lu, who assisted with figures; generations of UBC students, who gave helpful comments on earlier drafts; Daphne Koller, Nir Friedman, and Chris Manning, for letting me use their latex style files; Stanford University, Google Research and Skyline College for hosting me during part of my sabbatical; and various Canadian funding agencies (NSERC, CRC and CIFAR) who have supported me financially over the years.

In addition, I would like to thank the following people for giving me helpful feedback on parts of the book, and/or for sharing figures, code, exercises or even (in some cases) text: David Blei,

Preface

Hannes Bretschneider, Greg Corrado, Arnaud Doucet, Mario Figueiredo, Nando de Freitas, Mark Girolami, Gabriel Goh, Tom Griffiths, Katherine Heller, Geoff Hinton, Aapo Hyvarinen, Tommi Jaakkola, Mike Jordan, Charles Kemp, Emtiyaz Khan, Bonnie Kirkpatrick, Daphne Koller, Zico Kolter, Honglak Lee, Julien Mairal, Tom Minka, Ian Nabney, Arthur Pope, Carl Rassmussen, Ryan Rifkin, Ruslan Salakhutdinov, Mark Schmidt, David Sontag, Erik Sudderth, Josh Tenenbaum, Kai Yu, Martin Wainwright, Yair Weiss.

Kevin Murphy Palo Alto, California March 2012