Contents

Pr	eface	xxvii	
1	Intro	duction	1
	1.1	Machine	learning: what and why?
		1.1.1	Types of machine learning 2
	1.2	Supervis	ed learning 3
		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 13
		1.3.4	Matrix completion 14
	1.4	Some ba	sic concepts in machine learning 16
		1.4.1	Parametric vs non-parametric models 16
		1.4.2	A simple non-parametric classifier: K -nearest neighbors 16
		1.4.3	The curse of dimensionality 18
		1.4.4	Parametric models for classification and regression 19
		1.4.5	Linear regression 19
		1.4.6	Logistic regression 21
		1.4.7	Overfitting 22
		1.4.8	Model selection 22
		1.4.9	No free lunch theorem 24
2	Probe	ability	27
	2.1	Introduc	tion 27
	2.2	A brief r	eview of probability theory 28
		2.2.1	Discrete random variables 28
		2.2.2	Fundamental rules 28
		2.2.3	Bayes rule 29
		2.2.4	Independence and conditional independence 30
		2.2.5	Continuous random variables 32

viii CONTENTS

	2.2.6	Quantiles 33
	2.2.7	Mean and variance 33
2.3	Some o	common discrete distributions 34
	2.3.1	The binomial and Bernoulli distributions 34
	2.3.2	The multinomial and multinoulli distributions 35
	2.3.3	The Poisson distribution 37
	2.3.4	The empirical distribution 37
2.4	Some of	common continuous distributions 38
	2.4.1	Gaussian (normal) distribution 38
	2.4.2	Degenerate pdf 39
	2.4.3	The Laplace distribution 41
	2.4.4	The gamma distribution 41
	2.4.5	The beta distribution 42
	2.4.6	Pareto distribution 43
2.5	-	robability distributions 44
	2.5.1	Covariance and correlation 44
	2.5.2	
	2.5.3	
	2.5.4	Dirichlet distribution 47
2.6		rmations of random variables 49
	2.6.1	Zarreur trumstormunomo 10
	2.6.2	General transformations 50
	2.6.3	Central limit theorem 51
2.7		Carlo approximation 52
	2.7.1	Example: change of variables, the MC way 53
	2.7.2	Example: estimating π by Monte Carlo integration 54
	2.7.3	Accuracy of Monte Carlo approximation 54
2.8		ation theory 56
	2.8.1	Entropy 56
	2.8.2	KL divergence 57
	2.8.3	Mutual information 59
Gene	rative m	odels for discrete data 65
3.1	Introdu	action 65
3.2	Bayesia	n concept learning 65
	3.2.1	Likelihood 67
	3.2.2	Prior 67
	3.2.3	Posterior 68
	3.2.4	Posterior predictive distribution 71
	3.2.5	A more complex prior 72
3.3	The be	ta-binomial model 72
	3.3.1	Likelihood 73
	3.3.2	Prior 74
	3.3.3	Posterior 75
	3.3.4	Posterior predictive distribution 77

3

	3.4	The Diri	chlet-multinomial model 78
		3.4.1	Likelihood 79
		3.4.2	Prior 79
		3.4.3	Posterior 79
		3.4.4	Posterior predictive 81
	3.5	Naive Ba	ayes classifiers 82
		3.5.1	Model fitting 83
		3.5.2	Using the model for prediction 85
		3.5.3	The log-sum-exp trick 86
		3.5.4	Feature selection using mutual information 86
		3.5.5	Classifying documents using bag of words 87
4	Gaus	sian moa	lels 97
	4.1	Introduc	etion 97
	1.1	4.1.1	Notation 97
		4.1.2	
		4.1.3	
		4.1.4	Maximum entropy derivation of the Gaussian * 101
	4.2		discriminant analysis 101
	4.2	4.2.1	Quadratic discriminant analysis (QDA) 102
		4.2.2	Linear discriminant analysis (LDA) 102
		4.2.3	Two-class LDA 104
		4.2.4	MLE for discriminant analysis 106
		4.2.4	· ·
		4.2.5	Strategies for preventing overfitting 106 Regularized LDA * 107
		4.2.7	Diagonal LDA 108
		4.2.7	Nearest shrunken centroids classifier * 109
	4.3		e in jointly Gaussian distributions 110
	4.3	4.3.1	Statement of the result 111
		4.3.2	Examples 111
		4.3.3	Information form 115
		4.3.4	Proof of the result * 116
	4.4		Gaussian systems 119
	4.4	4.4.1	Statement of the result 119
		4.4.1	Examples 120
		4.4.3	Proof of the result * 124
	4.5		on: The Wishart distribution * 125
	4.5		
		4.5.1 4.5.2	
	4 G		0
	4.6		g the parameters of an MVN 127
		4.6.1	Posterior distribution of μ 128
		4.6.2	Posterior distribution of Σ^* 128
		4.6.3	Posterior distribution of μ and Σ^* 132
		4.6.4	Sensor fusion with unknown precisions * 138

X CONTENTS

Вауе	esian statistic	s 149
5.1	Introduction	n 149
5.2	Summarizin	ng posterior distributions 149
	5.2.1 M.	AP estimation 149
	5.2.2 Cr	redible intervals 152
	5.2.3 In:	ference for a difference in proportions 154
5.3	Bayesian mo	odel selection 155
		yesian Occam's razor 156
	5.3.2 Co	omputing the marginal likelihood (evidence) 158
		yes factors 163
		ffreys-Lindley paradox * 164
5.4		65
		ninformative priors 165
		ffreys priors * 166
		bust priors 168
		ixtures of conjugate priors 168
5.5	Hierarchical	·
		cample: modeling related cancer rates 171
5.6	Empirical Ba	
		tample: beta-binomial model 173
		tample: Gaussian-Gaussian model 173
5.7	-	ecision theory 176
		syes estimators for common loss functions 177
		ne false positive vs false negative tradeoff 180
	5.7.3 Ot	ther topics * 184
Freq	uentist statisi	tics 191
6.1	Introduction	n 191
6.2	Sampling di	istribution of an estimator 191
	6.2.1 Bo	potstrap 192
		arge sample theory for the MLE * 193
6.3	-	decision theory 194
		yes risk 195
		inimax risk 196
		lmissible estimators 197
6.4	-	roperties of estimators 200
		onsistent estimators 200
		abiased estimators 200
		inimum variance estimators 201
0.5		ne bias-variance tradeoff 202
6.5		sk minimization 204
		egularized risk minimization 205
		ructural risk minimization 206
		timating the risk using cross validation 206
	6.5.4 Up	oper bounding the risk using statistical learning theory * 209

CONTENTS xi

		6.5.5 Surrogate loss functions 210
	6.6	Pathologies of frequentist statistics * 211
		6.6.1 Counter-intuitive behavior of confidence intervals 212
		6.6.2 p-values considered harmful 213
		6.6.3 The likelihood principle 214
		6.6.4 Why isn't everyone a Bayesian? 215
7	Linea	r regression 217
	7.1	Introduction 217
	7.2	Model specification 217
	7.3	Maximum likelihood estimation (least squares) 217
		7.3.1 Derivation of the MLE 219
		7.3.2 Geometric interpretation 220
		7.3.3 Convexity 221
	7.4	Robust linear regression * 223
	7.5	Ridge regression 225
		7.5.1 Basic idea 225
		7.5.2 Numerically stable computation * 227
		7.5.3 Connection with PCA * 228
		7.5.4 Regularization effects of big data 230
	7.6	Bayesian linear regression 231
		7.6.1 Computing the posterior 232
		7.6.2 Computing the posterior predictive 233
		7.6.3 Bayesian inference when σ^2 is unknown * 234
		7.6.4 EB for linear regression (evidence procedure) 238
8	Logis	tic regression 245
	8.1	Introduction 245
	8.2	Model specification 245
	8.3	Model fitting 245
		8.3.1 MLE 246
		8.3.2 Steepest descent 247
		8.3.3 Newton's method 249
		8.3.4 Iteratively reweighted least squares (IRLS) 250
		8.3.5 Quasi-Newton (variable metric) methods 251
		8.3.6 ℓ_2 regularization 252
		8.3.7 Multi-class logistic regression 252
	8.4	Bayesian logistic regression 254
		8.4.1 Laplace approximation 255
		8.4.2 Derivation of the BIC 255
		8.4.3 Gaussian approximation for logistic regression 256
		8.4.4 Approximating the posterior predictive 256
		8.4.5 Residual analysis (outlier detection) * 260
	8.5	Online learning and stochastic optimization 261
		8.5.1 Online learning and regret minimization 262

xii CONTENTS

		8.5.3	Stochastic optimization and risk minimization 262 The LMS algorithm 264 The perceptron algorithm 265
			A Bayesian view 266
	8.6		e vs discriminative classifiers 267
	0.0		Pros and cons of each approach 268
			Dealing with missing data 269
			Fisher's linear discriminant analysis (FLDA) * 271
9	Gene		ear models and the exponential family 281
	9.1	Introducti	
	9.2	minounce	nential family 281
	0.2		Definition 282
			Examples 282
			Log partition function 284
			MLE for the exponential family 286
			Bayes for the exponential family * 287
			Maximum entropy derivation of the exponential family * 289
	9.3		ed linear models (GLMs) 290
			Basics 290
		9.3.2	ML and MAP estimation 292
		9.3.3	Bayesian inference 293
	9.4	Probit reg	ression 293
		9.4.1	ML/MAP estimation using gradient-based optimization 294
		9.4.2	Latent variable interpretation 294
		9.4.3	Ordinal probit regression * 295
		9.4.4	Multinomial probit models * 295
	9.5	Multi-task	9
			Hierarchical Bayes for multi-task learning 296
			Application to personalized email spam filtering 296
			Application to domain adaptation 297
			Other kinds of prior 297
	9.6		ed linear mixed models * 298
			Example: semi-parametric GLMMs for medical data 298
			Computational issues 300
	9.7	Learning	
			The pointwise approach 301
			The pairwise approach 301
			The listwise approach 302
			Loss functions for ranking 303
10			ical models (Bayes nets) 307
	10.1	Introducti	
			Chain rule 307
		10.1.2	Conditional independence 308

CONTENTS xiii

	10.1.3	Graphical models 308
	10.1.4	Graph terminology 309
	10.1.5	Directed graphical models 310
10.2	Exampl	es 311
	10.2.1	Naive Bayes classifiers 311
	10.2.2	Markov and hidden Markov models 312
	10.2.3	Medical diagnosis 313
	10.2.4	Genetic linkage analysis * 315
	10.2.5	Directed Gaussian graphical models * 318
10.3	Inferen	ce 319
10.4	Learnin	ng 320
	10.4.1	Plate notation 320
	10.4.2	Learning from complete data 322
	10.4.3	Learning with missing and/or latent variables 323
10.5	Conditi	onal independence properties of DGMs 324
	10.5.1	d-separation and the Bayes Ball algorithm (global Markov
		properties) 324
	10.5.2	Other Markov properties of DGMs 327
	10.5.3	Markov blanket and full conditionals 327
10.6	Influen	ce (decision) diagrams * 328
Mixt	ure mod	els and the EM algorithm 337
11.1	Latent	variable models 337
11.2	Mixture	e models 337
	11.2.1	Mixtures of Gaussians 339
	11.2.2	Mixture of multinoullis 340
	11.2.3	
	11.2.4	Mixtures of experts 342
11.3	Parame	ter estimation for mixture models 345
	11.3.1	Unidentifiability 346
	11.3.2	Computing a MAP estimate is non-convex 347
11.4	The EM	I algorithm 348
	11.4.1	Basic idea 349
	11.4.2	EM for GMMs 350
	11.4.3	1
	11.4.4	
	11.4.5	EM for the Student distribution * 359
	11.4.6	EM for probit regression * 362
	11.4.7	Theoretical basis for EM * 363
	11.4.8	Online EM 365
	11.4.9	Other EM variants * 367
11.5		selection for latent variable models 370
	11.5.1	Model selection for probabilistic models 370
	11.5.2	Model selection for non-probabilistic methods 370
11.6	Fitting	models with missing data 372

11

xiv CONTENTS

		11.6.1	EM for the MLE of an MVN with missing data 373
12	Laten	t linear 1	nodels 381
	12.1	Factor ar	nalysis 381
		12.1.1	FA is a low rank parameterization of an MVN 381
		12.1.2	Inference of the latent factors 382
		12.1.3	Unidentifiability 383
		12.1.4	Mixtures of factor analysers 385
		12.1.5	EM for factor analysis models 386
		12.1.6	Fitting FA models with missing data 387
	12.2	_	components analysis (PCA) 387
		12.2.1	Classical PCA: statement of the theorem 387
		12.2.2	Proof * 389
		12.2.3	•
		12.2.4	Probabilistic PCA 395
	10.0	12.2.5	EM algorithm for PCA 396
	12.3		g the number of latent dimensions 398
		12.3.1	Model selection for FA/PPCA 398
	10.4	12.3.2	Model selection for PCA 399
	12.4 12.5		categorical data 402 paired and multi-view data 404
	12.3	12.5.1	paired and multi-view data 404 Supervised PCA (latent factor regression) 405
		12.5.1	Partial least squares 406
		12.5.2	Canonical correlation analysis 407
	12.6		dent Component Analysis (ICA) 407
	12.0	12.6.1	Maximum likelihood estimation 410
		12.6.2	The FastICA algorithm 411
		12.6.3	Using EM 414
		12.6.4	Other estimation principles * 415
13	Snars	e linear 1	models 421
10	13.1	Introduc	
	13.2		variable selection 422
		13.2.1	The spike and slab model 424
		13.2.2	From the Bernoulli-Gaussian model to ℓ_0 regularization 425
		13.2.3	Algorithms 426
	13.3	ℓ_1 regula	arization: basics 429
		13.3.1	Why does ℓ_1 regularization yield sparse solutions? 430
		13.3.2	Optimality conditions for lasso 431
		13.3.3	Comparison of least squares, lasso, ridge and subset selection 435
		13.3.4	Regularization path 436
		13.3.5	Model selection 439
		13.3.6	Bayesian inference for linear models with Laplace priors 440
	13.4	_	arization: algorithms 441
		13.4.1	Coordinate descent 441

		13.4.2	LARS and other homotopy methods 441
		13.4.3	Proximal and gradient projection methods 442
		13.4.4	EM for lasso 447
	13.5	ℓ_1 regula	arization: extensions 449
		13.5.1	
		13.5.2	Fused lasso 454
		13.5.3	
	13.6	Non-con	vex regularizers 457
		13.6.1	Bridge regression 458
		13.6.2	Hierarchical adaptive lasso 458
		13.6.3	Other hierarchical priors 462
	13.7	Automat	ic relevance determination (ARD)/sparse Bayesian learning (SBL) 463
		13.7.1	ARD for linear regression 463
		13.7.2	Whence sparsity? 465
		13.7.3	Connection to MAP estimation 465
		13.7.4	Algorithms for ARD * 466
		13.7.5	ARD for logistic regression 468
	13.8	Sparse c	oding * 468
		13.8.1	Learning a sparse coding dictionary 469
		13.8.2	Results of dictionary learning from image patches 470
		13.8.3	Compressed sensing 472
		13.8.4	Image inpainting and denoising 472
		10.0.1	mage inputiting and deficiently
14	Kerne		79
14		els 4	79
14	14.1	els 47	79 ttion 479
14		e ls 4 Introduc Kernel fu	79 tion 479 unctions 479
14	14.1	Introduc Kernel fu 14.2.1	79 etion 479 unctions 479 RBF kernels 480
14	14.1	Introduc Kernel fu 14.2.1 14.2.2	79 etion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480
14	14.1	Introduc Kernel fu 14.2.1 14.2.2 14.2.3	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481
14	14.1	Introduc Kernel fo 14.2.1 14.2.2 14.2.3 14.2.4	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482
14	14.1	Introduc Kernel ft 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482
14	14.1	Introduct Kernel ft 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483
14	14.1	Introduct Kernel fu 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484
14	14.1	Introduct Kernel fu 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485
14	14.1 14.2	Introduct Kernel fu 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485
14	14.1 14.2	Introduct Kernel for 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8 Using ke	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485 ernels inside GLMs 486
14	14.1 14.2	Introduct Kernel for 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8 Using ke 14.3.1	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485 ernels inside GLMs 486 Kernel machines 486 LIVMs, RVMs, and other sparse vector machines 487
14	14.1 14.2	Introduct Kernel fr 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8 Using ke 14.3.1 14.3.2	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485 ernels inside GLMs 486 Kernel machines 486 LIVMs, RVMs, and other sparse vector machines 487
14	14.1 14.2	Introduct Kernel fu 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8 Using ke 14.3.1 14.3.2 The kern	rtion 479 cunctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485 ernels inside GLMs 486 Kernel machines 486 L1VMs, RVMs, and other sparse vector machines 487 nel trick 488
14	14.1 14.2	Introduct Kernel fu 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8 Using ke 14.3.1 14.3.2 The kern 14.4.1	rtion 479 cunctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485 ernels inside GLMs 486 Kernel machines 486 L1VMs, RVMs, and other sparse vector machines 487 nel trick 488 Kernelized nearest neighbor classification 489
14	14.1 14.2	Introduct Kernel for 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8 Using ker 14.3.1 14.3.2 The kerr 14.4.1 14.4.2	rtion 479 cunctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485 ernels inside GLMs 486 Kernel machines 486 LIVMs, RVMs, and other sparse vector machines 487 nel trick 488 Kernelized nearest neighbor classification 489 Kernelized K-medoids clustering 489
14	14.1 14.2	Introduct Kernel ft 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8 Using ke 14.3.1 14.3.2 The kern 14.4.1 14.4.2 14.4.3 14.4.4	rtion 479 unctions 479 RBF kernels 480 Kernels for comparing documents 480 Mercer (positive definite) kernels 481 Linear kernels 482 Matern kernels 482 String kernels 483 Pyramid match kernels 484 Kernels derived from probabilistic generative models 485 ernels inside GLMs 486 Kernel machines 486 LIVMs, RVMs, and other sparse vector machines 487 nel trick 488 Kernelized nearest neighbor classification 489 Kernelized K-medoids clustering 489 Kernelized ridge regression 492
14	14.1 14.2	Introduct Kernel ft 14.2.1 14.2.2 14.2.3 14.2.4 14.2.5 14.2.6 14.2.7 14.2.8 Using ke 14.3.1 14.3.2 The kern 14.4.1 14.4.2 14.4.3 14.4.4	rtion 479 Interior 480 Interior 480 Interior 481 Interior 482 Interior 483 Interior 483 Interior 484 Interior 483 Interior 484 Interior 486 Interior 486 Interior 486 Interior 486 Interior 488 Interior

xvi CONTENTS

		14.5.3 14.5.4	Choosing C 504 Summary of key points 504	
		14.5.5	A probabilistic interpretation of SVMs 505	
	14.6	Compari	ison of discriminative kernel methods 505	
	14.7	Kernels	for building generative models 507	
		14.7.1	Smoothing kernels 507	
		14.7.2	Kernel density estimation (KDE) 508	
		14.7.3	From KDE to KNN 509	
		14.7.4	Kernel regression 510	
		14.7.5	Locally weighted regression 512	
15		sian proc		
	15.1	Introduc		
	15.2		regression 516	
		15.2.1	Predictions using noise-free observations 517	
		15.2.2	Predictions using noisy observations 518	
		15.2.3	Effect of the kernel parameters 519	
		15.2.4	Estimating the kernel parameters 521	
		15.2.5	Computational and numerical issues * 524	
	15.0	15.2.6	Semi-parametric GPs * 524	
	15.3	GPs mee		
		15.3.1	Binary classification 525	
		15.3.2	Multi-class classification 528	
	15 /	15.3.3	GPs for Poisson regression 531	
	15.4		ion with other methods 532	
		15.4.1 15.4.2	Linear models compared to GPs 532 Linear smoothers compared to GPs 533	
		15.4.2	Linear smoothers compared to GPs 533 SVMs compared to GPs 534	
		15.4.4	LIVM and RVMs compared to GPs 534	
		15.4.5	Neural networks compared to GPs 535	
		15.4.6	Smoothing splines compared to GPs * 536	
		15.4.7	RKHS methods compared to GPs * 538	
	15.5		t variable model 540	
	15.6		nation methods for large datasets 542	
16	Adap	tive basis	s function models 543	
	16.1	Introduc	tion 543	
	16.2	Classific	ation and regression trees (CART) 544	
		16.2.1	Basics 544	
		16.2.2	Growing a tree 545	
		16.2.3	Pruning a tree 549	
		16.2.4	Pros and cons of trees 550	
		16.2.5	Random forests 550	
		16.2.6	CART compared to hierarchical mixture of experts *	55]
	16.3	Generali	zed additive models 552	

CONTENTS xvii

		16.3.1	Backfitting 552
		16.3.2	Computational efficiency 553
		16.3.3	Multivariate adaptive regression splines (MARS) 553
	16.4	Boosting	
		16.4.1	Forward stagewise additive modeling 555
		16.4.2	L2boosting 557
		16.4.3	AdaBoost 558
		16.4.4	LogitBoost 559
		16.4.5	Boosting as functional gradient descent 560
		16.4.6	Sparse boosting 561
		16.4.7	Multivariate adaptive regression trees (MART) 562
		16.4.8	Why does boosting work so well? 562
		16.4.9	A Bayesian view 563
	16.5	Feedforv	vard neural networks (multilayer perceptrons) 563
		16.5.1	Convolutional neural networks 564
		16.5.2	Other kinds of neural networks 568
		16.5.3	A brief history of the field 568
		16.5.4	The backpropagation algorithm 569
		16.5.5	Identifiability 572
		16.5.6	Regularization 572
		16.5.7	Bayesian inference * 576
	16.6		e learning 580
		16.6.1	Stacking 580
		16.6.2	Error-correcting output codes 581
		16.6.3	Ensemble learning is not equivalent to Bayes model averaging 581
	16.7	-	ental comparison 582
		16.7.1	Low-dimensional features 582
	10.0	16.7.2	High-dimensional features 583
	16.8	Interpret	ing black-box models 585
17	Mark	ov and h	idden Markov models 589
	17.1	Introduc	tion 589
	17.2	Markov	models 589
		17.2.1	Transition matrix 589
		17.2.2	Application: Language modeling 591
		17.2.3	Stationary distribution of a Markov chain * 596
		17.2.4	Application: Google's PageRank algorithm for web page ranking * 600
	17.3	Hidden 1	Markov models 603
		17.3.1	Applications of HMMs 604
	17.4		e in HMMs 606
		17.4.1	Types of inference problems for temporal models 606
		17.4.2	The forwards algorithm 609
		17.4.3	The forwards-backwards algorithm 610
		17.4.4	The Viterbi algorithm 612
		17.4.5	Forwards filtering, backwards sampling 616

xviii *CONTENTS*

	17.5	Learning	for HMMs 617	
		17.5.1	Training with fully observed data 617	
		17.5.2	EM for HMMs (the Baum-Welch algorithm) 618	
		17.5.3	Bayesian methods for "fitting" HMMs * 620	
		17.5.4	Discriminative training 620	
		17.5.5	Model selection 621	
	17.6	Generaliz	eations of HMMs 621	
		17.6.1	Variable duration (semi-Markov) HMMs 622	
		17.6.2	Hierarchical HMMs 624	
		17.6.3	Input-output HMMs 625	
		17.6.4	Auto-regressive and buried HMMs 626	
		17.6.5	Factorial HMM 627	
		17.6.6	Coupled HMM and the influence model 628	
		17.6.7	Dynamic Bayesian networks (DBNs) 628	
18	State	space mo	dels 631	
10	18.1	Introduct		
	18.2		ons of SSMs 632	
	10.2	18.2.1	SSMs for object tracking 632	
		18.2.2	Robotic SLAM 633	
		18.2.3	Online parameter learning using recursive least squares 636	
		18.2.4	SSM for time series forecasting * 637	
	18.3		in I.G-SSM 640	
	10.3	18.3.1		
		18.3.2	The Kalman filtering algorithm 640 The Kalman smoothing algorithm 643	
	10 /		8 8	
	18.4	18.4.1		
			Identifiability and numerical stability 646	
		18.4.2	Training with fully observed data 647	
		18.4.3	EM for LG-SSM 647	
		18.4.4	Subspace methods 647	
	10.5	18.4.5	Bayesian methods for "fitting" LG-SSMs 647	
	18.5		nate online inference for non-linear, non-Gaussian SSMs 647	
		18.5.1	Extended Kalman filter (EKF) 648	
		18.5.2	Unscented Kalman filter (UKF) 650	
	10.0	18.5.3	Assumed density filtering (ADF) 652	
	18.6	-	iscrete/continuous SSMs 655	
		18.6.1	Inference 656	
			Application: data association and multi-target tracking 658	
		18.6.3	Application: fault diagnosis 659	
		18.6.4	Application: econometric forecasting 660	
19	Undir	ected gra	phical models (Markov random fields) 661	
	19.1	Introduct	ion 661	
	19.2	Condition	nal independence properties of UGMs 661	
		19.2.1	Key properties 661	

CONTENTS xix

		19.2.2	An undirected alternative to d-separation 663
		19.2.3	Comparing directed and undirected graphical models 664
	19.3	Paramet	erization of MRFs 665
		19.3.1	The Hammersley-Clifford theorem 665
		19.3.2	Representing potential functions 667
	19.4	Example	es of MRFs 668
		19.4.1	Ising model 668
		19.4.2	Hopfield networks 669
		19.4.3	Potts model 671
		19.4.4	Gaussian MRFs 672
		19.4.5	Markov logic networks * 674
	19.5	Learning	
		19.5.1	Training maxent models using gradient methods 676
		19.5.2	Training partially observed maxent models 677
		19.5.3	Approximate methods for computing the MLEs of MRFs 678
		19.5.4	Pseudo likelihood 678
		19.5.5	Stochastic maximum likelihood 679
		19.5.6	Feature induction for maxent models * 680
		19.5.7	Iterative proportional fitting (IPF) * 681
	19.6	Conditio	onal random fields (CRFs) 684
		19.6.1	Chain-structured CRFs, MEMMs and the label-bias problem 684
		19.6.2	Applications of CRFs 686
		19.6.3	CRF training 692
	19.7	Structura	al SVMs 693
		19.7.1	SSVMs: a probabilistic view 693
		19.7.2	SSVMs: a non-probabilistic view 695
		19.7.3	Cutting plane methods for fitting SSVMs 698
		19.7.4	Online algorithms for fitting SSVMs 700
		19.7.5	Latent structural SVMs 701
20	Exact	inferenc	re for graphical models 707
20	20.1	Introduc	
	20.1		ropagation for trees 707
	20.2	20.2.1	Serial protocol 707
		20.2.2	Parallel protocol 709
		20.2.3	Gaussian BP * 710
		20.2.4	Other BP variants * 712
	20.3		able elimination algorithm 714
	20.5	20.3.1	The generalized distributive law * 717
		20.3.2	Computational complexity of VE 717
		20.3.3	A weakness of VE 720
	20.4		ction tree algorithm * 720
	20.1	20.4.1	Creating a junction tree 720
		20.4.2	Message passing on a junction tree 722
		20.4.3	Computational complexity of JTA 725

		20.4.4 JTA generalizations * 726
	20.5	Computational intractability of exact inference in the worst case 726
		20.5.1 Approximate inference 727
21	Varia	tional inference 731
	21.1	Introduction 731
	21.2	Variational inference 732
		21.2.1 Alternative interpretations of the variational objective 733
		21.2.2 Forward or reverse KL? * 733
	21.3	The mean field method 735
		21.3.1 Derivation of the mean field update equations 736
		21.3.2 Example: mean field for the Ising model 737
	21.4	Structured mean field * 739
		21.4.1 Example: factorial HMM 740
	21.5	Variational Bayes 742
		21.5.1 Example: VB for a univariate Gaussian 742
	01.0	21.5.2 Example: VB for linear regression 746
	21.6	Variational Bayes EM 749
	21.7	21.6.1 Example: VBEM for mixtures of Gaussians * 750
	21.7 21.8	Variational message passing and VIBES 756 Local variational bounds * 756
	21.0	21.8.1 Motivating applications 756
		21.8.2 Bohning's quadratic bound to the log-sum-exp function 758
		21.8.3 Bounds for the sigmoid function 760
		21.8.4 Other bounds and approximations to the log-sum-exp function * 762
		21.8.5 Variational inference based on upper bounds 763
22	More	variational inference 767
22	22.1	Introduction 767
	22.2	Loopy belief propagation: algorithmic issues 767
		22.2.1 A brief history 767
		22.2.2 LBP on pairwise models 768
		22.2.3 LBP on a factor graph 769
		22.2.4 Convergence 771
		22.2.5 Accuracy of LBP 774
		22.2.6 Other speedup tricks for LBP * 775
	22.3	Loopy belief propagation: theoretical issues * 776
		22.3.1 UGMs represented in exponential family form 776
		22.3.2 The marginal polytope 777
		22.3.3 Exact inference as a variational optimization problem 778
		22.3.4 Mean field as a variational optimization problem 779
		22.3.5 LBP as a variational optimization problem 779
	00.4	22.3.6 Loopy BP vs mean field 783
	22.4	Extensions of belief propagation * 783
		22.4.1 Generalized belief propagation 783

CONTENTS xxi

		22.4.2	Convex belief propagation 785	
	22.5	Expectation	on propagation 787	
		22.5.1	EP as a variational inference problem 788	
		22.5.2	Optimizing the EP objective using moment matching	789
		22.5.3	EP for the clutter problem 791	
		22.5.4	LBP is a special case of EP 792	
		22.5.5	Ranking players using TrueSkill 793	
		22.5.6	Other applications of EP 799	
	22.6	MAP state	e estimation 799	
		22.6.1	Linear programming relaxation 799	
		22.6.2	Max-product belief propagation 800	
		22.6.3	Graphcuts 801	
		22.6.4	Experimental comparison of graphcuts and BP 804	
		22.6.5	Dual decomposition 806	
22	Mont	o Carlo in	ference 815	
23	23.1	e Carlo in Introduct		
	23.2		ion 815 from standard distributions 815	
	23.2		Using the cdf 815	
			9	
	23.3		Sampling from a Gaussian (Box-Muller method) 817 sampling 817	
	23.3	-	Basic idea 817	
			Example 818	
			Application to Bayesian statistics 819	
			Adaptive rejection sampling 819	
			Rejection sampling in high dimensions 820	
	23.4		ce sampling 820	
	23.4	-	Basic idea 820	
			Handling unnormalized distributions 821	
			Importance sampling for a DGM: likelihood weighting	822
			Sampling importance resampling (SIR) 822	022
	23.5	Particle fi		
	20.0		Sequential importance sampling 824	
			The degeneracy problem 825	
			The resampling step 825	
			The proposal distribution 827	
			Application: robot localization 828	
			Application: visual object tracking 828	
			Application: time series forecasting 831	
	23.6		cwellised particle filtering (RBPF) 831	
			RBPF for switching LG-SSMs 831	
			Application: tracking a maneuvering target 832	
			Application: Fast SLAM 834	
			11	

xxii CONTENTS

	24.1	Introduc	
	24.2	Gibbs sa	
		24.2.1	Basic idea 838
		24.2.2	Example: Gibbs sampling for the Ising model 838
		24.2.3	Example: Gibbs sampling for inferring the parameters of a GMM 840
		24.2.4	Collapsed Gibbs sampling * 841
		24.2.5	Gibbs sampling for hierarchical GLMs 844
		24.2.6	BUGS and JAGS 846
		24.2.7	The Imputation Posterior (IP) algorithm 847
		24.2.8	Blocking Gibbs sampling 847
	24.3	-	lis Hastings algorithm 848
		24.3.1	Basic idea 848
		24.3.2	Gibbs sampling is a special case of MH 849
		24.3.3	Proposal distributions 850
		24.3.4	Adaptive MCMC 853
		24.3.5	Initialization and mode hopping 854
		24.3.6	Why MH works * 854
		24.3.7	Reversible jump (trans-dimensional) MCMC * 855
	24.4	Speed ar	nd accuracy of MCMC 856
		24.4.1	The burn-in phase 856
		24.4.2	Mixing rates of Markov chains * 857
		24.4.3	Practical convergence diagnostics 858
		24.4.4	Accuracy of MCMC 860
		24.4.5	How many chains? 862
	24.5	Auxiliary	variable MCMC * 863
		24.5.1	Auxiliary variable sampling for logistic regression 863
		24.5.2	Slice sampling 864
		24.5.3	Swendsen Wang 866
		24.5.4	Hybrid/Hamiltonian MCMC * 868
	24.6	Annealin	g methods 868
		24.6.1	Simulated annealing 869
		24.6.2	Annealed importance sampling 871
		24.6.3	Parallel tempering 871
	24.7	Approxim	nating the marginal likelihood 872
		24.7.1	The candidate method 872
		24.7.2	Harmonic mean estimate 872
		24.7.3	Annealed importance sampling 873
25	Cluste	ering	875
	25.1	Introduc	tion 875
		25.1.1	Measuring (dis)similarity 875
		25.1.2	Evaluating the output of clustering methods * 876
	25.2	Dirichlet	process mixture models 879
		25.2.1	From finite to infinite mixture models 879
		25.2.2	The Dirichlet process 882

CONTENTS xxiii

		25.2.3 Applying Dirichlet processes to mixture modeling 885
	25.3	25.2.4 Fitting a DP mixture model 886 Affinity propagation 887
	25.4	Spectral clustering 890
	20.1	25.4.1 Graph Laplacian 891
		25.4.2 Normalized graph Laplacian 892
		25.4.3 Example 893
	25.5	Hierarchical clustering 893
	20.0	25.5.1 Agglomerative clustering 895
		25.5.2 Divisive clustering 898
		25.5.3 Choosing the number of clusters 899
		25.5.4 Bayesian hierarchical clustering 899
	25.6	Clustering datapoints and features 901
		25.6.1 Biclustering 903
		25.6.2 Multi-view clustering 903
26	Cuanl	
20	26.1	nical model structure learning 907 Introduction 907
	26.2	Structure learning for knowledge discovery 908
	20.2	26.2.1 Relevance networks 908
		26.2.2 Dependency networks 909
	26.3	Learning tree structures 910
	_0.0	26.3.1 Directed or undirected tree? 911
		26.3.2 Chow-Liu algorithm for finding the ML tree structure 912
		26.3.3 Finding the MAP forest 912
		26.3.4 Mixtures of trees 914
	26.4	Learning DAG structures 914
		26.4.1 Markov equivalence 914
		26.4.2 Exact structural inference 916
		26.4.3 Scaling up to larger graphs 920
	26.5	Learning DAG structure with latent variables 922
		26.5.1 Approximating the marginal likelihood when we have missing data 922
		26.5.2 Structural EM 925
		26.5.3 Discovering hidden variables 926
		26.5.4 Case study: Google's Rephil 928
		26.5.5 Structural equation models * 929
	26.6	Learning causal DAGs 931
		26.6.1 Causal interpretation of DAGs 931
		26.6.2 Using causal DAGs to resolve Simpson's paradox 933
		26.6.3 Learning causal DAG structures 935
	26.7	Learning undirected Gaussian graphical models 938
		26.7.1 MLE for a GGM 938
		26.7.2 Graphical lasso 939
		26.7.3 Bayesian inference for GGM structure * 941
		26.7.4 Handling non-Gaussian data using copulas * 942

	26.8	Learning undirected discrete 26.8.1 Graphical lasso		
		26.8.2 Thin junction to	rees 944	
27	Laten	t variable models for dis	crete data 945	
	27.1	Introduction 945		
	27.2	Distributed state LVMs fo		
		27.2.1 Mixture models		
		27.2.2 Exponential fan	· ·	
		27.2.3 LDA and mPCA		
			non-negative matrix factorization 949	
	27.3	Latent Dirichlet allocation	n (LDA) 950	
		27.3.1 Basics 950		
		_	iscovery of topics 953	
		•	valuating LDA as a language model 953	
			ollapsed) Gibbs sampling 955	
		27.3.5 Example 95		
			tch variational inference 957 line variational inference 959	
			line variational inference 959 e number of topics 960	
	27.4	Extensions of LDA 96	•	
	21.4	27.4.1 Correlated topic	· -	
		27.4.2 Dynamic topic		
			963	
		27.4.4 Supervised LDA		
	27.5	LVMs for graph-structure		
		27.5.1 Stochastic block		
		27.5.2 Mixed members	ship stochastic block model 973	
		27.5.3 Relational topic	model 974	
	27.6	LVMs for relational data	975	
		27.6.1 Infinite relations		
			trix factorization for collaborative filtering 97	9
	27.7	Restricted Boltzmann ma		
		27.7.1 Varieties of RBN		
		27.7.2 Learning RBMs	987	
		27.7.3 Applications of	RBMs 991	
28	Deep	learning 995		
	28.1	Introduction 995		
	28.2	Deep generative models	995	
		28.2.1 Deep directed r		
		28.2.2 Deep Boltzman		
		28.2.3 Deep belief net		
	00.0		se learning of DBNs 998	
	28.3	Deep neural networks	999	

CONTENTS xxv

	28.3.1	Deep multi-layer perceptrons 999	
	28.3.2	Deep auto-encoders 1000	
	28.3.3	Stacked denoising auto-encoders 1001	
28.4	Applicati	ons of deep networks 1001	
	28.4.1	Handwritten digit classification using DBNs 1001	
	28.4.2	Data visualization and feature discovery using deep auto-encoders	1002
	28.4.3	Information retrieval using deep auto-encoders (semantic hashing)	1003
	28.4.4	Learning audio features using 1d convolutional DBNs 1004	
	28.4.5	Learning image features using 2d convolutional DBNs 1005	
28.5	Discussion	on 1005	

Notation 1009

Bibliography 1015

Indexes 1047

Index to code 1047 Index to keywords 1050