

Contents

Preface xxvii

1	<i>Introduction</i>	1
1.1	Machine learning: what and why?	1
1.1.1	Types of machine learning	2
1.2	Supervised learning	3
1.2.1	Classification	3
1.2.2	Regression	8
1.3	Unsupervised 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 basic 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	<i>Probability</i>	27
2.1	Introduction	27
2.2	A brief review 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

2.2.6	Quantiles	33
2.2.7	Mean and variance	33
2.3	Some 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 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	Joint probability distributions	44
2.5.1	Covariance and correlation	44
2.5.2	The multivariate Gaussian	46
2.5.3	Multivariate Student t distribution	46
2.5.4	Dirichlet distribution	47
2.6	Transformations of random variables	49
2.6.1	Linear transformations	49
2.6.2	General transformations	50
2.6.3	Central limit theorem	51
2.7	Monte 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	Information theory	56
2.8.1	Entropy	56
2.8.2	KL divergence	57
2.8.3	Mutual information	59
3	<i>Generative models for discrete data</i>	65
3.1	Introduction	65
3.2	Bayesian 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 beta-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

3.4	The Dirichlet-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 Bayes 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	Gaussian models	97
4.1	Introduction	97
4.1.1	Notation	97
4.1.2	Basics	97
4.1.3	MLE for an MVN	99
4.1.4	Maximum entropy derivation of the Gaussian *	101
4.2	Gaussian discriminant analysis	101
4.2.1	Quadratic discriminant analysis (QDA)	102
4.2.2	Linear discriminant analysis (LDA)	103
4.2.3	Two-class LDA	104
4.2.4	MLE for discriminant analysis	106
4.2.5	Strategies for preventing overfitting	106
4.2.6	Regularized LDA *	107
4.2.7	Diagonal LDA	108
4.2.8	Nearest shrunken centroids classifier *	109
4.3	Inference in jointly Gaussian distributions	110
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	Linear Gaussian systems	119
4.4.1	Statement of the result	119
4.4.2	Examples	120
4.4.3	Proof of the result *	124
4.5	Digression: The Wishart distribution *	125
4.5.1	Inverse Wishart distribution	126
4.5.2	Visualizing the Wishart distribution *	127
4.6	Inferring 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

5 Bayesian statistics	149
5.1	Introduction 149
5.2	Summarizing posterior distributions 149
5.2.1	MAP estimation 149
5.2.2	Credible intervals 152
5.2.3	Inference for a difference in proportions 154
5.3	Bayesian model selection 155
5.3.1	Bayesian Occam's razor 156
5.3.2	Computing the marginal likelihood (evidence) 158
5.3.3	Bayes factors 163
5.3.4	Jeffreys-Lindley paradox * 164
5.4	Priors 165
5.4.1	Uninformative priors 165
5.4.2	Jeffreys priors * 166
5.4.3	Robust priors 168
5.4.4	Mixtures of conjugate priors 168
5.5	Hierarchical Bayes 171
5.5.1	Example: modeling related cancer rates 171
5.6	Empirical Bayes 172
5.6.1	Example: beta-binomial model 173
5.6.2	Example: Gaussian-Gaussian model 173
5.7	Bayesian decision theory 176
5.7.1	Bayes estimators for common loss functions 177
5.7.2	The false positive vs false negative tradeoff 180
5.7.3	Other topics * 184
6 Frequentist statistics	191
6.1	Introduction 191
6.2	Sampling distribution of an estimator 191
6.2.1	Bootstrap 192
6.2.2	Large sample theory for the MLE * 193
6.3	Frequentist decision theory 194
6.3.1	Bayes risk 195
6.3.2	Minimax risk 196
6.3.3	Admissible estimators 197
6.4	Desirable properties of estimators 200
6.4.1	Consistent estimators 200
6.4.2	Unbiased estimators 200
6.4.3	Minimum variance estimators 201
6.4.4	The bias-variance tradeoff 202
6.5	Empirical risk minimization 204
6.5.1	Regularized risk minimization 205
6.5.2	Structural risk minimization 206
6.5.3	Estimating the risk using cross validation 206
6.5.4	Upper bounding the risk using statistical learning theory * 209

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	Linear 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	Logistic 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

8.5.2	Stochastic optimization and risk minimization	262
8.5.3	The LMS algorithm	264
8.5.4	The perceptron algorithm	265
8.5.5	A Bayesian view	266
8.6	Generative vs discriminative classifiers	267
8.6.1	Pros and cons of each approach	268
8.6.2	Dealing with missing data	269
8.6.3	Fisher's linear discriminant analysis (FLDA) *	271
9	Generalized linear models and the exponential family	281
9.1	Introduction	281
9.2	The exponential family	281
9.2.1	Definition	282
9.2.2	Examples	282
9.2.3	Log partition function	284
9.2.4	MLE for the exponential family	286
9.2.5	Bayes for the exponential family *	287
9.2.6	Maximum entropy derivation of the exponential family *	289
9.3	Generalized linear models (GLMs)	290
9.3.1	Basics	290
9.3.2	ML and MAP estimation	292
9.3.3	Bayesian inference	293
9.4	Probit regression	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 learning	296
9.5.1	Hierarchical Bayes for multi-task learning	296
9.5.2	Application to personalized email spam filtering	296
9.5.3	Application to domain adaptation	297
9.5.4	Other kinds of prior	297
9.6	Generalized linear mixed models *	298
9.6.1	Example: semi-parametric GLMMs for medical data	298
9.6.2	Computational issues	300
9.7	Learning to rank *	300
9.7.1	The pointwise approach	301
9.7.2	The pairwise approach	301
9.7.3	The listwise approach	302
9.7.4	Loss functions for ranking	303
10	Directed graphical models (Bayes nets)	307
10.1	Introduction	307
10.1.1	Chain rule	307
10.1.2	Conditional independence	308

10.1.3	Graphical models	308
10.1.4	Graph terminology	309
10.1.5	Directed graphical models	310
10.2	Examples	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	Inference	319
10.4	Learning	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	Conditional 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	Influence (decision) diagrams *	328
II	Mixture models and the EM algorithm	337
11.1	Latent variable models	337
11.2	Mixture models	337
11.2.1	Mixtures of Gaussians	339
11.2.2	Mixture of multinoullis	340
11.2.3	Using mixture models for clustering	340
11.2.4	Mixtures of experts	342
11.3	Parameter 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 algorithm	348
11.4.1	Basic idea	349
11.4.2	EM for GMMs	350
11.4.3	EM for mixture of experts	357
11.4.4	EM for DGMs with hidden variables	358
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	Model 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

11.6.1	EM for the MLE of an MVN with missing data	373
12 Latent linear models		381
12.1	Factor analysis	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	Principal components analysis (PCA)	387
12.2.1	Classical PCA: statement of the theorem	387
12.2.2	Proof * 389	
12.2.3	Singular value decomposition (SVD)	392
12.2.4	Probabilistic PCA	395
12.2.5	EM algorithm for PCA	396
12.3	Choosing the number of latent dimensions	398
12.3.1	Model selection for FA/PPCA	398
12.3.2	Model selection for PCA	399
12.4	PCA for categorical data	402
12.5	PCA for paired and multi-view data	404
12.5.1	Supervised PCA (latent factor regression)	405
12.5.2	Partial least squares	406
12.5.3	Canonical correlation analysis	407
12.6	Independent Component Analysis (ICA)	407
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 Sparse linear models		421
13.1	Introduction	421
13.2	Bayesian 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 regularization: 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	ℓ_1 regularization: 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 regularization: extensions	449
13.5.1	Group Lasso	449
13.5.2	Fused lasso	454
13.5.3	Elastic net (ridge and lasso combined)	455
13.6	Non-convex regularizers	457
13.6.1	Bridge regression	458
13.6.2	Hierarchical adaptive lasso	458
13.6.3	Other hierarchical priors	462
13.7	Automatic 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 coding *	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
14	Kernels	479
14.1	Introduction	479
14.2	Kernel functions	479
14.2.1	RBF kernels	480
14.2.2	Kernels for comparing documents	480
14.2.3	Mercer (positive definite) kernels	481
14.2.4	Linear kernels	482
14.2.5	Matern kernels	482
14.2.6	String kernels	483
14.2.7	Pyramid match kernels	484
14.2.8	Kernels derived from probabilistic generative models	485
14.3	Using kernels inside GLMs	486
14.3.1	Kernel machines	486
14.3.2	LIVMs, RVMs, and other sparse vector machines	487
14.4	The kernel trick	488
14.4.1	Kernelized nearest neighbor classification	489
14.4.2	Kernelized K-medoids clustering	489
14.4.3	Kernelized ridge regression	492
14.4.4	Kernel PCA	493
14.5	Support vector machines (SVMs)	496
14.5.1	SVMs for regression	497
14.5.2	SVMs for classification	498

14.5.3	Choosing C	504
14.5.4	Summary of key points	504
14.5.5	A probabilistic interpretation of SVMs	505
14.6	Comparison 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	Gaussian processes	515
15.1	Introduction	515
15.2	GPs for 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
15.2.6	Semi-parametric GPs *	524
15.3	GPs meet GLMs	525
15.3.1	Binary classification	525
15.3.2	Multi-class classification	528
15.3.3	GPs for Poisson regression	531
15.4	Connection with other methods	532
15.4.1	Linear models compared to GPs	532
15.4.2	Linear smoothers compared to GPs	533
15.4.3	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	GP latent variable model	540
15.6	Approximation methods for large datasets	542
16	Adaptive basis function models	543
16.1	Introduction	543
16.2	Classification 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 *	551
16.3	Generalized additive models	552

16.3.1	Backfitting	552
16.3.2	Computational efficiency	553
16.3.3	Multivariate adaptive regression splines (MARS)	553
16.4	Boosting	554
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	Feedforward 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	Ensemble 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	Experimental comparison	582
16.7.1	Low-dimensional features	582
16.7.2	High-dimensional features	583
16.8	Interpreting black-box models	585
17	<i>Markov and hidden Markov models</i>	589
17.1	Introduction	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 Markov models	603
17.3.1	Applications of HMMs	604
17.4	Inference 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

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	Generalizations 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	<i>State space models</i>	631
18.1	Introduction	631
18.2	Applications of SSMs	632
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	Inference in LG-SSM	640
18.3.1	The Kalman filtering algorithm	640
18.3.2	The Kalman smoothing algorithm	643
18.4	Learning for LG-SSM	646
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
18.4.5	Bayesian methods for “fitting” LG-SSMs	647
18.5	Approximate 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
18.5.3	Assumed density filtering (ADF)	652
18.6	Hybrid discrete/continuous SSMs	655
18.6.1	Inference	656
18.6.2	Application: data association and multi-target tracking	658
18.6.3	Application: fault diagnosis	659
18.6.4	Application: econometric forecasting	660
19	<i>Undirected graphical models (Markov random fields)</i>	661
19.1	Introduction	661
19.2	Conditional independence properties of UGMs	661
19.2.1	Key properties	661

19.2.2	An undirected alternative to d-separation	663
19.2.3	Comparing directed and undirected graphical models	664
19.3	Parameterization of MRFs	665
19.3.1	The Hammersley-Clifford theorem	665
19.3.2	Representing potential functions	667
19.4	Examples 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	676
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	Conditional 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	Structural 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	<i>Exact inference for graphical models</i>	707
20.1	Introduction	707
20.2	Belief propagation for trees	707
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	The variable elimination algorithm	714
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	The junction tree algorithm *	720
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	Variational 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
21.5.2	Example: VB for linear regression	746
21.6	Variational Bayes EM	749
21.6.1	Example: VBEM for mixtures of Gaussians *	750
21.7	Variational message passing and VIBES	756
21.8	Local variational bounds *	756
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
22.1	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
22.3.6	Loopy BP vs mean field	783
22.4	Extensions of belief propagation *	783
22.4.1	Generalized belief propagation	783

22.4.2	Convex belief propagation	785
22.5	Expectation 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 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
23	Monte Carlo inference	815
23.1	Introduction	815
23.2	Sampling from standard distributions	815
23.2.1	Using the cdf	815
23.2.2	Sampling from a Gaussian (Box-Muller method)	817
23.3	Rejection sampling	817
23.3.1	Basic idea	817
23.3.2	Example	818
23.3.3	Application to Bayesian statistics	819
23.3.4	Adaptive rejection sampling	819
23.3.5	Rejection sampling in high dimensions	820
23.4	Importance sampling	820
23.4.1	Basic idea	820
23.4.2	Handling unnormalized distributions	821
23.4.3	Importance sampling for a DGM: likelihood weighting	822
23.4.4	Sampling importance resampling (SIR)	822
23.5	Particle filtering	823
23.5.1	Sequential importance sampling	824
23.5.2	The degeneracy problem	825
23.5.3	The resampling step	825
23.5.4	The proposal distribution	827
23.5.5	Application: robot localization	828
23.5.6	Application: visual object tracking	828
23.5.7	Application: time series forecasting	831
23.6	Rao-Blackwellised particle filtering (RBPF)	831
23.6.1	RBPF for switching LG-SSMs	831
23.6.2	Application: tracking a maneuvering target	832
23.6.3	Application: Fast SLAM	834
24	Markov chain Monte Carlo (MCMC) inference	837

24.1	Introduction	837
24.2	Gibbs sampling	838
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	Metropolis 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 and 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	Annealing methods	868
24.6.1	Simulated annealing	869
24.6.2	Annealed importance sampling	871
24.6.3	Parallel tempering	871
24.7	Approximating 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	Clustering	875
25.1	Introduction	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

25.2.3	Applying Dirichlet processes to mixture modeling	885
25.2.4	Fitting a DP mixture model	886
25.3	Affinity propagation	887
25.4	Spectral clustering	890
25.4.1	Graph Laplacian	891
25.4.2	Normalized graph Laplacian	892
25.4.3	Example	893
25.5	Hierarchical clustering	893
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	<i>Graphical model structure learning</i>	907
26.1	Introduction	907
26.2	Structure learning for knowledge discovery	908
26.2.1	Relevance networks	908
26.2.2	Dependency networks	909
26.3	Learning tree structures	910
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 graphical models	942
26.8.1	Graphical lasso for MRFs/CRFs	942
26.8.2	Thin junction trees	944
27	<i>Latent variable models for discrete data</i>	945
27.1	Introduction	945
27.2	Distributed state LVMs for discrete data	946
27.2.1	Mixture models	946
27.2.2	Exponential family PCA	947
27.2.3	LDA and mPCA	948
27.2.4	GaP model and non-negative matrix factorization	949
27.3	Latent Dirichlet allocation (LDA)	950
27.3.1	Basics	950
27.3.2	Unsupervised discovery of topics	953
27.3.3	Quantitatively evaluating LDA as a language model	953
27.3.4	Fitting using (collapsed) Gibbs sampling	955
27.3.5	Example	956
27.3.6	Fitting using batch variational inference	957
27.3.7	Fitting using online variational inference	959
27.3.8	Determining the number of topics	960
27.4	Extensions of LDA	961
27.4.1	Correlated topic model	961
27.4.2	Dynamic topic model	962
27.4.3	LDA-HMM	963
27.4.4	Supervised LDA	967
27.5	LVMs for graph-structured data	970
27.5.1	Stochastic block model	971
27.5.2	Mixed membership stochastic block model	973
27.5.3	Relational topic model	974
27.6	LVMs for relational data	975
27.6.1	Infinite relational model	976
27.6.2	Probabilistic matrix factorization for collaborative filtering	979
27.7	Restricted Boltzmann machines (RBMs)	983
27.7.1	Varieties of RBMs	985
27.7.2	Learning RBMs	987
27.7.3	Applications of RBMs	991
28	<i>Deep learning</i>	995
28.1	Introduction	995
28.2	Deep generative models	995
28.2.1	Deep directed networks	996
28.2.2	Deep Boltzmann machines	996
28.2.3	Deep belief networks	997
28.2.4	Greedy layer-wise learning of DBNs	998
28.3	Deep neural networks	999

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	Applications 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	1005
<i>Notation</i>		1009
<i>Bibliography</i>		1015
<i>Indexes</i>		1047
Index to code		1047
Index to keywords		1050