

Contents

Preface	vii
Mathematical notation	xi
Contents	xiii
1 Introduction	1
1.1 Example: Polynomial Curve Fitting	4
1.2 Probability Theory	12
1.2.1 Probability densities	17
1.2.2 Expectations and covariances	19
1.2.3 Bayesian probabilities	21
1.2.4 The Gaussian distribution	24
1.2.5 Curve fitting re-visited	28
1.2.6 Bayesian curve fitting	30
1.3 Model Selection	32
1.4 The Curse of Dimensionality	33
1.5 Decision Theory	38
1.5.1 Minimizing the misclassification rate	39
1.5.2 Minimizing the expected loss	41
1.5.3 The reject option	42
1.5.4 Inference and decision	42
1.5.5 Loss functions for regression	46
1.6 Information Theory	48
1.6.1 Relative entropy and mutual information	55
Exercises	58

2	Probability Distributions	67
2.1	Binary Variables	68
2.1.1	The beta distribution	71
2.2	Multinomial Variables	74
2.2.1	The Dirichlet distribution	76
2.3	The Gaussian Distribution	78
2.3.1	Conditional Gaussian distributions	85
2.3.2	Marginal Gaussian distributions	88
2.3.3	Bayes' theorem for Gaussian variables	90
2.3.4	Maximum likelihood for the Gaussian	93
2.3.5	Sequential estimation	94
2.3.6	Bayesian inference for the Gaussian	97
2.3.7	Student's t-distribution	102
2.3.8	Periodic variables	105
2.3.9	Mixtures of Gaussians	110
2.4	The Exponential Family	113
2.4.1	Maximum likelihood and sufficient statistics	116
2.4.2	Conjugate priors	117
2.4.3	Noninformative priors	117
2.5	Nonparametric Methods	120
2.5.1	Kernel density estimators	122
2.5.2	Nearest-neighbour methods	124
	Exercises	127
3	Linear Models for Regression	137
3.1	Linear Basis Function Models	138
3.1.1	Maximum likelihood and least squares	140
3.1.2	Geometry of least squares	143
3.1.3	Sequential learning	143
3.1.4	Regularized least squares	144
3.1.5	Multiple outputs	146
3.2	The Bias-Variance Decomposition	147
3.3	Bayesian Linear Regression	152
3.3.1	Parameter distribution	152
3.3.2	Predictive distribution	156
3.3.3	Equivalent kernel	159
3.4	Bayesian Model Comparison	161
3.5	The Evidence Approximation	165
3.5.1	Evaluation of the evidence function	166
3.5.2	Maximizing the evidence function	168
3.5.3	Effective number of parameters	170
3.6	Limitations of Fixed Basis Functions	172
	Exercises	173

4	Linear Models for Classification	179
4.1	Discriminant Functions	181
4.1.1	Two classes	181
4.1.2	Multiple classes	182
4.1.3	Least squares for classification	184
4.1.4	Fisher's linear discriminant	186
4.1.5	Relation to least squares	189
4.1.6	Fisher's discriminant for multiple classes	191
4.1.7	The perceptron algorithm	192
4.2	Probabilistic Generative Models	196
4.2.1	Continuous inputs	198
4.2.2	Maximum likelihood solution	200
4.2.3	Discrete features	202
4.2.4	Exponential family	202
4.3	Probabilistic Discriminative Models	203
4.3.1	Fixed basis functions	204
4.3.2	Logistic regression	205
4.3.3	Iterative reweighted least squares	207
4.3.4	Multiclass logistic regression	209
4.3.5	Probit regression	210
4.3.6	Canonical link functions	212
4.4	The Laplace Approximation	213
4.4.1	Model comparison and BIC	216
4.5	Bayesian Logistic Regression	217
4.5.1	Laplace approximation	217
4.5.2	Predictive distribution	218
	Exercises	220
5	Neural Networks	225
5.1	Feed-forward Network Functions	227
5.1.1	Weight-space symmetries	231
5.2	Network Training	232
5.2.1	Parameter optimization	236
5.2.2	Local quadratic approximation	237
5.2.3	Use of gradient information	239
5.2.4	Gradient descent optimization	240
5.3	Error Backpropagation	241
5.3.1	Evaluation of error-function derivatives	242
5.3.2	A simple example	245
5.3.3	Efficiency of backpropagation	246
5.3.4	The Jacobian matrix	247
5.4	The Hessian Matrix	249
5.4.1	Diagonal approximation	250
5.4.2	Outer product approximation	251
5.4.3	Inverse Hessian	252

5.4.4	Finite differences	252
5.4.5	Exact evaluation of the Hessian	253
5.4.6	Fast multiplication by the Hessian	254
5.5	Regularization in Neural Networks	256
5.5.1	Consistent Gaussian priors	257
5.5.2	Early stopping	259
5.5.3	Invariances	261
5.5.4	Tangent propagation	263
5.5.5	Training with transformed data	265
5.5.6	Convolutional networks	267
5.5.7	Soft weight sharing	269
5.6	Mixture Density Networks	272
5.7	Bayesian Neural Networks	277
5.7.1	Posterior parameter distribution	278
5.7.2	Hyperparameter optimization	280
5.7.3	Bayesian neural networks for classification	281
	Exercises	284
6	Kernel Methods	291
6.1	Dual Representations	293
6.2	Constructing Kernels	294
6.3	Radial Basis Function Networks	299
6.3.1	Nadaraya-Watson model	301
6.4	Gaussian Processes	303
6.4.1	Linear regression revisited	304
6.4.2	Gaussian processes for regression	306
6.4.3	Learning the hyperparameters	311
6.4.4	Automatic relevance determination	312
6.4.5	Gaussian processes for classification	313
6.4.6	Laplace approximation	315
6.4.7	Connection to neural networks	319
	Exercises	320
7	Sparse Kernel Machines	325
7.1	Maximum Margin Classifiers	326
7.1.1	Overlapping class distributions	331
7.1.2	Relation to logistic regression	336
7.1.3	Multiclass SVMs	338
7.1.4	SVMs for regression	339
7.1.5	Computational learning theory	344
7.2	Relevance Vector Machines	345
7.2.1	RVM for regression	345
7.2.2	Analysis of sparsity	349
7.2.3	RVM for classification	353
	Exercises	357

8	Graphical Models	359
8.1	Bayesian Networks	360
8.1.1	Example: Polynomial regression	362
8.1.2	Generative models	365
8.1.3	Discrete variables	366
8.1.4	Linear-Gaussian models	370
8.2	Conditional Independence	372
8.2.1	Three example graphs	373
8.2.2	D-separation	378
8.3	Markov Random Fields	383
8.3.1	Conditional independence properties	383
8.3.2	Factorization properties	384
8.3.3	Illustration: Image de-noising	387
8.3.4	Relation to directed graphs	390
8.4	Inference in Graphical Models	393
8.4.1	Inference on a chain	394
8.4.2	Trees	398
8.4.3	Factor graphs	399
8.4.4	The sum-product algorithm	402
8.4.5	The max-sum algorithm	411
8.4.6	Exact inference in general graphs	416
8.4.7	Loopy belief propagation	417
8.4.8	Learning the graph structure	418
	Exercises	418
9	Mixture Models and EM	423
9.1	K -means Clustering	424
9.1.1	Image segmentation and compression	428
9.2	Mixtures of Gaussians	430
9.2.1	Maximum likelihood	432
9.2.2	EM for Gaussian mixtures	435
9.3	An Alternative View of EM	439
9.3.1	Gaussian mixtures revisited	441
9.3.2	Relation to K -means	443
9.3.3	Mixtures of Bernoulli distributions	444
9.3.4	EM for Bayesian linear regression	448
9.4	The EM Algorithm in General	450
	Exercises	455
10	Approximate Inference	461
10.1	Variational Inference	462
10.1.1	Factorized distributions	464
10.1.2	Properties of factorized approximations	466
10.1.3	Example: The univariate Gaussian	470
10.1.4	Model comparison	473
10.2	Illustration: Variational Mixture of Gaussians	474

10.2.1	Variational distribution	475
10.2.2	Variational lower bound	481
10.2.3	Predictive density	482
10.2.4	Determining the number of components	483
10.2.5	Induced factorizations	485
10.3	Variational Linear Regression	486
10.3.1	Variational distribution	486
10.3.2	Predictive distribution	488
10.3.3	Lower bound	489
10.4	Exponential Family Distributions	490
10.4.1	Variational message passing	491
10.5	Local Variational Methods	493
10.6	Variational Logistic Regression	498
10.6.1	Variational posterior distribution	498
10.6.2	Optimizing the variational parameters	500
10.6.3	Inference of hyperparameters	502
10.7	Expectation Propagation	505
10.7.1	Example: The clutter problem	511
10.7.2	Expectation propagation on graphs	513
	Exercises	517
11	Sampling Methods	523
11.1	Basic Sampling Algorithms	526
11.1.1	Standard distributions	526
11.1.2	Rejection sampling	528
11.1.3	Adaptive rejection sampling	530
11.1.4	Importance sampling	532
11.1.5	Sampling-importance-resampling	534
11.1.6	Sampling and the EM algorithm	536
11.2	Markov Chain Monte Carlo	537
11.2.1	Markov chains	539
11.2.2	The Metropolis-Hastings algorithm	541
11.3	Gibbs Sampling	542
11.4	Slice Sampling	546
11.5	The Hybrid Monte Carlo Algorithm	548
11.5.1	Dynamical systems	548
11.5.2	Hybrid Monte Carlo	552
11.6	Estimating the Partition Function	554
	Exercises	556
12	Continuous Latent Variables	559
12.1	Principal Component Analysis	561
12.1.1	Maximum variance formulation	561
12.1.2	Minimum-error formulation	563
12.1.3	Applications of PCA	565
12.1.4	PCA for high-dimensional data	569

12.2	Probabilistic PCA	570
12.2.1	Maximum likelihood PCA	574
12.2.2	EM algorithm for PCA	577
12.2.3	Bayesian PCA	580
12.2.4	Factor analysis	583
12.3	Kernel PCA	586
12.4	Nonlinear Latent Variable Models	591
12.4.1	Independent component analysis	591
12.4.2	Autoassociative neural networks	592
12.4.3	Modelling nonlinear manifolds	595
	Exercises	599
13	Sequential Data	605
13.1	Markov Models	607
13.2	Hidden Markov Models	610
13.2.1	Maximum likelihood for the HMM	615
13.2.2	The forward-backward algorithm	618
13.2.3	The sum-product algorithm for the HMM	625
13.2.4	Scaling factors	627
13.2.5	The Viterbi algorithm	629
13.2.6	Extensions of the hidden Markov model	631
13.3	Linear Dynamical Systems	635
13.3.1	Inference in LDS	638
13.3.2	Learning in LDS	642
13.3.3	Extensions of LDS	644
13.3.4	Particle filters	645
	Exercises	646
14	Combining Models	653
14.1	Bayesian Model Averaging	654
14.2	Committees	655
14.3	Boosting	657
14.3.1	Minimizing exponential error	659
14.3.2	Error functions for boosting	661
14.4	Tree-based Models	663
14.5	Conditional Mixture Models	666
14.5.1	Mixtures of linear regression models	667
14.5.2	Mixtures of logistic models	670
14.5.3	Mixtures of experts	672
	Exercises	674
Appendix A	Data Sets	677
Appendix B	Probability Distributions	685
Appendix C	Properties of Matrices	695

Appendix D	Calculus of Variations	703
Appendix E	Lagrange Multipliers	707
References		711
Index		729