Contents

P	reface	XXX	vii
Li	st of l	Figures	xxix
1	Intro	$\mathbf{duction}$	1
	1.1	What is	machine learning? 1
	1.2	Supervis	sed learning 1
		1.2.1	Classification 2
		1.2.2	Regression 8
		1.2.3	Overfitting and generalization 12
		1.2.4	No free lunch theorem 13
	1.3	Unsuper	vised learning 13
		1.3.1	Clustering 14
		1.3.2	Discovering latent "factors of variation" 15
		1.3.3	Self-supervised learning 16
		1.3.4	Evaluating unsupervised learning 16
	1.4	Reinforc	ement learning 17
	1.5	Data	18
		1.5.1	Some common image datasets 18
		1.5.2	Some common text datasets 21
		1.5.3	Preprocessing discrete input data 22
		1.5.4	Preprocessing text data 23
		1.5.5	Handling missing data 26
	1.6	Discussion	on 27
		1.6.1	The relationship between ML and other fields 27
		1.6.2	Structure of the book 27
		1.6.3	Caveats 27

31

I Foundations 29

2 Probability: Univariate Models

X CONTENTS

2.1	Introdu	action 31
	2.1.1	What is probability? 31
	2.1.2	Types of uncertainty 31
	2.1.3	Probability as an extension of logic 32
2.2	Rando	m variables 33
	2.2.1	Discrete random variables 33
	2.2.2	Continuous random variables 35
	2.2.3	Sets of related random variables 36
	2.2.4	Independence and conditional independence 37
	2.2.5	Moments of a distribution 38
	2.2.6	Limitations of summary statistics 41
2.3	Bayes'	rule 43
	2.3.1	Example: Testing for COVID-19 44
	2.3.2	Example: The Monty Hall problem 46
	2.3.3	Inverse problems * 47
2.4	Bernou	alli and binomial distributions 48
	2.4.1	Definition 48
	2.4.2	Sigmoid (logistic) function 49
	2.4.3	Binary logistic regression 51
2.5	Catego	rical and multinomial distributions 51
	2.5.1	Definition 52
	2.5.2	Softmax function 52
	2.5.3	Multiclass logistic regression 53
	2.5.4	Log-sum-exp trick 54
2.6		iate Gaussian (normal) distribution 55
	2.6.1	Cumulative distribution function 55
	2.6.2	Probability density function 57
	2.6.3	Regression 58
	2.6.4	Why is the Gaussian distribution so widely used? 59
	2.6.5	Dirac delta function as a limiting case 59
2.7		other common univariate distributions * 60
	2.7.1	Student t distribution 60
	2.7.2	Cauchy distribution 61
	2.7.3	Laplace distribution 62
	2.7.4	Beta distribution 62
	2.7.5	Gamma distribution 63
	2.7.6	Empirical distribution 64
2.8		ormations of random variables * 65
	2.8.1	Discrete case 65
	2.8.2	Continuous case 65
	2.8.3	Invertible transformations (bijections) 65
	2.8.4	Moments of a linear transformation 67
	2.8.5	The convolution theorem 68
	2.8.6	Central limit theorem 70
	2.8.7	Monte Carlo approximation 71

CONTENTS xi

	2.9	EXERCISES 12
3	Prob	pability: Multivariate Models 75
	3.1	Joint distributions for multiple random variables 75
		3.1.1 Covariance 75
		3.1.2 Correlation 76
		3.1.3 Uncorrelated does not imply independent 77
		3.1.4 Correlation does not imply causation 77
		3.1.5 Simpsons' paradox 78
	3.2	The multivariate Gaussian (normal) distribution 78
		3.2.1 Definition 79
		3.2.2 Mahalanobis distance 81
		3.2.3 Marginals and conditionals of an MVN * 82
		3.2.4 Example: Imputing missing values * 83
	3.3	Linear Gaussian systems * 83
		3.3.1 Example: inferring a latent vector from a noisy sensor 85
		3.3.2 Example: inferring a latent vector from multiple noisy sensors 86
	3.4	The exponential family 86
		3.4.1 Definition 86
		3.4.2 Example 87
		3.4.3 Log partition function is cumulant generating function 88
		3.4.4 Maximum entropy derivation of the exponential family 88
	3.5	Mixture models 89
		3.5.1 Gaussian mixture models 90
	2.6	3.5.2 Mixtures of Bernoullis 91
	3.6	Probabilistic graphical models * 92
		3.6.1 Representation 93 3.6.2 Inference 95
	3.7	3.6.3 Learning 96 Exercises 96
	5.1	Exercises 90
4	Stat	istics 101
	4.1	Introduction 101
	4.2	Maximum likelihood estimation (MLE) 101
		4.2.1 Definition 101
		4.2.2 Justification for MLE 102
		4.2.3 Example: MLE for the Bernoulli distribution 104
		4.2.4 Example: MLE for the categorical distribution 105
		4.2.5 Example: MLE for the univariate Gaussian 105
		4.2.6 Example: MLE for the multivariate Gaussian 106
	4.0	4.2.7 Example: MLE for linear regression 108
	4.3	Empirical risk minimization (ERM) 109
		4.3.1 Example: minimizing the misclassification rate 109
	4 4	4.3.2 Surrogate loss 110
	4.4	Other estimation methods * 110

xii CONTENTS

	4.4.1	The method of moments 110
	4.4.2	Online (recursive) estimation 112
4.5	Regular	ization 114
	4.5.1	Example: MAP estimation for the Bernoulli distribution 115
	4.5.2	Example: MAP estimation for the multivariate Gaussian * 116
	4.5.3	Example: weight decay 117
	4.5.4	Picking the regularizer using a validation set 118
	4.5.5	Cross-validation 119
	4.5.6	Early stopping 120
	4.5.7	Using more data 121
4.6	Bayesia	n statistics * 121
	4.6.1	Conjugate priors 123
	4.6.2	The beta-binomial model 123
	4.6.3	The Dirichlet-multinomial model 131
	4.6.4	The Gaussian-Gaussian model 134
	4.6.5	Beyond conjugate priors 137
	4.6.6	Credible intervals 139
	4.6.7	Bayesian machine learning 140
	4.6.8	Computational issues 145
4.7	Frequer	itist statistics * 147
	4.7.1	Sampling distributions 148
	4.7.2	Gaussian approximation of the sampling distribution of the MLE 148
	4.7.3	Bootstrap approximation of the sampling distribution of any estimator 149
	4.7.4	Confidence intervals 150
	4.7.5	Caution: Confidence intervals are not credible 151
	4.7.6	The bias-variance tradeoff 152
4.8	Exercise	es 157
Deci	sion Th	eory 161
5.1		n decision theory 161
0.1	5.1.1	Basics 161
	5.1.1 $5.1.2$	Classification problems 163
	5.1.3	ROC curves 165
	5.1.4	Precision-recall curves 167
	5.1.5	Regression problems 170
	5.1.6	Probabilistic prediction problems 171
5.2		n hypothesis testing 173
0.2		Example: Testing if a coin is fair 174
	5.2.2	Bayesian model selection 174
	5.2.3	Occam's razor 176
	5.2.4	Connection between cross validation and marginal likelihood 178
	5.2.5	Information criteria 179
5.3		atist decision theory 180
0.0	5.3.1	Computing the risk of an estimator 180
	0.0.1	Computing the risk of an estimator 100

5

CONTENTS xiii

		5.3.3	Admissible estimators 183
	5.4	Empiric	al risk minimization 184
		5.4.1	Empirical risk 184
		5.4.2	Structural risk 186
		5.4.3	Cross-validation 187
		5.4.4	Statistical learning theory * 187
	5.5	Frequen	tist hypothesis testing * 189
		5.5.1	Likelihood ratio test 189
		5.5.2	Null hypothesis significance testing (NHST) 190
		5.5.3	p-values 191
		5.5.4	p-values considered harmful 191
		5.5.5	Why isn't everyone a Bayesian? 193
	5.6	Exercise	s 195
6	Info	rmation	Theory 197
	6.1	Entropy	
		6.1.1	Entropy for discrete random variables 197
		6.1.2	Cross entropy 199
		6.1.3	Joint entropy 199
		6.1.4	Conditional entropy 200
		6.1.5	Perplexity 201
		6.1.6	Differential entropy for continuous random variables * 202
	6.2	Relative	e entropy (KL divergence) * 203
		6.2.1	Definition 203
		6.2.2	Interpretation 204
		6.2.3	Example: KL divergence between two Gaussians 204
		6.2.4	Non-negativity of KL 204
		6.2.5	KL divergence and MLE 205
		6.2.6	Forward vs reverse KL 206
	6.3		information * 207
		6.3.1	Definition 207
		6.3.2	Interpretation 208
		6.3.3	Example 208
		6.3.4	Conditional mutual information 209
		6.3.5	MI as a "generalized correlation coefficient" 210
		6.3.6	Normalized mutual information 211
		6.3.7	Maximal information coefficient 211
		6.3.8	Data processing inequality 213
		6.3.9	Sufficient Statistics 214
	0.4	6.3.10	Fano's inequality * 215
	6.4	Exercise	es 216
7	Line	ar Algel	ora 219
	7.1	Introduc	
		7.1.1	Notation 219

xiv CONTENTS

	719	Vector and cod 922
	7.1.2	Vector spaces 222
	7.1.3	
	7.1.4	•
7.0	7.1.5	Special types of matrices 229
7.2		multiplication 232
	7.2.1	Vector-Vector Products 232
	7.2.2	
	7.2.3	
	7.2.4	11 0
	7.2.5	*
	7.2.6	
7.3		inversion 239
	7.3.1	The inverse of a square matrix 239
	7.3.2	*
	7.3.3	
	7.3.4	
7.4		alue decomposition (EVD) 242
	7.4.1	Basics 242
	7.4.2	0
	7.4.3	e v
	7.4.4	v i
	7.4.5	<u> </u>
	7.4.6	Power method 245
	7.4.7	
	7.4.8	Eigenvectors optimize quadratic forms 247
7.5	Singula	ar value decomposition (SVD) 248
	7.5.1	
	7.5.2	Connection between SVD and EVD 249
	7.5.3	Pseudo inverse 249
	7.5.4	SVD and the range and null space of a matrix * 250
	7.5.5	
7.6	Other	matrix decompositions * 252
	7.6.1	
	7.6.2	QR decomposition 253
	7.6.3	Cholesky decomposition 254
7.7	Solving	g systems of linear equations * 254
	7.7.1	Solving square systems 255
	7.7.2	Solving underconstrained systems (least norm estimation) 256
	7.7.3	Solving overconstrained systems (least squares estimation) 257
7.8	Matrix	calculus 258
	7.8.1	Derivatives 258
	7.8.2	Gradients 259
	7.8.3	Directional derivative 259
	7.8.4	Total derivative * 260
	7.8.5	Jacobian 260

CONTENTS

		7.8.6	Hessian 261
		7.8.7	Gradients of commonly used functions 261
	7.9	Exercis	ses 263
8	Opti	mizatio	on 265
	8.1	Introdu	action 265
		8.1.1	Local vs global optimization 265
		8.1.2	Constrained vs unconstrained optimization 267
		8.1.3	Convex vs nonconvex optimization 267
		8.1.4	Smooth vs nonsmooth optimization 271
	8.2	First-o	rder methods 272
		8.2.1	Descent direction 273
		8.2.2	Step size (learning rate) 274
		8.2.3	Convergence rates 276
		8.2.4	Momentum methods 277
	8.3	Second	-order methods 278
		8.3.1	Newton's method 279
		8.3.2	BFGS and other quasi-Newton methods 280
		8.3.3	Trust region methods 281
		8.3.4	Natural gradient descent * 282
	8.4	Stocha	stic gradient descent 285
		8.4.1	Application to finite sum problems 286
		8.4.2	Example: SGD for fitting linear regression 286
		8.4.3	Choosing the step size (learning rate) 287
		8.4.4	Iterate averaging 290
		8.4.5	Variance reduction * 290
		8.4.6	Preconditioned SGD 291
	8.5	Constr	ained optimization 294
		8.5.1	Lagrange multipliers 295
		8.5.2	The KKT conditions 296
		8.5.3	Linear programming 298
		8.5.4	Quadratic programming 299
		8.5.5	Mixed integer linear programming * 300
	8.6	Proxim	nal gradient method * 300
		8.6.1	Projected gradient descent 301
		8.6.2	Proximal operator for ℓ_1 -norm regularizer 302
		8.6.3	Proximal operator for quantization 303
	8.7	Bound	optimization * 304
		8.7.1	The general algorithm 305
		8.7.2	The EM algorithm 305
		8.7.3	Example: EM for a GMM 308
	8.8	Blackb	ox and derivative free optimization 312
	8.9	Exercis	ses 313

xvi CONTENTS

IILinear models 315

9

9	Line	ar Discriminant Analysis 317	
	9.1	Introduction 317	
	9.2	Gaussian discriminant analysis 317	
		9.2.1 Quadratic decision boundaries 318	
		9.2.2 Linear decision boundaries 319	
		9.2.3 The connection between LDA and logistic regression 319	
		9.2.4 Model fitting 320	
		9.2.5 Nearest centroid classifier 322	
		9.2.6 Fisher's linear discriminant analysis * 322	
	9.3	Naive Bayes classifiers 326	
		9.3.1 Example models 326	
		9.3.2 Model fitting 327	
		9.3.3 Bayesian naive Bayes 328	
		9.3.4 The connection between naive Bayes and logistic regression 32	9
	9.4	Generative vs discriminative classifiers 330	
		9.4.1 Advantages of discriminative classifiers 330	
		9.4.2 Advantages of generative classifiers 331	
		9.4.3 Handling missing features 331	
	9.5	Exercises 332	
10	Logi	stic regression 333	
	10.1	Introduction 333	
	10.2	Binary logistic regression 333	
		10.2.1 Linear classifiers 333	
		10.2.2 Nonlinear classifiers 334	
		10.2.3 Maximum likelihood estimation 336	
		10.2.4 Stochastic gradient descent 339	
		10.2.5 Perceptron algorithm 339	
		10.2.6 Iteratively reweighted least squares 340	
		10.2.7 MAP estimation 341	
		10.2.8 Standardization 343	
	10.3	Multinomial logistic regression 344	
		10.3.1 Linear and nonlinear classifiers 344	
		10.3.2 Maximum likelihood estimation 345	
		10.3.3 Gradient-based optimization 347	
		10.3.4 Bound optimization 347	
		10.3.5 MAP estimation 349	
		10.3.6 Maximum entropy classifiers 350	
		10.3.7 Hierarchical classification 351	
		10.3.8 Handling large numbers of classes 352	
	10.4	Robust logistic regression * 353	
		10.4.1 Mixture model for the likelihood 353	
		10.4.2 Bi-tempered loss 354	

CONTENTS

10.5	Bayesian logistic regression * 357
	10.5.1 Laplace approximation 357
	10.5.2 Approximating the posterior predictive 358
10.6	Exercises 361
11 Line	ar Regression 363
	_
	Introduction 363
11.2	Least squares linear regression 363
	11.2.1 Terminology 363
	11.2.2 Least squares estimation 364 11.2.3 Other approaches to computing the MLE 368
	11.2.3 Other approaches to computing the MLE 368 11.2.4 Measuring goodness of fit 372
11.3	Ridge regression 373
11.5	11.3.1 Computing the MAP estimate 374
	11.3.2 Connection between ridge regression and PCA 376
	11.3.3 Choosing the strength of the regularizer 377
11.4	Lasso regression 377
11.4	11.4.1 MAP estimation with a Laplace prior (ℓ_1 regularization) 378
	11.4.2 Why does ℓ_1 regularization yield sparse solutions? 379
	11.4.3 Hard vs soft thresholding 380
	11.4.4 Regularization path 381
	11.4.5 Comparison of least squares, lasso, ridge and subset selection 383
	11.4.6 Variable selection consistency 384
	11.4.7 Group lasso 386
	11.4.8 Elastic net (ridge and lasso combined) 387
	11.4.9 Optimization algorithms 389
11.5	Regression splines * 391
	11.5.1 B-spline basis functions 392
	11.5.2 Fitting a linear model using a spline basis 393
	11.5.3 Smoothing splines 394
	11.5.4 Generalized additive models 394
11.6	Robust linear regression * 394
	11.6.1 Laplace likelihood 394
	11.6.2 Student-t likelihood 396
	11.6.3 Huber loss 396
11 -	11.6.4 RANSAC 397
11.7	Bayesian linear regression * 397
	11.7.1 Priors 397
	11.7.2 Posteriors 397
	11.7.3 Example 398 11.7.4 Computing the posterior predictive 399
	11.7.5 The advantage of centering 400 11.7.6 Dealing with multicollinearity 401
11.8	· ·
11.0	LACTOROD TUU

xviii CONTENTS

12 Gene	eralized Linear Models 405
12.1	Introduction 405
12.2	Examples 405
	12.2.1 Linear regression 406
	12.2.2 Binomial regression 406
	12.2.3 Poisson regression 407
12.3	GLMs with non-canonical link functions 407
12.4	Maximum likelihood estimation 408
12.5	Worked example: predicting insurance claims 409
III D	Deep neural networks 413
13 Neu	ral Networks for Structured Data 415
13.1	Introduction 415
13.2	Multilayer perceptrons (MLPs) 416
	13.2.1 The XOR problem 417
	13.2.2 Differentiable MLPs 418
	13.2.3 Activation functions 418
	13.2.4 Example models 419
	13.2.5 The importance of depth 424
	13.2.6 The "deep learning revolution" 424
	13.2.7 Connections with biology 425
13.3	Backpropagation 427
	13.3.1 Forward vs reverse mode differentiation 428
	13.3.2 Reverse mode differentiation for multilayer perceptrons 430
	13.3.3 Vector-Jacobian product for common layers 431
	13.3.4 Computation graphs 434
13.4	Training neural networks 436
	13.4.1 Tuning the learning rate 436
	13.4.2 Vanishing and exploding gradients 436
	13.4.3 Non-saturating activation functions 437
	13.4.4 Residual connections 440
	13.4.5 Parameter initialization 442
40 5	13.4.6 Parallel training 444
13.5	Regularization 445
	13.5.1 Early stopping 446
	13.5.2 Weight decay 446
	13.5.3 Sparse DNNs 446
	13.5.4 Dropout 447
	13.5.5 Bayesian neural networks 448
19.6	13.5.6 Regularization effects of (stochastic) gradient descent * 448 Other kinds of feedforward networks 450
13.6	
	13.6.1 Radial basis function networks 450 13.6.2 Mixtures of experts 451
	13.0.4 IVIIXTUIES OF EXPERTS 401

CONTENTSxix

13.7	Exercises 454
14 N eu	ral Networks for Images 457
14.1	Introduction 457
14.2	Common layers 458
	14.2.1 Convolutional layers 458
	14.2.2 Pooling layers 465
	14.2.3 Putting it altogether 466
	14.2.4 Normalization layers 466
14.3	Common architectures for image classification 469
	14.3.1 LeNet 469
	14.3.2 AlexNet 470
	14.3.3 GoogLeNet (Inception) 471
	14.3.4 ResNet 471
	14.3.5 DenseNet 474
	14.3.6 Neural architecture search 474
14.4	Other forms of convolution * 475
	14.4.1 Dilated convolution 475
	14.4.2 Transposed convolution 475
	14.4.3 Depthwise separable convolution 477
14.5	Solving other discriminative vision tasks with CNNs 478
	14.5.1 Image tagging 478
	14.5.2 Object detection 478
	14.5.3 Instance segmentation 479
	14.5.4 Semantic segmentation 480
440	14.5.5 Human pose estimation 481
14.6	Generating images by inverting CNNs * 482
	14.6.1 Converting a trained classifier into a generative model 482
	14.6.2 Image priors 483
	14.6.3 Visualizing the features learned by a CNN 484
	14.6.4 Deep Dream 485
	14.6.5 Neural style transfer 486
15 Neu	ral networks for sequences 491
15.1	Introduction 491
15.2	Recurrent neural networks (RNNs) 491
	15.2.1 Vec2Seq (sequence generation) 491
	15.2.2 Seq2Vec (sequence classification) 494
	15.2.3 Seq2Seq (sequence translation) 495
	15.2.4 Teacher forcing 497
	15.2.5 Backpropagation through time 498
	15.2.6 Vanishing and exploding gradients 499
	15.2.7 Gating and long term memory 500
	15.2.8 Beam search 503
15.3	1d CNNs 504

Author: Kevin P. Murphy. (C) MIT Press. CC-BY-NC-ND license

15.3 1d CNNs

XX CONTENTS

	15.3.1	1d CNNs for sequence classification 504
	15.3.2	Causal 1d CNNs for sequence generation 505
15.4	Attenti	
	15.4.1	Attention as soft dictionary lookup 506
	15.4.2	Kernel regression as non-parametric attention 507
	15.4.3	Parametric attention 508
	15.4.4	Seq2Seq with attention 509
	15.4.5	Seq2vec with attention (text classification) 511
	15.4.6	Seq+Seq2Vec with attention (text pair classification) 511
	15.4.7	Soft vs hard attention 513
15.5	Transfo	
	15.5.1	
	15.5.2	Multi-headed attention 514
		Positional encoding 515
		Putting it altogether 517
	15.5.5	Comparing transformers, CNNs and RNNs 518
	15.5.6	Transformers for images * 519
	15.5.7	Other transformer variants * 520
15.6		t transformers * 520
	15.6.1	Fixed non-learnable localized attention patterns 521
	15.6.2	Learnable sparse attention patterns 521
	15.6.3	Memory and recurrence methods 522
	15.6.4	Low-rank and kernel methods 522
15.7	0	ge models and unsupervised representation learning 524
	15.7.1	ELMo 524
	15.7.2	BERT 525
		GPT 529
		T5 530
	15.7.5	Discussion 530
IV N	onpar	ametric models 531
16 Exer	nplar-b	ased Methods 533
16.1	K neare	est neighbor (KNN) classification 533
		Example 534
	16.1.2	The curse of dimensionality 534
	16.1.3	Reducing the speed and memory requirements 536
	16.1.4	Open set recognition 536
16.2		g distance metrics 537
	16.2.1	Linear and convex methods 538
	16.2.2	Deep metric learning 539
	16.2.3	Classification losses 540
	16.2.4	Ranking losses 540
	16.2.5	Speeding up ranking loss optimization 542

Draft of "Probabilistic Machine Learning: An Introduction". July 20, 2021

CONTENTS

	16.2.6 Other training tricks for DML 545
16.3	Kernel density estimation (KDE) 545
	16.3.1 Density kernels 546
	16.3.2 Parzen window density estimator 546
	16.3.3 How to choose the bandwidth parameter 548
	16.3.4 From KDE to KNN classification 548
	16.3.5 Kernel regression 549
17 Keri	nel Methods 553
17.1	Inferring functions from data 553
	17.1.1 Smoothness prior 554
	17.1.2 Inference from noise-free observations 554
	17.1.3 Inference from noisy observations 556
17.2	Mercer kernels 556
	17.2.1 Mercer's theorem 557
	17.2.2 Some popular Mercer kernels 557
17.3	Gaussian processes 562
	17.3.1 Noise-free observations 562
	17.3.2 Noisy observations 563
	17.3.3 Comparison to kernel regression 565
	17.3.4 Weight space vs function space 565
	17.3.5 Numerical issues 566
	17.3.6 Estimating the kernel 566
	17.3.7 GPs for classification 569
	17.3.8 Connections with deep learning 571
17.4	Scaling GPs to large datasets 571
	17.4.1 Sparse (inducing-point) approximations 571
	17.4.2 Exploiting parallelization and kernel matrix structure 571
	17.4.3 Random feature approximation 572
17.5	Support vector machines (SVMs) 573
	17.5.1 Large margin classifiers 573
	17.5.2 The dual problem 576
	17.5.3 Soft margin classifiers 577
	17.5.4 The kernel trick 578
	17.5.5 Converting SVM outputs into probabilities 579
	17.5.6 Connection with logistic regression 580
	17.5.7 Multi-class classification with SVMs 580
	17.5.8 How to choose the regularizer C 581
	17.5.9 Kernel ridge regression 583
17.6	17.5.10 SVMs for regression 584 Sparse vector machines 585
17.6	1
	17.6.1 Relevance vector machines (RVMs) 587 17.6.2 Comparison of sparse and dense kernel methods 587
177	Exercises 590
11.1	LIACI CIDCO 000

XXII CONTENTS

591

18 Trees, Forests, Bagging and Boosting

	18.1	Classifi	cation and regression trees (CART) 591
		18.1.1	Model definition 591
		18.1.2	Model fitting 593
		18.1.3	Regularization 594
		18.1.4	Handling missing input features 594
		18.1.5	Pros and cons 594
	18.2	Ensemb	ole learning 596
		18.2.1	Stacking 596
		18.2.2	Ensembling is not Bayes model averaging 597
	18.3	Baggin	g = 597
	18.4	Randor	m forests 598
	18.5	Boostin	ng 599
		18.5.1	Forward stagewise additive modeling 600
		18.5.2	Quadratic loss and least squares boosting 600
		18.5.3	Exponential loss and AdaBoost 601
		18.5.4	LogitBoost 604
		18.5.5	Gradient boosting 604
	18.6	Interpr	eting tree ensembles 608
		18.6.1	Feature importance 609
		18.6.2	Partial dependency plots 610
. 7	ъ		. 11
V	Ве	yond	supervised learning 613
19	Lear	ning wi	ith Fewer Labeled Examples 615
	19.1	Data a	ugmentation 615
		19.1.1	Examples 615
		19.1.2	Theoretical justification 616
	19.2	Transfe	er learning 616
		19.2.1	Fine-tuning 617
		19.2.2	Adapters 618
		19.2.3	Supervised pre-training 619
		19.2.4	Unsupervised pre-training (self-supervised learning) 620
		19.2.5	Domain adaptation 625
	19.3	Semi-su	pervised learning 625
		4004	Self-training and pseudo-labeling 626
		19.3.1	2
		19.3.1 19.3.2	Entropy minimization 627
			Entropy minimization 627
		19.3.2	Entropy minimization 627
		19.3.2 19.3.3	Entropy minimization 627 Co-training 630 Label propagation on graphs 630 Consistency regularization 631
		19.3.2 19.3.3 19.3.4	Entropy minimization 627 Co-training 630 Label propagation on graphs 630
		19.3.2 19.3.3 19.3.4 19.3.5	Entropy minimization 627 Co-training 630 Label propagation on graphs 630 Consistency regularization 631
	19.4	19.3.2 19.3.3 19.3.4 19.3.5 19.3.6 19.3.7	Entropy minimization 627 Co-training 630 Label propagation on graphs 630 Consistency regularization 631 Deep generative models * 633

Draft of "Probabilistic Machine Learning: An Introduction". July 20, 2021

CONTENTS xxiii

			Information-theoretic approach 638	
			Batch active learning 639	
	19.5	Meta-lea		
				639
	19.6		t learning 640	
			Matching networks 641	
	19.7		supervised learning 642	
	19.8	Exercise	es 643	
20	Dime	ensional	ity Reduction 645	
	20.1	Principa	al components analysis (PCA) 645	
		20.1.1	Examples 645	
		20.1.2	Derivation of the algorithm 647	
		20.1.3	Computational issues 650	
		20.1.4	Choosing the number of latent dimensions	652
	20.2	Factor a	nalysis * 654	
			Generative model 655	
		20.2.2	Probabilistic PCA 656	
		20.2.3	EM algorithm for FA/PPCA 657	
		20.2.4	Unidentifiability of the parameters 659	
		20.2.5	Nonlinear factor analysis 661	
		20.2.6	Mixtures of factor analysers 662	
		20.2.7	Exponential family factor analysis 663	
		20.2.8	1	65
	20.3	Autoend		
			Bottleneck autoencoders 668	
		20.3.2	Denoising autoencoders 669	
		20.3.3	Contractive autoencoders 670	
		20.3.4	Sparse autoencoders 671	
		20.3.5	Variational autoencoders 671	
	20.4		d learning * 676	
			What are manifolds? 677	
		20.4.2	The manifold hypothesis 677	
		20.4.3	Approaches to manifold learning 678	
		20.4.4	Multi-dimensional scaling (MDS) 679	
		20.4.5	Isomap 682	
		20.4.6	Kernel PCA 683	
			Maximum variance unfolding (MVU) 688	5
		20.4.8	Local linear embedding (LLE) 685	
		20.4.9	Laplacian eigenmaps 686	
			t-SNE 689	
	20.5		nbeddings 693	
		20.5.1	Latent semantic analysis / indexing 693	
		20.5.2	Word2vec 695	
		20.5.3	GloVE 697	

xxiv CONTENTS

		20.5.4	Word analogies 698
		20.5.5	RAND-WALK model of word embeddings 699
		20.5.6	arphi
	20.6	Exercise	\sim 700
21	Clust	tering	703
	21.1	Introduc	etion 703
		21.1.1	Evaluating the output of clustering methods 703
	21.2	Hierarch	nical agglomerative clustering 705
		21.2.1	The algorithm 706
		21.2.2	Example 708
		21.2.3	Extensions 709
	21.3		s clustering 710
			The algorithm 710
		21.3.2	Examples 710
			Vector quantization 712
		21.3.4	The K-means++ algorithm 713
		21.3.5	The K-medoids algorithm 713
		21.3.6	Speedup tricks 714
		21.3.7	Choosing the number of clusters K 715
	21.4		ng using mixture models 718
		21.4.1	Mixtures of Gaussians 718
	~ -	21.4.2	Mixtures of Bernoullis 722
	21.5		clustering * 722
			Normalized cuts 722
			Eigenvectors of the graph Laplacian encode the clustering 723
			Example 724
	01.0	21.5.4	Connection with other methods 724
	21.6	Bicluste	· ·
			Basic biclustering 725
		21.6.2	Nested partition models (Crosscat) 726
22	Reco	\mathbf{mmend}	er Systems 729
	22.1	Explicit	feedback 729
		22.1.1	Datasets 729
			Collaborative filtering 730
		22.1.3	Matrix factorization 731
		22.1.4	Autoencoders 733
	22.2	_	feedback 734
		22.2.1	Bayesian personalized ranking 735
		22.2.2	Factorization machines 735
		22.2.3	Neural matrix factorization 736
	22.3	_	ing side information 737
	22.4	Explora	tion-exploitation tradeoff 738
72	Cran	h Embe	addings 7/1

CONTENTSxxv

	23.1	Introduction 741
	23.2	Graph Embedding as an Encoder/Decoder Problem 742
	23.3	Shallow graph embeddings 744
		23.3.1 Unsupervised embeddings 745
		23.3.2 Distance-based: Euclidean methods 745
		23.3.3 Distance-based: non-Euclidean methods 746
		23.3.4 Outer product-based: Matrix factorization methods 746
		23.3.5 Outer product-based: Skip-gram methods 747
		23.3.6 Supervised embeddings 749
	23.4	T T
		23.4.1 Message passing GNNs 750
		23.4.2 Spectral Graph Convolutions 751
		23.4.3 Spatial Graph Convolutions 751
		23.4.4 Non-Euclidean Graph Convolutions 753
	23.5	Deep graph embeddings 753
		23.5.1 Unsupervised embeddings 754
	22.0	23.5.2 Semi-supervised embeddings 756
	23.6	Applications 757
		23.6.1 Unsupervised applications 757
		23.6.2 Supervised applications 759
\mathbf{A}	ppend	lices 761
\mathbf{V}	I A	ppendix 763
A	Nota	ation 765
		Introduction 765
	A.3	
		v
	11.0	Functions 766
	11.0	Functions 766 A.3.1 Common functions of one argument 766
	11.0	Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766
		Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766
	A.4	Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767
		Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767
		Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767 A.4.2 Vectors 767
		Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767 A.4.2 Vectors 767 A.4.3 Matrices 767
	A.4	Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767 A.4.2 Vectors 767 A.4.3 Matrices 767 A.4.4 Matrix calculus 768
	A.4 A.5	Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767 A.4.2 Vectors 767 A.4.3 Matrices 767 A.4.4 Matrix calculus 768 Optimization 768
	A.4 A.5 A.6	Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767 A.4.2 Vectors 767 A.4.3 Matrices 767 A.4.4 Matrix calculus 768 Optimization 768 Probability 769
	A.4 A.5 A.6 A.7	Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767 A.4.2 Vectors 767 A.4.3 Matrices 767 A.4.4 Matrix calculus 768 Optimization 768 Probability 769 Information theory 769
	A.4 A.5 A.6	Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767 A.4.2 Vectors 767 A.4.3 Matrices 767 A.4.4 Matrix calculus 768 Optimization 768 Probability 769 Information theory 769 Statistics and machine learning 769
	A.4 A.5 A.6 A.7	Functions 766 A.3.1 Common functions of one argument 766 A.3.2 Common functions of two arguments 766 A.3.3 Common functions of > 2 arguments 766 Linear algebra 767 A.4.1 General notation 767 A.4.2 Vectors 767 A.4.3 Matrices 767 A.4.4 Matrix calculus 768 Optimization 768 Probability 769 Information theory 769 Statistics and machine learning 769

Author: Kevin P. Murphy. (C) MIT Press. CC-BY-NC-ND license

XXVI CONTENTS

A.9 Abbreviations 771

Bibliography 784