Contents

	Preface		<i>page</i> xi		
1	Introduction				
	1.1	Teaching a computer to distinguish cats from dogs	1		
		1.1.1 The pipeline of a typical machine learning problem	5		
	1.2	Predictive learning problems	6		
		1.2.1 Regression	6		
		1.2.2 Classification	9		
	1.3	Feature design	12		
	1.4	Numerical optimization	15		
	1.5	Summary	16		
Part I	Fundame	ental tools and concepts	19		
2	Fundamentals of numerical optimization				
	2.1	Calculus-defined optimality	21		
		2.1.1 Taylor series approximations	21		
		2.1.2 The first order condition for optimality	22		
		2.1.3 The convenience of convexity	24		
	2.2				
		2.2.1 The big picture	27		
		2.2.2 Stopping condition	27		
		2.2.3 Gradient descent	29		
		2.2.4 Newton's method	33		
	2.3	Summary	38		
	2.4	Exercises	38		
3	Regression				
	3.1	3.1 The basics of linear regression			
		3.1.1 Notation and modeling	45		
		3.1.2 The Least Squares cost function for linear regression	n 47		
		3.1.3 Minimization of the Least Squares cost function	48		

		3.1.4	The efficacy of a learned model	50	
		3.1.5	•	50	
	3.2		edge-driven feature design for regression	51	
		3.2.1	General conclusions	54	
	3.3	Nonlin	hear regression and ℓ_2 regularization	56	
		3.3.1	Logistic regression	56	
		3.3.2	Non-convex cost functions and ℓ_2 regularization	59	
	3.4	Summa		61	
	3.5	Exercis		62	
4	Class	Classification			
	4.1	The pe	erceptron cost functions	73	
		4.1.1	The basic perceptron model	73	
		4.1.2	The softmax cost function	75	
		4.1.3	The margin perceptron	78	
		4.1.4		80	
		4.1.5	The accuracy of a learned classifier	82	
		4.1.6	Predicting the value of new input data	83	
		4.1.7	Which cost function produces the best results?	84	
		4.1.8	The connection between the perceptron and counting		
			costs	85	
	4.2	The log	gistic regression perspective on the softmax cost	86	
		4.2.1	Step functions and classification	87	
		4.2.2	Convex logistic regression	89	
	4.3	The su	ipport vector machine perspective on the margin		
		percep		91	
		4.3.1	A quest for the hyperplane with maximum margin	91	
		4.3.2	The hard-margin SVM problem	93	
		4.3.3	The soft-margin SVM problem	93	
		4.3.4	Support vector machines and logistic regression	95	
	4.4	Multic	lass classification	95	
		4.4.1	One-versus-all multiclass classification	96	
		4.4.2	Multiclass softmax classification	99	
		4.4.3	The accuracy of a learned multiclass classifier	103	
		4.4.4	Which multiclass classification scheme works best?	104	
	4.5	Knowl	edge-driven feature design for classification	104	
		4.5.1	General conclusions	106	
	4.6	Histog	ram features for real data types	107	
		4.6.1	Histogram features for text data	109	
		4.6.2	Histogram features for image data	112	
		4.6.3	Histogram features for audio data	115	
	4.7	Summa	_	117	
	4.8	Exercis	·	118	

			Contents VII			
Dart II	Tools for	fully data-driven machine learning	129			
raitii	10015 101	Tuny data-driven machine learning	129			
5	Auto	matic feature design for regression	131			
	5.1	Automatic feature design for the ideal regression scenari	o 131			
		5.1.1 Vector approximation	132			
		5.1.2 From vectors to continuous functions	133			
		5.1.3 Continuous function approximation	134			
		5.1.4 Common bases for continuous function approxi	mation 135			
		5.1.5 Recovering weights	140			
		5.1.6 Graphical representation of a neural network	140			
	5.2	Automatic feature design for the real regression scenario	141			
		5.2.1 Approximation of discretized continuous function	ons 142			
		5.2.2 The real regression scenario	142			
	5.3	Cross-validation for regression	146			
		5.3.1 Diagnosing the problem of overfitting/underfitting	ng 149			
		5.3.2 Hold out cross-validation	149			
		5.3.3 Hold out calculations	151			
		5.3.4 <i>k</i> -fold cross-validation	152			
	5.4	Which basis works best?	155			
		5.4.1 Understanding of the phenomenon underlying the	he data 156			
		5.4.2 Practical considerations	156			
		5.4.3 When the choice of basis is arbitrary	156			
	5.5	Summary	158			
	5.6	Exercises	158			
	5.7	Notes on continuous function approximation	165			
6	Auto	Automatic feature design for classification				
	6.1	Automatic feature design for the ideal classification scen	ario 166			
		6.1.1 Approximation of piecewise continuous function	ns 166			
		6.1.2 The formal definition of an indicator function	168			
		6.1.3 Indicator function approximation	170			
		6.1.4 Recovering weights	170			
	6.2	Automatic feature design for the real classification scena	rio 171			
		6.2.1 Approximation of discretized indicator function	s 171			
		6.2.2 The real classification scenario	172			
		6.2.3 Classifier accuracy and boundary definition	178			
	6.3	Multiclass classification	179			
		6.3.1 One-versus-all multiclass classification	179			
		6.3.2 Multiclass softmax classification	180			
	6.4	Cross-validation for classification				
		6.4.1 Hold out cross-validation	182			
		6.4.2 Hold out calculations	182			

		6.4.3	k-fold cross-validation	184
		6.4.4	<i>k</i> -fold cross-validation for one-versus-all multiclass	
			classification	187
	6.5	Which	basis works best?	187
	6.6	Summa		188
	6.7	Exercis		189
7	Kern	els, back	propagation, and regularized cross-validation	195
	7.1		feature kernels	195
		7.1.1	The fundamental theorem of linear algebra	196
		7.1.2		197
		7.1.3		197
		7.1.4	Examples of kernels	199
		7.1.5	_	201
	7.2	The ba	ckpropagation algorithm	202
		7.2.1	Computing the gradient of a two layer network cost	
			function	203
		7.2.2	Three layer neural network gradient calculations	205
		7.2.3		206
	7.3	Cross-	validation via ℓ_2 regularization	208
		7.3.1	ℓ_2 regularization and cross-validation	209
		7.3.2	Regularized <i>k</i> -fold cross-validation for regression	210
		7.3.3	Regularized cross-validation for classification	211
	7.4	Summa	_	212
	7.5		r kernel calculations	212
		7.5.1	Kernelizing various cost functions	212
		7.5.2	Fourier kernel calculations – scalar input	214
		7.5.3		215
Part III	Method	s for lar	ge scale machine learning	217
	_		- -	
8		_	dient schemes	219
	8.1		step length rules for gradient descent	219
			Gradient descent and simple quadratic surrogates	219
		8.1.2	Functions with bounded curvature and optimally conservative	
			step length rules	221
		8.1.3	How to use the conservative fixed step length rule	224
	8.2	_	ve step length rules for gradient descent	225
		8.2.1	Adaptive step length rule via backtracking line search	226
		8.2.2	How to use the adaptive step length rule	227
	8.3		stic gradient descent	229
		8.3.1	Decomposing the gradient	229
		8.3.2	The stochastic gradient descent iteration	230
		8.3.3	The value of stochastic gradient descent	232

		8.3.4 Step length rules for stochastic gradient descent	233
		8.3.5 How to use the stochastic gradient method in practice	234
	8.4	Convergence proofs for gradient descent schemes	235
		8.4.1 Convergence of gradient descent with Lipschitz constant fix	ed
		step length	236
		8.4.2 Convergence of gradient descent with backtracking line	
		search	236
		8.4.3 Convergence of the stochastic gradient method	238
		8.4.4 Convergence rate of gradient descent for convex functions	
		with fixed step length	239
	8.5	Calculation of computable Lipschitz constants	241
	8.6	Summary	243
	8.7	Exercises	243
9	Dime	ension reduction techniques	245
	9.1	Techniques for data dimension reduction	245
		9.1.1 Random subsampling	245
		9.1.2 K-means clustering	246
		9.1.3 Optimization of the <i>K</i> -means problem	249
	9.2	Principal component analysis	250
		9.2.1 Optimization of the PCA problem	256
	9.3	Recommender systems	256
		9.3.1 Matrix completion setup	257
		9.3.2 Optimization of the matrix completion model	258
	9.4	Summary	259
	9.5	Exercises	260
Pa	rt IV Append	ices	263
	Dania waatau		265
Α		and matrix operations	265
	A.1	Vector operations	265
	A.2	Matrix operations	266
В	Basics of vec	tor calculus	268
	B.1	Basic definitions	268
	B.2	Commonly used rules for computing derivatives	269
	B.3	Examples of gradient and Hessian calculations	269
C	Fundamental	matrix factorizations and the pseudo-inverse	274
	C.1	Fundamental matrix factorizations	274
		C.1.1 The singular value decomposition	274
		C.1.2 Eigenvalue decomposition	276
		C.1.3 The pseudo-inverse	277

Contents

İΧ

Contents

Index

Χ

D	Convex geometry			278
	D.1	Definit	tions of convexity	278
		D.1.1	Zeroth order definition of a convex function	278
		D.1.2	First order definition of a convex function	279
	Refer	rences		280

285