Contents

Preface xxxv							
1	Introduction 1						
Ι	Fundamentals 3						
2	Prob	ability	5				
	2.1	Introdu	ction 5				
	2.2	Some co	ommon probability distributions 5				
		2.2.1	Discrete distributions 5				
		2.2.2	Continuous distributions on \mathbb{R} 6				
		2.2.3	Continuous distributions on \mathbb{R}^+ 9				
		2.2.4	Continuous distributions on $[0,1]$ 12				
		2.2.5	The multivariate Gaussian (normal) distribution 13				
		2.2.6	Some other multivariate continuous distributions 24				
	2.3	The exp	ponential family 29				
		2.3.1	Definition 30				
		2.3.2	Examples 31				
		2.3.3	Log partition function is cumulant generating function 35				
		2.3.4	Canonical (natural) vs mean (moment) parameters 37				
		2.3.5	MLE for the exponential family 38				
		2.3.6	Exponential dispersion family 39				
		2.3.7	Maximum entropy derivation of the exponential family 39				
	2.4	Fisher i	nformation matrix (FIM) 40				
		2.4.1	Definition 40				
		2.4.2	Equivalence between the FIM and the Hessian of the NLL 40				
		2.4.3	Examples 42				
		2.4.4	Approximating KL divergence using FIM 43				
		2.4.5	Fisher information matrix for exponential family 43				
	2.5		rmations of random variables 44				
		2.5.1	Invertible transformations (bijections) 45				
		2.5.2	Monte Carlo approximation 45				
		2.5.3	Probability integral transform 46				
	2.6	Markov					
		2.6.1	Parameterization 47				
		2.6.2	Application: Language modeling 50				
		2.6.3	Parameter estimation 50				
		2.6.4	Stationary distribution of a Markov chain 52				
	2.7	Diverge	nce measures between probability distributions 56				

x

47

```
1
               2.7.1
                        f-divergence
                                         56
2
                2.7.2
                        Integral probability metrics
3
                2.7.3
                        Maximum mean discrepancy (MMD)
                                                                   59
4
                        Total variation distance
                2.7.4
5
               2.7.5
                        Comparing distributions using binary classifiers
                                                                              61
6
      3 Bayesian statistics
                                     65
7
               Introduction
                                 65
         3.1
8
                        Frequentist statistics
               3.1.1
               3.1.2
                        Bayesian statistics
9
               3.1.3
                        Arguments for the Bayesian approach
                                                                    66
10
               3.1.4
                        Arguments against the Bayesian approach
                                                                        67
11
               3.1.5
                        Why not just use MAP estimation?
                                                                  67
12
         3.2
               Closed-form analysis using conjugate priors
                                                                 72
               3.2.1
                         The binomial model
13
               3.2.2
                         The multinomial model
14
               3.2.3
                        The univariate Gaussian model
                                                             74
<u>15</u>
         3.3
                Conjugate Bayesian analysis for the multivariate Gaussian
                                                                                79
16
                3.3.1
                        Posterior of \mu given \Sigma
                                                    79
                        Posterior of \Sigma given \mu
                                                    80
               3.3.2
17
               3.3.3
                        Posterior of \Sigma and \mu
18
                3.3.4
                        Conjugate-exponential models
                                                            85
<u>19</u>
         3.4
               Beyond conjugate priors
               3.4.1
                        Robust (heavy-tailed) priors
                                                          88
20
                3.4.2
                        Priors for variance parameters
                                                            88
21
         3.5
               Noninformative priors
                                           89
22
                3.5.1
                        Maximum entropy priors
                                                       90
23
               3.5.2
                        Jeffreys priors
                                            91
24
               3.5.3
                        Invariant priors
                                             94
                3.5.4
                        Reference priors
                                              95
25
         3.6
               Hierarchical priors
26
                         A hierarchical binomial model
               3.6.1
                                                            96
27
                3.6.2
                        A hierarchical Gaussian model
                                                             98
               Empirical Bayes
                                     101
         3.7
28
               3.7.1
                         A hierarchical binomial model
                                                            102
29
               3.7.2
                         A hierarchical Gaussian model
                                                             103
30
               3.7.3
                        Hierarchical Bayes for n-gram smoothing
                                                                       104
31
               Model selection and evaluation
         3.8
                                                    106
               3.8.1
                        Bayesian model selection
32
                                                                 107
               3.8.2
                        Estimating the marginal likelihood
33
               3.8.3
                        Connection between cross validation and marginal likelihood
                                                                                           108
\underline{34}
               3.8.4
                        Pareto-Smoothed Importance Sampling LOO estimate
35
               3.8.5
                        Information criteria
                                                 110
               3.8.6
                         Posterior predictive checks
                                                        112
36
               3.8.7
                        Bayesian p-values
                                               113
37
      4 Probabilistic graphical models
                                                   117
38
                Introduction
                                 117
         4.1
39
         4.2
                Directed graphical models (Bayes nets)
40
                        Representing the joint distribution
                4.2.1
41
                4.2.2
                        Examples
                                       118
42
                4.2.3
                        Gaussian Bayes nets
                4.2.4
                        Conditional independence properties
                                                                   123
43
               4.2.5
                        Generation (sampling)
44
               4.2.6
                        Inference
                                      128
<u>45</u>
               4.2.7
                         Learning
                                      130
46
                4.2.8
                        Plate notation
                                            135
```

```
1
              Undirected graphical models (Markov random fields)
                                                                       138
2
        4.3
              4.3.1
                       Representing the joint distribution
3
              4.3.2
                       Fully visible MRFs (Ising, Potts, Hopfield, etc)
                                                                          140
4
              4.3.3
                                                                                  146
                       MRFs with latent variables (Boltzmann machines, etc)
5
              4.3.4
                       Maximum entropy models
                                                     148
              4.3.5
6
                       Gaussian MRFs
                                           150
              4.3.6
                       Conditional independence properties
                                                                153
7
              4.3.7
                       Generation (sampling)
                                                  155
8
              4.3.8
                       Inference
                                    155
9
              4.3.9
                       Learning
                                    156
10
        4.4
              Conditional random fields (CRFs)
                                                    160
              4.4.1
                       1d CRFs
                                    160
11
              4.4.2
                       2d CRFs
                                    163
12
              4.4.3
                       Parameter estimation
                                                 166
13
              4.4.4
                       Other approaches to structured prediction
                                                                     167
14
        4.5
              Comparing directed and undirected PGMs
                                        167
              4.5.1
                       CI properties
15
              4.5.2
                       Converting between a directed and undirected model
<u>16</u>
              4.5.3
                       Conditional directed vs undirected PGMs and the label bias problem
                                                                                                170
17
              4.5.4
                       Combining directed and undirected graphs
18
              4.5.5
                       Comparing directed and undirected Gaussian PGMs
                                                                               173
        4.6
              PGM extensions
                                   175
19
              4.6.1
                       Factor graphs
                                         175
20
              4.6.2
                       Probabilistic circuits
                                                178
21
              4.6.3
                       Directed relational PGMs
                                                     178
22
                                                        180
              4.6.4
                       Undirected relational PGMs
              4.6.5
                       Open-universe probability models
                                                             183
23
              4.6.6
                       Programs as probability models
                                                           184
24
              Structural causal models
                                           184
25
              4.7.1
                       Example: causal impact of education on wealth
                                                                           185
26
              4.7.2
                       Structural equation models
              4.7.3
                       Do operator and augmented DAGs
                                                              187
27
              4.7.4
                       Estimating average treatment effect using path analysis
                                                                                   188
28
              4.7.5
                       Counterfactuals
                                           189
29
                                    193
     5 Information theory
30
              KL divergence
                                 193
        5.1
31
              5.1.1
                       Desiderata
                                      194
32
              5.1.2
                       The KL divergence uniquely satisfies the desiderata
                                                                               195
33
              5.1.3
                       Thinking about KL
                                               198
34
              5.1.4
                       Properties of KL
                       KL divergence and MLE
              5.1.5
35
              5.1.6
                       KL divergence and Bayesian Inference
36
              5.1.7
                       KL divergence and Exponential Families
                                                                    204
37
              5.1.8
                       Bregman divergence
                                               205
38
        5.2
                           206
              Entropy
              5.2.1
                       Definition
39
              5.2.2
                       Differential entropy for continuous random variables
                                                                               207
40
                       Typical sets
              5.2.3
                                       208
41
              5.2.4
                       Cross entropy and perplexity
                                                        209
42
                                      210
        5.3
              Mutual information
                       Definition
                                     210
              5.3.1
43
              5.3.2
                                         210
                       Interpretation
44
              5.3.3
                       Data processing inequality
                                                      211
45
              5.3.4
                       Sufficient Statistics
46
                                                            212
              5.3.5
                       Multivariate mutual information
```

```
1
              5.3.6
                       Variational bounds on mutual information
                                                                       215
2
              5.3.7
                       Relevance networks
                                                217
3
              Data compression (source coding)
                                                      218
        5.4
4
              5.4.1
                       Lossless compression
5
              5.4.2
                       Lossy compression and the rate-distortion tradeoff
                                                                               219
              5.4.3
                       Bits back coding
                                             221
6
        5.5
              Error-correcting codes (channel coding)
                                                            222
7
        5.6
              The information bottleneck
                                               224
8
              5.6.1
                       Vanilla IB
9
              5.6.2
                       Variational IB
                                          225
              5.6.3
                       Conditional entropy bottleneck
                                                            226
10
11
       Optimization
                              229
12
              Introduction
                                229
13
        6.2
              Automatic differentiation
                                             229
                       Differentiation in functional form
                                                              229
14
              6.2.2
                       Differentiating chains, circuits, and programs
                                                                          234
15
        6.3
              Stochastic gradient descent
                                               239
16
        6.4
              Natural gradient descent
                                            240
<u>17</u>
                       Defining the natural gradient
                                                          240
              6.4.1
              6.4.2
                       Interpretations of NGD
                                                    241
18
              6.4.3
                       Benefits of NGD
                                             242
<u>19</u>
              6.4.4
                       Approximating the natural gradient
20
              6.4.5
                       Natural gradients for the exponential family
                                                                         244
21
              Gradients of stochastic functions
              6.5.1
                       Minibatch approximation to finite-sum objectives
                                                                              247
<u>22</u>
              6.5.2
                       Optimizing parameters of a distribution
23
              6.5.3
                       Score function estimator (likelihood ratio trick)
                                                                            248
^{24}
              6.5.4
                       Reparameterization trick
                                                     249
25
              6.5.5
                       The delta method
                                              251
              6.5.6
                       Gumbel softmax trick
26
              6.5.7
                       Stochastic computation graphs
                                                           252
27
              6.5.8
                       Straight-through estimator
                                                       252
28
              Bound optimization (MM) algorithms
                                                          253
29
                       The general algorithm
              6.6.1
                                                   253
30
              6.6.2
                       Example: logistic regression
                                                        254
              6.6.3
                       The EM algorithm
                                               256
31
              6.6.4
                       Example: EM for an MVN with missing data
32
              6.6.5
                       Example: robust linear regression using Student-t likelihood
                                                                                         260
33
              6.6.6
                       Extensions to EM
                                              261
\underline{34}
        6.7
              The Bayesian learning rule
                                              263
              6.7.1
                       Deriving inference algorithms from BLR
<u>35</u>
              6.7.2
                       Deriving optimization algorithms from BLR
                                                                         266
36
              6.7.3
                       Variational optimization
                                                     270
37
              Bayesian optimization
                       Sequential model-based optimization
                                                                 271
38
              6.8.1
              6.8.2
                                                272
                       Surrogate functions
39
              6.8.3
                       Acquisition functions
                                                 273
40
              6.8.4
                       Other issues
                                        276
41
              Derivative free optimization
                                               277
42
                       Local search
                                        277
              6.9.1
              6.9.2
                       Simulated annealing
                                                280
43
                       Evolutionary algorithms
                                                     283
              6.9.3
44
              6.9.4
                       Estimation of distribution (EDA) algorithms
                                                                          284
45
              6.9.5
                                                  287
                       Cross-entropy method
46
              6.9.6
                       Evolutionary strategies
                                                   287
```

1					
2		6.10	Optimal Transport 289		
3			6.10.1 Warm-up: Matching optimally two families of points 289		
			6.10.2 From Optimal Matchings to Kantorovich and Monge formulations 289		
4		0.11	6.10.3 Solving optimal transport 292		
<u>5</u>		6.11	Submodular optimization 297		
<u>6</u>			6.11.1 Intuition, Examples, and Background 297 6.11.2 Submodular Basic Definitions 300		
<u>7</u>			6.11.3 Example Submodular Functions 300 6.11.3 Example Submodular Functions 301		
8			6.11.4 Submodular Optimization 303		
9			6.11.5 Applications of Submodularity in Machine Learning and AI 308		
_ 10			6.11.6 Sketching, CoreSets, Distillation, and Data Subset & Feature Selection 308		
			6.11.7 Combinatorial Information Functions 312		
11			6.11.8 Clustering, Data Partitioning, and Parallel Machine Learning 313		
<u>12</u>			6.11.9 Active and Semi-Supervised Learning 313		
<u>13</u>			6.11.10 Probabilistic Modeling 314		
$\underline{14}$			6.11.11 Structured Norms and Loss Functions 316		
<u>15</u>			6.11.12 Conclusions 316		
16					
<u>17</u>	Π	I	nference 317		
18					
	7		rence algorithms: an overview 319		
<u>19</u>		7.1	Introduction 319		
<u>20</u>		7.2	Common inference patterns 319		
<u>21</u>			7.2.1 Global latents 320 7.2.2 Local latents 320		
<u>22</u>			7.2.3 Global and local latents 321		
23		7.3	Exact inference algorithms 321		
$\underline{24}$		7.4	Approximate inference algorithms 322		
			7.4.1 MAP estimation 322		
26			7.4.2 Grid approximation 322		
			7.4.3 Laplace (quadratic) approximation 323		
<u>27</u>			7.4.4 Variational inference 324		
<u>28</u>			7.4.5 Markov Chain Monte Carlo (MCMC) 326		
<u>29</u>			7.4.6 Sequential Monte Carlo 327 7.4.7 Challenging posteriors 328		
<u>30</u>		7.5	Evaluating approximate inference algorithms 328		
31					
32	8	Infe	erence for state-space models 331		
33		8.1	Introduction 331		
		8.2	Inference for discrete chains 331		
34			8.2.1 Example: casino HMM 332		
<u>35</u>			8.2.2 Forwards filtering 333 8.2.3 Backwards smoothing 335		
<u>36</u>			8.2.4 The forwards-backwards algorithm 337		
<u>37</u>			8.2.5 Numerically stable implementation 338		
38			8.2.6 Time and space complexity 340		
39			8.2.7 The Viterbi algorithm 340		
40			8.2.8 Forwards filtering, backwards sampling 343		
41		8.3	Inference for linear-Gaussian chains 344		
			8.3.1 Examples 344		
42			8.3.2 The Kalman filter 347		
<u>43</u>			8.3.3 The Kalman (RTS) smoother 349 8.3.4 Information form filtering and smoothing 351		
$\underline{44}$		8.4	8.3.4 Information form filtering and smoothing 351 Inference for non-linear and/or non-Gaussian chains 351		
$\underline{45}$		8.5	Inference based on local linearization 351		
<u>46</u>		2.0	8.5.1 Taylor series expansion 353		

 $\underline{47}$

xiv

```
1
             8.5.2
                                                               355
                      The extended Kalman filter (EKF)
2
             8.5.3
                      The extended Kalman smoother
                                                            358
3
             Inference based on the unscented transform
                                                              358
4
             8.6.1
                      The unscented transform
<u>5</u>
             8.6.2
                      The unscented Kalman filter (UKF)
                                                                360
             8.6.3
                      The unscented Kalman smoother
                                                             362
<u>6</u>
       8.7
                      ariants of the Kalman filter
             Other
7
             8.7.1
                      Ensemble Kalman filter
                                                   362
8
             8.7.2
                                                  364
                      Robust Kalman filters
9
             8.7.3
                      Gaussian filtering
                                             364
       8.8
             Assumed density filtering
                                            366
10
             8.8.1
                      Gaussian sum filter
                                               367
11
                      ADF for logistic regression
             8.8.2
                                                      369
12
             8.8.3
                      ADF for DNNs
<u>13</u>
                                                 373
       Inference for graphical models
14
             Introduction
                               373
15
       9.2
             Belief propagation on trees
                                              374
16
             9.2.1
                      BP for undirected graphs with pairwise potentials
                                                                              374
             9.2.2
                      Max product belief propagation
<u>17</u>
       9.3
             Loopy belief propagation
                                           377
18
             9.3.1
                      Loopy BP for factor graphs
                                                       377
<u>19</u>
             9.3.2
                      Gaussian belief propagation
                                                       378
             9.3.3
20
                      Convergence
                                        380
             9.3.4
                      Accuracy
                                    382
21
             9.3.5
                      Generalized belief propagation
                                                          383
<u>22</u>
             9.3.6
                      Convex BP
                                      383
23
             9.3.7
                      Application: error correcting codes
                                                              383
24
             9.3.8
                      Application: Affinity propagation
                                                             385
             9.3.9
                      Emulating BP with graph neural nets
                                                                  386
25
       9.4
             The variable elimination (VE) algorithm
                                                            387
26
             9.4.1
                      Derivation of the algorithm
                                                       387
27
             9.4.2
                      Computational complexity of VE
                                                             388
             9.4.3
                      Computational complexity of exact inference
                                                                         390
28
             9.4.4
                      Drawbacks of VE
                                             391
29
       9.5
             The junction tree algorithm (JTA)
                                                     392
30
             Inference as optimization
                                            392
31
             9.6.1
                      Inference as backpropagation
                                                        393
             9.6.2
                      Perturb and MAP
                                              395
32
33
                                      397
    10 Variational inference
\underline{34}
       10.1
             Introduction
              10.1.1
                      Variational free energy
35
                                                          398
              10.1.2
                      Evidence lower bound (ELBO)
36
       10.2 Mean field VI
                                399
37
              10.2.1
                                                                           399
                      Coordinate ascent variational inference (CAVI)
38
              10.2.2
                      Example: CAVI for the Ising model
             10.2.3
                      Variational Bayes
                                             402
39
              10.2.4
                      Example: VB for a univariate Gaussian
                                                                   403
40
                      Variational Bayes EM
              10.2.5
41
              10.2.6
                      Example: VBEM for a GMM
                                                         407
42
              10.2.7
                      Variational message passing (VMP)
                                                               413
              10.2.8
                      Autoconj
                                    414
43
       10.3 Fixed-form VI
                                 414
44
                      Stochastic variational inference
              10.3.1
                                                           414
45
              10.3.2
                      Black-box variational inference
                                                          415
46
              10.3.3
                      Reparameterization VI
```

```
1
                      Full-rank Gaussian VI
                                                 418
2
              10.3.4
              10.3.5
                      Low-rank Gaussian VI
                                                 418
3
              10.3.6
                      Automatic differentiation VI
                                                       420
4
              10.3.7
                      Sparse Gaussian VI
5
              10.3.8
                      Non-Gaussian reparameterized VI
                                                             426
              10.3.9
                      Amortized inference
                                               427
6
                                                      429
        10.4
              More accurate variational posteriors
7
              10.4.1
                      Structured mean field
8
              10.4.2
                      Hierarchical (auxiliary variable) posteriors
                                                                     429
9
              10.4.3
                      Normalizing flow posteriors
                                                      430
              10.4.4
                      Implicit posteriors
                                             432
10
              10.4.5
                      Combining VI with MCMC inference
                                                                432
11
        10.5 Lower bounds
                                432
12
              10.5.1
                      Multi-sample ELBO (IWAE bound)
                                                               432
13
              10.5.2
                      The thermodynamic variational objective (TVO)
                                                                           433
        10.6 Upper bounds
                                434
14
              10.6.1
                      Minimizing the \chi-divergence upper bound
                                                                     435
15
                      Minimizing the evidence upper bound
              10.6.2
16
        10.7 Expectation propagation (EP)
17
              10.7.1
                      Minimizing forwards vs reverse KL
                                                              436
              10.7.2
                      EP as generalized ADF
                                                  438
18
              10.7.3
                      Algorithm
                                     439
19
              10.7.4
                      Example
                                    440
20
                      Optimization issues
              10.7.5
                                              441
              10.7.6
                      Power EP and \alpha-divergence
                                                      441
21
              10.7.7
                      Stochastic EP
                                         441
22
              10.7.8
                      Applications
                                       442
23
    11 Monte Carlo inference
                                       443
24
        11.1 Introduction
25
        11.2 Monte Carlo integration
                                          443
26
              11.2.1
                      Example: estimating \pi by Monte Carlo integration
                                                                             444
27
                      Accuracy of Monte Carlo integration
28
        11.3 Generating random samples from simple distributions
                                                                        446
              11.3.1
                      Sampling using the inverse cdf
29
              11.3.2
                      Sampling from a Gaussian (Box-Muller method)
                                                                           447
30
        11.4 Rejection sampling
                                     447
31
              11.4.1
                      Basic idea
                                     448
32
              11.4.2
                      Example
                                    449
              11.4.3
                      Adaptive rejection sampling
                                                       449
33
              11.4.4
                      Rejection sampling in high dimensions
                                                                 450
34
        11.5 Importance sampling
                                       450
35
              11.5.1
                      Direct importance sampling
              11.5.2
                      Self-normalized importance sampling
                                                               451
36
              11.5.3
                      Choosing the proposal
37
              11.5.4
                       Annealed importance sampling (AIS)
                                                                453
38
        11.6 Controlling Monte Carlo variance
                                                    454
39
              11.6.1
                      Common random numbers
                                                     454
              11.6.2
                      Rao-Blackwellisation
                                               454
40
              11.6.3
                      Control variates
                                           455
41
              11.6.4
                      Antithetic sampling
                                               456
42
              11.6.5
                      Quasi Monte Carlo (QMC)
                                                      457
<u>43</u>
    12 Markov Chain Monte Carlo inference
                                                         459
44
             Introduction
45
                                                460
        12.2
              Metropolis Hastings algorithm
46
              12.2.1 Basic idea
                                     460
47
```

xvi

```
1
             12.2.2
                      Why MH works
                                          461
2
             12.2.3
                                                462
                      Proposal distributions
3
             12.2.4
                     Initialization
                                       465
4
       12.3 Gibbs sampling
                                 465
<u>5</u>
             12.3.1
                     Basic idea
                                    465
             12.3.2
                     Gibbs sampling is a special case of MH
                                                                 466
<u>6</u>
             12.3.3
                     Example: Gibbs sampling for Ising models
                                                                    466
7
                     Example: Gibbs sampling for Potts models
                                                                     468
             12.3.4
8
             12.3.5
                     Example: Gibbs sampling for GMMs
                                                               468
9
             12.3.6
                                                             470
                     Sampling from the full conditionals
             12.3.7
                     Blocked Gibbs sampling
10
             12.3.8
                     Collapsed Gibbs sampling
                                                    472
11
       12.4
            Auxiliary variable MCMC
                                           474
12
             12.4.1
                     Slice sampling
                                        475
13
             12.4.2
                     Swendsen Wang
                                          476
       12.5 Hamiltonian Monte Carlo (HMC)
                                                   478
14
                     Hamiltonian mechanics
                                                 478
             12.5.1
15
             12.5.2
                     Integrating Hamilton's equations
                                                          479
16
             12.5.3
                      The HMC algorithm
                                              480
17
             12.5.4
                     Tuning HMC
             12.5.5
                                                   482
18
                     Riemann Manifold HMC
                     Langevin Monte Carlo (MALA)
             12.5.6
                                                          483
19
             12.5.7
                     Connection between SGD and Langevin sampling
                                                                           484
20
             12.5.8
                      Applying HMC to constrained parameters
21
             12.5.9
                     Speeding up HMC
       12.6 MCMC convergence
                                     487
22
                     Mixing rates of Markov chains
                                                        488
             12.6.1
23
             12.6.2
                      Practical convergence diagnostics
                                                           488
24
             12.6.3
                     Improving speed of convergence
                                                         496
25
             12.6.4
                     Non-centered parameterizations and Neal's funnel
                                                                           496
26
            Stochastic gradient MCMC
                                            497
             12.7.1
                     Stochastic Gradient Langevin Dynamics (SGLD)
                                                                          498
27
             12.7.2
                     Preconditionining
                                           498
28
             12.7.3
                     Reducing the variance of the gradient estimate
                                                                        499
29
                     SG-HMC
             12.7.4
                                   500
                     Underdamped Langevin Dynamics
30
             12.7.5
       12.8 Reversible jump (trans-dimensional) MCMC
                                                             502
31
             12.8.1
                     Basic idea
                                    502
32
             12.8.2
                     Example
                                   504
33
             12.8.3
                     Discussion
                                    505
\underline{34}
            Annealing methods
                                    505
             12.9.1
                     Parallel tempering
                                            506
35
<u>36</u>
   13 Sequential Monte Carlo inference
                                                   507
37
       13.1 Introduction
                              507
                                             507
38
             13.1.1
                     Problem statement
             13.1.2
                     Particle filtering for state-space models
39
             13.1.3
                     SMC samplers for static parameter estimation
                                                                        509
40
       13.2 Particle filtering
                                 509
41
             13.2.1
                     Importance sampling
42
             13.2.2
                     Sequential importance sampling
             13.2.3
                     Sequential importance sampling with resampling
                                                                          511
43
             13.2.4
                     Resampling methods
                                              514
44
             13.2.5
                     Adaptive resampling
                                              516
45
            Proposal distributions
                                       517
46
                     Locally optimal proposal
                                                   517
```

<u>1</u>		
2		13.3.2 Proposals based on the Laplace approximation 518
<u>3</u>		13.3.3 Proposals based on the extended and unscented Kalman filter 518
		13.3.4 Proposals based on SMC 520
<u>4</u>		13.3.5 Learned ("neural") proposals (Unfinished) 520
<u>5</u>	13.4	Rao-Blackwellised particle filtering (RBPF) 521
<u>6</u>		13.4.1 Mixture of Kalman filters 521
<u>7</u>		13.4.2 Example: tracking a maneuvering object 523
		13.4.3 Example: Simultaneous localization and mapping (SLAM) 523
8	13.5	Extensions of the particle filter 527
9	13.6	SMC samplers 528
<u>10</u>		13.6.1 Ingredients of an SMC sampler 528
<u>11</u>		13.6.2 Likelihood tempering (geometric path) 529 13.6.3 Data tempering 532
12		13.6.4 Sampling rare events and extrema 533
13		13.6.5 SMC-ABC and likelihood-free inference 534
		13.6.6 SMC ² 534
<u>14</u>		10.0.0 (514)
$\underline{15}$		
<u>16</u>	III]	Prediction 537
<u>17</u>		
<u>18</u>		lictive models: an overview 539
<u>19</u>	14.1	
		14.1.1 Types of model 539
<u>20</u>		14.1.2 Model fitting using ERM, MLE and MAP 540
<u>21</u>	14.9	14.1.3 Model fitting using Bayes, VI and generalized Bayes 541 Evaluating predictive models 542
$\underline{22}$	14.2	14.2.1 Proper scoring rules 542
23		14.2.2 Calibration 542
24		14.2.3 Beyond evaluating marginal probabilities 546
	14.3	Conformal prediction 549
<u>25</u>		14.3.1 Conformalizing classification 550
<u>26</u>		14.3.2 Conformalizing regression 551
$\underline{27}$		14.3.3 Conformalizing Bayes 552
28		14.3.4 What do we do if we don't have a calibration set? 553
<u>29</u>	15 Gene	eralized linear models 555
<u>30</u>		Introduction 555
31	10.1	15.1.1 Examples 555
		15.1.2 GLMs with non-canonical link functions 558
<u>32</u>		15.1.3 Maximum likelihood estimation 558
<u>33</u>		15.1.4 Bayesian inference 559
$\underline{34}$	15.2	Linear regression 560
<u>35</u>		15.2.1 Conjugate priors 560
<u>36</u>		15.2.2 Uninformative priors 562
		15.2.3 Informative priors 564
<u>37</u>		15.2.4 Spike and slab prior 566
<u>38</u>		15.2.5 Laplace prior (Bayesian lasso) 567
<u>39</u>		15.2.6 Horseshoe prior 568
<u>40</u>		15.2.7 Automatic relevancy determination 569
41	15.3	Logistic regression 571
		15.3.1 Binary logistic regression 572
42		15.3.2 Multinomial logistic regression 572
<u>43</u>		15.3.3 Priors 573
$\underline{44}$		15.3.4 Posteriors 574 15.3.5 Laplace approximation 574
$\underline{45}$		15.3.6 MCMC inference 577
<u>46</u>		15.3.7 Variational inference 578
		10.0., , all autoliar illiciones 010

 $\underline{47}$

```
1
                                                    578
             15.3.8
                     Assumed density filtering
2
      15.4 Probit regression
                                  578
3
             15.4.1
                     Latent variable interpretation
                                                        578
4
             15.4.2
                     Maximum likelihood estimation
                                                          579
5
             15.4.3
                     Bayesian inference
             15.4.4
                     Ordinal probit regression
                                                   581
6
                                                      582
             15.4.5
                     Multinomial probit models
7
            Multi-level GLMs
                                   582
8
             15.5.1
                     Generalized linear mixed models (GLMMs)
                                                                      583
9
             15.5.2
                     Model fitting
                                       583
            15.5.3
                     Example: radon regression
                                                     583
10
11 16 Deep neural networks
                                      587
12
            Introduction
                                                          587
      16.2
            Building blocks of differentiable circuits
13
             16.2.1
                     Linear layers
                                       588
14
             16.2.2
                     Non-linearities
15
             16.2.3
                                               589
                     Convolutional layers
16
             16.2.4
                     Residual (skip) connections
                                                      590
             16.2.5
                     Normalization layers
17
             16.2.6
                     Dropout layers
                                         591
18
             16.2.7
                     Attention layers
                                          592
<u>19</u>
            16.2.8
                                          595
                     Recurrent layers
             16.2.9
                     Multiplicative layers
                                               595
20
             16.2.10 Implicit layers
                                        596
21
      16.3 Canonical examples of neural networks
                                                         596
<u>22</u>
                     Multi-layer perceptrons (MLP)
                                                          597
23
             16.3.2
                     Convolutional neural networks (CNN)
                                                                 597
24
             16.3.3
                     Recurrent neural networks (RNN)
                                                             597
             16.3.4
                     Transformers
                                       599
25
             16.3.5
                     Graph neural networks (GNNs)
                                                          603
27 17 Bayesian neural networks
                                          609
            Introduction
                              609
28
            Priors for BNNs
                                  609
      17.2
29
             17.2.1
                     Gaussian priors
30
                                                    612
             17.2.2
                     Sparsity-promoting priors
             17.2.3
                     Learning the prior
                                             612
31
             17.2.4
                     Priors in function space
                                                  612
32
             17.2.5
                     Architectural priors
                                              612
33
      17.3 Likelihoods for BNNs
                                       613
<u>34</u>
            Posteriors for BNNs
             17.4.1
                     Laplace approximation
                                                 614
35
            17.4.2
                     Variational inference
                                               615
36
            17.4.3
                     Expectation propagation
                                                   616
37
            17.4.4
                     Last layer methods
                                             616
38
             17.4.5
                     Dropout
                     MCMC methods
            17.4.6
                                           617
39
                     Methods based on the SGD trajectory
            17.4.7
                                                                 617
40
            17.4.8
                     Deep ensembles
                                          619
41
             17.4.9
                     Approximating the posterior predictive distibution
                                                                              623
\underline{42}
            Generalization in Bayesian deep learning
             17.5.1
                     Sharp vs flat minima
43
             17.5.2
                     Effective dimensionality of a model
                                                              626
44
            17.5.3
                     The hypothesis space of DNNs
                                                         626
<u>45</u>
            17.5.4
                     Double descent
                                         627
46
             17.5.5
                     A Bayesian Resolution to Double Descent
                                                                     630
```

```
1
                       PAC-Bayes
                                       632
2
              17.5.6
              17.5.7
                       Out-of-Distribution Generalization for BNNs
                                                                        632
3
        17.6 Online inference
                                   635
4
                       Extended Kalman Filtering for DNNs
              17.6.1
                                                                 635
5
              17.6.2
                       Assumed Density Filtering for DNNs
                                                                 638
              17.6.3
                       Sequential Laplace for DNNs
6
              17.6.4
                       Variational methods
7
              Hierarchical Bayesian neural networks
                                                         640
8
              17.7.1
                      Solving multiple related classification problems
                                                                          641
9
     18 Gaussian processes
                                    645
10
        18.1 Introduction
                               645
11
              18.1.1
                       GPs: What and why?
                                                 645
12
        18.2
              Mercer kernels
                                 647
                       Some popular Mercer kernels
                                                        648
              18.2.1
13
              18.2.2
                       Mercer's theorem
14
              18.2.3
                       Kernels from Spectral Densities
                                                           655
15
        18.3 GPs with Gaussian likelihoods
16
              18.3.1
                       Predictions using noise-free observations
                                                                    656
              18.3.2
                       Predictions using noisy observations
                                                                658
17
              18.3.3
                       Weight space vs function space
                                                           659
18
              18.3.4
                       Semi-parametric GPs
                                                 659
19
              18.3.5
                       Marginal likelihood
                                               660
20
              18.3.6
                       Computational and numerical issues
                                                                661
              18.3.7
                       Kernel ridge regression
21
        18.4 GPs with non-Gaussian likelihoods
                                                      664
22
              18.4.1
                       Binary classification
23
              18.4.2
                       Multi-class classification
                                                    666
24
              18.4.3
                       GPs for Poisson regression (Cox process)
                                                                    667
                       Other likelihoods
              18.4.4
25
        18.5
              Scaling GP inference to large datasets
                                                         668
26
              18.5.1
                       Subset of data
                                          668
27
              18.5.2
                       Nyström approximation
                                                   669
              18.5.3
                                                   670
28
                       Inducing point methods
              18.5.4
                       Sparse variational methods
                                                      673
29
              18.5.5
                       Exploiting parallelization and structure via kernel matrix multiplies
                                                                                               677
30
              18.5.6
                       Converting a GP to a SSM
                                                      679
31
        18.6 Learning the kernel
                                      679
              18.6.1
                       Empirical Bayes for the kernel parameters
                                                                      680
32
              18.6.2
                       Bayesian inference for the kernel parameters
                                                                        682
33
              18.6.3
                       Multiple kernel learning for additive kernels
                                                                       683
34
              18.6.4
                       Automatic search for compositional kernels
                                                                       685
35
                       Spectral mixture kernel learning
              18.6.5
              18.6.6
                       Deep kernel learning
36
        18.7 GPs and DNNs
                                  691
37
              18.7.1
                       Kernels derived from random DNNs (NN-GP)
38
              18.7.2
                       Kernels derived from trained DNNs (neural tangent kernel)
                                                                                       694
39
              18.7.3
                       Deep GPs
                                     696
        18.8
              Gaussian processes for timeseries forecasting
                                                               701
40
                       Example: Mauna Loa
                                                 701
41
                                             703
42
     19 Beyond the iid assumption
        19.1 Introduction
43
        19.2 Distribution shift
                                    703
44
              19.2.1
                       Motivating examples
45
                       A causal view of distribution shift
              19.2.2
                                                             705
<u>46</u>
              19.2.3
                       Covariate shift
                                          705
47
```

```
1
               19.2.4
                        Domain shift
                                          706
2
                                                707
               19.2.5
                        Label / prior shift
3
              19.2.6
                        Concept shift
                                           707
4
              19.2.7
                        Manifestation shift
                                                707
5
              19.2.8
                        Selection bias
                                           708
        19.3
              Training-time techniques for distribution shift
                                                                    708
<u>6</u>
               19.3.1
                        Importance weighting for covariate shift
                                                                      709
7
               19.3.2
                        Domain adaptation
                                                 710
8
               19.3.3
                        Domain randomization
                                                     710
9
              19.3.4
                        Data augmentation
                                                 711
                        Unsupervised label shift estimation
               19.3.5
                                                                  711
10
                                                                   712
               19.3.6
                        Distributionally robust optimization
11
        19.4 Test-time techniques for distribution shift
12
                                                                        712
               19.4.1
                        Detecting shifts using two-sample testing
13
               19.4.2
                                                                                 712
                        Detecting single out-of-distribution (OOD) inputs
               19.4.3
                        Selective prediction
                                                 715
14
                        Open world recognition
                                                     716
               19.4.4
<u>15</u>
               19.4.5
                        Online adaptation
                                                717
16
        19.5 Learning from multiple distributions
                                                          718
<u>17</u>
               19.5.1
                        Transfer learning
                                              719
               19.5.2
                        Few-shot learning
                                               720
18
               19.5.3
                        Prompt tuning
                                            720
<u>19</u>
               19.5.4
                        Zero-shot learning
                                                720
20
               19.5.5
                        Multi-task learning
                                                 721
21
               19.5.6
                        Domain generalization
               19.5.7
                        Invariant risk minimization
                                                         723
<u>22</u>
        19.6
              Meta-learning
                                  724
23
               19.6.1
                        Meta-learning as probabilistic inference for prediction
                                                                                     725
24
                        Gradient-based meta-learning
               19.6.2
                                                            726
25
               19.6.3
                        Metric-based few-shot learning
                                                             726
               19.6.4
                        VERSA
                                     726
26
               19.6.5
                        Neural processes
                                              727
27
              Continual learning
                                       727
        19.7
28
               19.7.1
                        Domain drift
                                          727
29
              19.7.2
                        Concept drift
                                           727
               19.7.3
                        Task incremental learning
                                                        729
30
              19.7.4
                        Catastrophic forgetting
                                                     730
31
               19.7.5
                        Online learning
                                             732
32
              Adversarial examples
33
               19.8.1
                        Whitebox (gradient-based) attacks
                                                                 735
\underline{34}
               19.8.2
                        Blackbox (gradient-free) attacks
                                                              735
               19.8.3
                        Real world adversarial attacks
<u>35</u>
                        Defenses based on robust optimization
                                                                     737
               19.8.4
36
              19.8.5
                        Why models have adversarial examples
                                                                      738
<u>37</u>
38
             Generation
                                       741
39
40
    20 Generative models: an overview
                                                      743
41
        20.1 Introduction
\underline{42}
              Types of generative model
                                               743
                                                  745
              Goals of generative modeling
43
                                             745
              20.3.1
                        Generating data
44
              20.3.2
                        Density estimation
                                                746
<u>45</u>
              20.3.3
                        Imputation
46
              20.3.4
                        Structure discovery
                                                 748
```

```
1
                       Latent space interpolation
                                                      749
2
              20.3.5
              20.3.6
                       Representation learning
                                                   750
3
        20.4 Evaluating generative models
                                                750
4
              20.4.1
                       Likelihood
                                      751
5
              20.4.2
                       Distances and divergences in feature space
                                                                      752
              20.4.3
                       Precision and recall metrics
6
                                                       753
              20.4.4
                       Statistical tests
7
              20.4.5
                       Challenges with using pretrained classifiers
                                                                      755
8
              20.4.6
                       Using model samples to train classifiers
9
              20.4.7
                       Assessing overfitting
                                               755
10
              20.4.8
                       Human evaluation
                                             755
11
     21 Variational autoencoders
                                           757
12
        21.1 Introduction
                               757
13
        21.2
              VAE basics
                              757
14
              21.2.1
                       Modeling assumptions
                                                 758
              21.2.2
                       Evidence lower bound
                                                 759
15
              21.2.3
                       Optimization
                                        760
16
              21.2.4
                       The reparameterization trick
17
              21.2.5
                       Computing the reparameterized ELBO
                                                                  762
18
              21.2.6
                       Comparison of VAEs and autoencoders
                                                                  763
              21.2.7
                       VAEs optimize in an augmented space
                                                                  764
<u>19</u>
        21.3 VAE generalizations
                                       767
20
              21.3.1
                      \sigma-VAE
                                  767
21
              21.3.2
                       β-VAE
                                  769
22
              21.3.3
                       InfoVAE
                                    771
              21.3.4
                       Multi-modal VAEs
                                              774
23
              21.3.5
                       VAEs with missing data
                                                   775
24
              21.3.6
                       Semi-supervised VAEs
25
              21.3.7
                       VAEs with sequential encoders/decoders
                                                                    778
26
        21.4 Avoiding posterior collapse
                                             781
              21.4.1
                       KL annealing
27
              21.4.2
                       Lower bounding the rate
                                                    782
28
              21.4.3
                       Free bits
                                    783
29
                       Adding skip connections
                                                    783
              21.4.4
                                                          783
30
              21.4.5
                       Improved variational inference
              21.4.6
                       Alternative objectives
31
              21.4.7
                       Enforcing identifiability
                                                   784
32
        21.5 VAEs with hierarchical structure
33
                                                             785
              21.5.1
                       Bottom-up vs top-down inference
34
              21.5.2
                       Example: Very deep VAE
              21.5.3
                                                                  788
                       Connection with autoregressive models
35
              21.5.4
                       Variational pruning
36
              21.5.5
                       Other optimization difficulties
                                                         790
37
              Vector quantization VAE
38
              21.6.1
                       Autoencoder with binary code
                                                          791
              21.6.2
                                           791
                       VQ-VAE model
39
              21.6.3
                       Learning the prior
                                             793
40
                       Hierarchical extension (VQ-VAE-2)
              21.6.4
                                                               793
41
              21.6.5
                       Discrete VAE
                                         794
42
              21.6.6
                                     795
                       VQ-GAN
              Wake-sleep algorithm
                                        796
        21.7
43
              21.7.1
                       Wake phase
                                       797
44
              21.7.2
                       Sleep phase
                                       797
45
              21.7.3
                       Daydream phase
                                            798
46
                                                  799
              21.7.4
                       Summary of algorithm
47
```

```
1
                                       801
   22 Auto-regressive models
2
      22.1 Introduction
                             801
3
      22.2 Neural autoregressive density estimators (NADE)
                                                                  802
4
                              802
            Causal CNNs
5
             22.3.1
                     1d causal CNN (Convolutional Markov models)
                                                                        803
6
            22.3.2
                     2d causal CNN (PixelCNN)
      22.4 Transformer decoders
                                      804
7
                     Text generation (GPT)
            22.4.1
                                                805
8
            22.4.2
                     Music generation
                                          805
9
            22.4.3
                     Text-to-image generation (DALL-E)
                                                             806
10
   23 Normalizing Flows
                                  809
11
      23.1 Introduction
                             809
12
            23.1.1
                     Preliminaries
                                      809
            23.1.2
                     Example
                                   811
13
            23.1.3
                     How to train a flow model
                                                   812
14
            Constructing Flows
                                    813
15
            23.2.1
                     Affine flows
16
            23.2.2
                     Elementwise flows
                                           814
            23.2.3
                     Coupling flows
                                        816
<u>17</u>
            23.2.4
                                             818
                     Autoregressive flows
18
            23.2.5
                     Residual flows
<u>19</u>
            23.2.6
                     Continuous-time flows
                                               825
20
      23.3 Applications
                             827
                     Density estimation
            23.3.1
                                            827
21
            23.3.2
                     Generative Modeling
                                              828
22
            23.3.3
                     Inference
                                  828
23
   24 Energy-based models
                                     831
^{24}
      24.1 Introduction
                             831
25
                     Example: Products of experts (PoE)
            24.1.1
                                                              832
26
                     Computational difficulties
                                                   832
27
      24.2 Maximum Likelihood Training
                                               833
                     Gradient-based MCMC methods
            24.2.1
                                                          834
28
                                                834
            24.2.2
                     Contrastive divergence
29
      24.3 Score Matching (SM)
30
            24.3.1
                     Basic score matching
31
            24.3.2
                     Denoising Score Matching (DSM)
                                                           839
            24.3.3
                     Sliced Score Matching (SSM)
32
            24.3.4
                     Connection to Contrastive Divergence
                                                               841
33
            24.3.5
                     Score-Based Generative Models
                                                        842
34
      24.4 Noise Contrastive Estimation
35
            24.4.1
                     Connection to Score Matching
                                                       846
      24.5
            Other Methods
                                847
36
            24.5.1
                     Minimizing Differences/Derivatives of KL Divergences
                                                                               847
37
            24.5.2
                     Minimizing the Stein Discrepancy
38
            24.5.3
                     Adversarial Training
39
   25 Diffusion models
                               851
40
            Variational diffusion models
                                            851
41
             25.1.1
                     Encoder
                                  851
42
             25.1.2
                     Decoder
                                  853
                     Model fitting
                                      855
            25.1.3
43
            25.1.4
                     Connection to DDPM
                                               858
44
            25.1.5
                     2d Example
                                     858
45
            25.1.6
                     Application to image generation
                                                         859
46
      25.2 Conditional diffusion models
                                             859
```

```
1
              25.2.1
                      Classifier guidance
                                             860
2
              25.2.2
                                                 860
                      Classifier-free guidance
3
              25.2.3
                      Conditional image generation
                                                        861
4
              25.2.4
                      Other forms of conditional generation
                                                                861
5
             Speeding up the generation process
6
    26 Generative adversarial networks
                                                  865
7
        26.1 Introduction
8
        26.2
              Learning by Comparison
                                           866
9
              26.2.1
                      Guiding principles
                                             867
              26.2.2
                      Class probability estimation
                                                      868
10
              26.2.3
                      Bounds on f-divergences
                                                   871
11
              26.2.4
                      Integral probability metrics
                                                      872
12
              26.2.5
                      Moment matching
                                             874
                                                           875
              26.2.6
                      On density ratios and differences
13
        26.3 Generative Adversarial Networks
14
              26.3.1
                      From learning principles to loss functions
                                                                    877
15
              26.3.2
                      Gradient Descent
                                            878
16
                      Challenges with GAN training
              26.3.3
                                                         879
                      Improving GAN optimization
              26.3.4
                                                        881
17
              26.3.5
                      Convergence of GAN training
                                                        881
18
        26.4
             Conditional GANs
                                     885
19
        26.5 Inference with GANs
                                       886
20
        26.6
              Neural architectures in GANs
                                                887
              26.6.1
                      The importance of discriminator architectures
                                                                        887
21
              26.6.2
                       Architectural inductive biases
                                                        887
22
              26.6.3
                      Attention in GANs
23
              26.6.4
                      Progressive generation
                                                 889
24
              26.6.5
                      Regularization
              26.6.6
                      Scaling up GAN models
                                                  891
25
        26.7
             Applications
                               891
26
              26.7.1
                      GANs for image generation
                                                      891
27
              26.7.2
                       Video generation
                                            893
              26.7.3
                                            894
28
                      Audio generation
              26.7.4
                      Text generation
                                          895
29
              26.7.5
                      Imitation Learning
                                             896
30
              26.7.6
                      Domain Adaptation
31
              26.7.7
                                                     897
                      Design, Art and Creativity
32
33
           Discovery
                                 899
34
                                                   901
35
    27 Discovery methods: an overview
        27.1 Introduction
36
        27.2
              Overview of Part V
                                      902
37
    28 Latent factor models
                                      903
38
        28.1
              Introduction
                               903
39
        28.2
                                  903
              Mixture models
40
              28.2.1
                      Gaussian mixture models (GMMs)
                                                             904
41
              28.2.2
                      Bernoulli mixture models
42
              28.2.3
                      Gaussian scale mixtures (GSMs)
                                                           906
              28.2.4
                      Using GMMs as a prior for inverse imaging problems
                                                                               908
43
              28.2.5
                      Using mixture models for classification problems
44
              Factor analysis
                                 913
45
              28.3.1
                      Factor analysis: the basics
                                                     913
46
              28.3.2
                      Probabilistic PCA
                                             917
47
```

```
1
                                                    919
            28.3.3
                     Mixture of factor analysers
2
            28.3.4
                     Factor analysis models for paired data
                                                               926
3
                     Factor analysis with exponential family likelihoods
                                                                            929
            28.3.5
4
            28.3.6
                     Factor analysis with DNN likelihoods
                                                              930
5
            28.3.7
                     Factor analysis with GP likelihoods (GP-LVM)
                                                                        931
      28.4 LFMs with non-Gaussian priors
                                                933
6
            28.4.1
                     Non-negative matrix factorization (NMF)
                                                                   933
7
            28.4.2
                     Multinomial PCA
                                           934
8
            Topic models
                              936
9
            28.5.1
                     Latent Dirichlet Allocation (LDA)
                                                           936
            28.5.2
                     Correlated topic model
                                                940
10
            28.5.3
                     Dynamic topic model
                                               940
11
            28.5.4
                     LDA-HMM
                                     941
12
      28.6 Independent components analysis (ICA)
                                                         945
13
                     Noiseless ICA model
                                              945
            28.6.1
            28.6.2
                     The need for non-Gaussian priors
                                                          946
14
            28.6.3
                                                         947
                     Maximum likelihood estimation
15
                     Alternatives to MLE
            28.6.4
16
            28.6.5
                     Sparse coding
                                       950
17
            28.6.6
                     Nonlinear ICA
                                        950
   29 State-space models
                                  953
<u>19</u>
      29.1 Introduction
                             953
20
            Hidden Markov models (HMMs)
                                                 954
21
            29.2.1
                    Conditional independence properties
                                                              954
            29.2.2
                     State transition model
                                               954
<u>22</u>
            29.2.3
                     Discrete likelihoods
                                             955
23
            29.2.4
                     Gaussian likelihoods
                                             955
24
            29.2.5
                     Autoregressive likelihoods
                                                   956
25
      29.3 HMMs: Applications
                                      958
            29.3.1
                     Time series segmentation
                                                  958
26
            29.3.2
                     Protein sequence alignment
                                                     960
27
            29.3.3
                     Spelling correction
                                            961
28
      29.4
            HMMs:
                    parameter learning
                                            964
29
                                                           964
            29.4.1
                     The Baum-Welch (EM) algorithm
            29.4.2
                     Parameter estimation using SGD
                                                          967
30
            29.4.3
                     Parameter estimation using spectral methods
                                                                      970
31
            29.4.4
                     Bayesian HMM
                                         970
32
            HMMs: Generalizations
                                        971
33
                                                              971
            29.5.1
                     Hidden semi-Markov model (HSMM)
            29.5.2
                     Hierarchical HMMs
                                            973
34
                                         975
            29.5.3
                     Factorial HMMs
35
            29.5.4
                     Coupled HMMs
                                         976
36
            29.5.5
                     Dynamic Bayes nets (DBN)
                                                     977
37
            29.5.6
                     Changepoint detection
                                                977
38
      29.6 Linear dynamical systems (LDS)
            29.6.1
                     Conditional independence properties
                                                              980
39
            29.6.2
                     Parameterization
                                          980
40
      29.7 LDS: Applications
                                   981
41
            29.7.1
                    Object tracking and state estimation
                                                              981
                     Timeseries forecasting
42
            29.7.2
                                               982
            29.7.3
                     Online linear regression
                                                 982
43
                                              982
      29.8
            Structural time series models
44
            29.8.1
                     Basics
                                983
<u>45</u>
            29.8.2
                     Details
                                983
                     Example: modeling CO_2 levels from Mauna Loa
                                                                         986
46
            29.8.3
<u>47</u>
```

```
1
                                                                  987
2
              29.8.4
                      Example: forecasting electricity demand
              29.8.5
                      Causal impact of a time series intervention
                                                                     987
3
              29.8.6
                      Prophet
                                  991
4
              29.8.7
                      Neural forecasting methods
                                                      993
5
        29.9 LDS: parameter learning
6
              29.9.1
                      EM for LDS
              29.9.2
                      Subspace identification methods
                                                          996
7
              29.9.3
                      Ensuring stability of the dynamical system
                                                                     997
8
              29.9.4
                      Bayesian LDS
                                        997
9
        29.10 Switching linear dynamical systems (SLDS)
                                                             997
10
              29.10.1 Parameterization
                                           998
              29.10.2 Posterior inference
                                             998
11
              29.10.3 Application: Multi-target tracking
                                                            999
12
        29.11 Non-linear dynamical systems
13
              29.11.1 Application: Nonlinear state estimation and tracking
                                                                               1002
14
        29.12 Deep SSMs
                             1003
              29.12.1 Deep Markov models
                                               1004
15
              29.12.2 Recurrent SSM
                                          1005
16
                                                           1005
              29.12.3 Improving multi-step predictions
17
              29.12.4 Variational RNNs
                                            1006
18
    30 Graph learning
                               1009
19
20
        30.1 Introduction
                              1009
              Latent variable models for graphs
                                                   1009
21
              30.2.1
                      Stochastic block model
                                                 1009
22
              30.2.2
                      Mixed membership stochastic block model
                                                                    1011
23
              30.2.3
                                                  1013
                      Infinite relational model
24
        30.3 Graphical model structure learning
                                                     1015
              30.3.1
                      Applications
                                       1016
25
              30.3.2
                      Methods
                                   1017
26
27
                                                   1019
    31 Non-parametric Bayesian models
28
        31.1 Introduction
                              1019
        31.2 Dirichlet processes
29
              31.2.1
                      Definition of a DP
                                             1020
30
              31.2.2
                      Stick breaking construction of the DP
                                                                1022
31
              31.2.3
                                                                 1023
                      The Chinese restaurant process (CRP)
32
        31.3 Dirichlet process mixture models
                                                   1024
33
              31.3.1
                      Model definition
              31.3.2
                                                                 1026
                      Fitting using collapsed Gibbs sampling
34
              31.3.3
                      Other fitting algorithms
                                                  1028
35
              31.3.4
                                                          1029
                      Choosing the hyper-parameters
36
                                                         1030
        31.4
              Generalizations of the Dirichlet process
37
              31.4.1
                      Pitman-Yor process
                                              1031
                                                                  1032
              31.4.2
                      Dependent random probability measures
38
        31.5 The Indian buffet process and the Beta process
                                                                 1034
39
        31.6 Small-variance asymptotics
                                             1037
40
        31.7 Completely random measures
                                               1040
41
        31.8 Lévy processes
                                 1041
42
             Point processes with repulsion and reinforcement
                                                                  1043
              31.9.1
                      Poisson process
                                          1043
43
              31.9.2
                      Renewal process
                                           1044
44
              31.9.3
                                          1045
                      Hawkes process
45
              31.9.4
                      Gibbs point process
                                              1047
46
              31.9.5
                      Determinantal point process
                                                       1048
```

47

```
1
  32 Representation learning (Unfinished)
                                                       1051
3
      32.1 CLIP
                      1051
4
  33 Interpretability
                             1053
5
      33.1 Introduction
                             1053
            33.1.1
                    The Role of Interpretability
                                                     1054
6
                    Terminology and Framework
                                                      1055
7
           Methods for Interpretable Machine Learning
                                                            1059
8
            33.2.1
                    Inherently Interpretable Models: The Model is its Explanation
                                                                                        1059
9
            33.2.2
                    Semi-Inherently Interpretable Models: Example-Based Methods
                                                                                        1062
10
            33.2.3
                    Post-hoc or Joint training: The Explanation gives a Partial View of the Model
                                                                                                       1062
            33.2.4
                    Transparency and Visualization
11
      33.3 Properties: The Abstraction Between Context and Method
12
                    Properties of Explanations from Interpretable Machine Learning
                                                                                         1068
13
                    Properties of Explanations from Cognitive Science
      33.4 Evaluation of Interpretable Machine Learning Models
14
                    Computational Evaluation: Does the Method have Desired Properties?
15
                                                                                                      1077
                    User Study-based Evaluation: Does the Method Help a User Perform a Task?
16
      33.5 Discussion: How to Think about Interpretable Machine Learning
17
          Action
                            1087
19
20 \over 34 Decision making under uncertainty
                                                    1089
      34.1 Bayesian decision theory
<u>22</u>
            34.1.1
                    Basics
                               1089
            34.1.2
                    Classification
                                      1090
23
            34.1.3
                    Regression
                                   1090
24
                    Structured prediction
                                              1091
            34.1.4
25
            34.1.5
                    Fairness
                                 1092
26
      34.2 Decision (influence) diagrams
                                             1092
                    Example: oil wildcatter
            34.2.1
                                                1092
27
            34.2.2
                    Information arcs
                                         1093
28
            34.2.3
                    Value of information
                                             1094
29
            34.2.4
                    Computing the optimal policy
                                                       1095
           A/B testing
30
                            1095
      34.3
            34.3.1
                    A Bayesian approach
                                              1096
31
            34.3.2
                    Example
                                  1099
32
      34.4 Contextual bandits
                                   1100
33
                                         1101
            34.4.1
                     Types of bandit
                                     1102
34
            34.4.2
                    Applications
            34.4.3
                    Exploration-exploitation tradeoff
                                                         1102
35
            34.4.4
                    The optimal solution
                                              1103
36
            34.4.5
                     Upper confidence bounds (UCB)
                                                         1104
37
            34.4.6
                     Thompson sampling
                                             1106
38
            34.4.7
                    Regret
                                1107
      34.5
           Markov decision problems
                                          1109
39
            34.5.1
                    Basics
                               1109
40
            34.5.2
                     Partially observed MDPs
                                                  1110
41
            34.5.3
                    Episodes and returns
                                              1110
42
            34.5.4
                     Value functions
                                        1112
            34.5.5
                    Optimal value functions and policies
                                                             1112
43
      34.6 Planning in an MDP
                                     1113
44
            34.6.1
                     Value iteration
                                        1114
<u>45</u>
            34.6.2
                     Policy iteration
                                        1115
46
            34.6.3
                    Linear programming
                                             1116
<u>47</u>
```

```
1
2
        34.7 Active learning
                                 1117
              34.7.1
                      Relationship to other forms of sequential decision making
                                                                                  1117
3
              34.7.2
                      Common heursitics
                                             1117
4
             34.7.3
                      Batch methods
                                         1118
5
    35 Reinforcement learning
                                        1119
6
        35.1 Introduction
7
             35.1.1
                      Overview of methods
                                               1119
8
              35.1.2
                      Value based methods
                                               1121
9
              35.1.3
                      Policy search methods
                                                1121
                      Model-based RL
             35.1.4
                                          1121
10
              35.1.5
                      Exploration-exploitation tradeoff
                                                          1122
11
        35.2
             Value-based RL
                                 1124
12
              35.2.1
                      Monte Carlo RL
              35.2.2
                      Temporal difference (TD) learning
                                                            1124
13
              35.2.3
                      TD learning with eligibility traces
                                                            1125
14
              35.2.4
                      SARSA: on-policy TD control
15
              35.2.5
                      Q-learning: off-policy TD control
                                                           1127
16
              35.2.6
                      Deep Q-network (DQN)
             Policy-based RL
        35.3
                                  1130
17
              35.3.1
                      The policy gradient theorem
                                                      1130
18
             35.3.2
                      REINFORCE
                                        1131
19
             35.3.3
                      Actor-critic methods
                                               1132
20
              35.3.4
                      Bound optimization methods
                                                       1134
              35.3.5
                      Deterministic policy gradient methods
                                                                1136
21
              35.3.6
                      Gradient-free methods
                                                1137
22
        35.4 Model-based RL
                                  1137
23
             35.4.1
                      Model predictive control (MPC)
24
              35.4.2
                      Combining model-based and model-free
                                                                 1139
              35.4.3
                      MBRL using Gaussian processes
25
             35.4.4
                      MBRL using DNNs
                                             1141
26
              35.4.5
                      MBRL using latent-variable models
                                                             1141
27
              35.4.6
                      Robustness to model errors
        35.5 Off-policy learning
28
                                    1144
              35.5.1
                      Basic techniques
                                           1145
29
             35.5.2
                      The curse of horizon
                                               1148
30
              35.5.3
                      The deadly triad
                                           1149
31
        35.6 Control as inference
                                      1150
              35.6.1
                      Maximum entropy reinforcement learning
                                                                   1150
32
              35.6.2
                      Other approaches
                                            1153
33
             35.6.3
                      Imitation learning
                                            1154
34
    36 Causality
                        1157
35
        36.1 Introduction
                              1157
36
        36.2
             Causal Formalism
                                    1159
37
              36.2.1
                      Structural Causal Models
                                                   1159
38
              36.2.2
                      Causal DAGs
                                        1161
             36.2.3
                                       1163
                      Identification
39
              36.2.4
                      Counterfactuals and the Causal Hierarchy
                                                                   1164
40
        36.3 Randomized Control Trials
                                            1166
41
        36.4 Confounder Adjustment
                                         1167
42
                      Causal Estimand, Statistical Estimand, and Identification
                                                                                   1167
             36.4.2
                      ATE Estimation with Observed Confounders
                                                                      1170
43
              36.4.3
                      Uncertainity Quantification
44
              36.4.4
                      Matching
                                   1175
45
                      Practical Considerations and Procedures
              36.4.5
                                                                  1176
46
              36.4.6
                      Summary and Practical Advice
47
```

xxviii

```
36.5 Instrumental Variable Strategies
                                                             1181
\underline{2}
                         Additive Unobserved Confounding
                                                                           1183
              36.5.1
3
                         Instrument Monotonicity and Local Average Treatment Effect
              36.5.2
                                                                                                              1184
4
              36.5.3
                        Two Stage Least Squares
                                                               1188
5
      36.6 Difference in Differences
              36.6.1
                         Estimation
                                             1192
      36.7
              Credibility Checks
                                            1192
7
              36.7.1
                         Placebo Checks
                                                   1193
8
              36.7.2
                         Sensitivity Analysis to Unobserved Confounding
                                                                                             1193
9
      36.8 The Do Calculus
                                          1201
              36.8.1
                         The three rules
                                                  1201
10
              36.8.2
                         Revisiting Backdoor Adjustment
                                                                         1202
11
                         Frontdoor Adjustment
              36.8.3
12
      36.9 Further Reading
                                         1205
\begin{array}{c} \underline{^{13}} \\ \textbf{Bibliography} \end{array}
                             1220
<u>15</u>
16
\underline{17}
<u>18</u>
<u>19</u>
<u>20</u>
21
<u>22</u>
<u>23</u>
24
25
26
<u>27</u>
28
29
30
31
32
<u>33</u>
\underline{34}
<u>35</u>
<u>36</u>
<u>37</u>
38
39
40
41
\underline{42}
\underline{43}
44
\underline{45}
<u>46</u>
\underline{47}
```