

Probabilistic Graphical Models

Principles and Techniques

Daphne Koller

Nir Friedman

The MIT Press
Cambridge, Massachusetts
London, England

Contents

Acknowledgments **xxiii**

List of Figures **xxv**

List of Algorithms **xxx**

List of Boxes **xxxiii**

1 Introduction **1**

- 1.1 Motivation 1
- 1.2 Structured Probabilistic Models 2
 - 1.2.1 Probabilistic Graphical Models 3
 - 1.2.2 Representation, Inference, Learning 5
- 1.3 Overview and Roadmap 6
 - 1.3.1 Overview of Chapters 6
 - 1.3.2 Reader's Guide 9
 - 1.3.3 Connection to Other Disciplines 11
- 1.4 Historical Notes 12

2 Foundations **15**

- 2.1 Probability Theory 15
 - 2.1.1 Probability Distributions 15
 - 2.1.2 Basic Concepts in Probability 18
 - 2.1.3 Random Variables and Joint Distributions 19
 - 2.1.4 Independence and Conditional Independence 23
 - 2.1.5 Querying a Distribution 25
 - 2.1.6 Continuous Spaces 27
 - 2.1.7 Expectation and Variance 31
- 2.2 Graphs 34
 - 2.2.1 Nodes and Edges 34
 - 2.2.2 Subgraphs 35
 - 2.2.3 Paths and Trails 36

2.2.4	Cycles and Loops	36
2.3	Relevant Literature	39
2.4	Exercises	39

I Representation 43

3 The Bayesian Network Representation 45

3.1	Exploiting Independence Properties	45
3.1.1	Independent Random Variables	45
3.1.2	The Conditional Parameterization	46
3.1.3	The Naive Bayes Model	48
3.2	Bayesian Networks	51
3.2.1	The Student Example Revisited	52
3.2.2	Basic Independencies in Bayesian Networks	56
3.2.3	Graphs and Distributions	60
3.3	Independencies in Graphs	68
3.3.1	D-separation	69
3.3.2	Soundness and Completeness	72
3.3.3	An Algorithm for d-Separation	74
3.3.4	I-Equivalence	76
3.4	From Distributions to Graphs	78
3.4.1	Minimal I-Maps	78
3.4.2	Perfect Maps	81
3.4.3	Finding Perfect Maps ★	83
3.5	Summary	92
3.6	Relevant Literature	93
3.7	Exercises	96

4 Undirected Graphical Models 103

4.1	The Misconception Example	103
4.2	Parameterization	106
4.2.1	Factors	106
4.2.2	Gibbs Distributions and Markov Networks	108
4.2.3	Reduced Markov Networks	110
4.3	Markov Network Independencies	114
4.3.1	Basic Independencies	114
4.3.2	Independencies Revisited	117
4.3.3	From Distributions to Graphs	120
4.4	Parameterization Revisited	122
4.4.1	Finer-Grained Parameterization	123
4.4.2	Overparameterization	128
4.5	Bayesian Networks and Markov Networks	134
4.5.1	From Bayesian Networks to Markov Networks	134
4.5.2	From Markov Networks to Bayesian Networks	137

4.5.3	Chordal Graphs	139
4.6	Partially Directed Models	142
4.6.1	Conditional Random Fields	142
4.6.2	Chain Graph Models ★	148
4.7	Summary and Discussion	151
4.8	Relevant Literature	152
4.9	Exercises	153
5	<i>Local Probabilistic Models</i>	157
5.1	Tabular CPDs	157
5.2	Deterministic CPDs	158
5.2.1	Representation	158
5.2.2	Independencies	159
5.3	Context-Specific CPDs	162
5.3.1	Representation	162
5.3.2	Independencies	171
5.4	Independence of Causal Influence	175
5.4.1	The Noisy-Or Model	175
5.4.2	Generalized Linear Models	178
5.4.3	The General Formulation	182
5.4.4	Independencies	184
5.5	Continuous Variables	185
5.5.1	Hybrid Models	189
5.6	Conditional Bayesian Networks	191
5.7	Summary	193
5.8	Relevant Literature	194
5.9	Exercises	195
6	<i>Template-Based Representations</i>	199
6.1	Introduction	199
6.2	Temporal Models	200
6.2.1	Basic Assumptions	201
6.2.2	Dynamic Bayesian Networks	202
6.2.3	State-Observation Models	207
6.3	Template Variables and Template Factors	212
6.4	Directed Probabilistic Models for Object-Relational Domains	216
6.4.1	Plate Models	216
6.4.2	Probabilistic Relational Models	222
6.5	Undirected Representation	228
6.6	Structural Uncertainty ★	232
6.6.1	Relational Uncertainty	233
6.6.2	Object Uncertainty	235
6.7	Summary	240
6.8	Relevant Literature	242
6.9	Exercises	243

7	<i>Gaussian Network Models</i>	247
7.1	Multivariate Gaussians	247
7.1.1	Basic Parameterization	247
7.1.2	Operations on Gaussians	249
7.1.3	Independencies in Gaussians	250
7.2	Gaussian Bayesian Networks	251
7.3	Gaussian Markov Random Fields	254
7.4	Summary	257
7.5	Relevant Literature	258
7.6	Exercises	258
8	<i>The Exponential Family</i>	261
8.1	Introduction	261
8.2	Exponential Families	261
8.2.1	Linear Exponential Families	263
8.3	Factored Exponential Families	266
8.3.1	Product Distributions	266
8.3.2	Bayesian Networks	267
8.4	Entropy and Relative Entropy	269
8.4.1	Entropy	269
8.4.2	Relative Entropy	272
8.5	Projections	273
8.5.1	Comparison	274
8.5.2	M-Projections	277
8.5.3	I-Projections	282
8.6	Summary	282
8.7	Relevant Literature	283
8.8	Exercises	283
II	<i>Inference</i>	285
9	<i>Variable Elimination</i>	287
9.1	Analysis of Complexity	288
9.1.1	Analysis of Exact Inference	288
9.1.2	Analysis of Approximate Inference	290
9.2	Variable Elimination: The Basic Ideas	292
9.3	Variable Elimination	296
9.3.1	Basic Elimination	297
9.3.2	Dealing with Evidence	303
9.4	Complexity and Graph Structure: Variable Elimination	306
9.4.1	Simple Analysis	306
9.4.2	Graph-Theoretic Analysis	306
9.4.3	Finding Elimination Orderings ★	310
9.5	Conditioning ★	315

9.5.1	The Conditioning Algorithm	315
9.5.2	Conditioning and Variable Elimination	318
9.5.3	Graph-Theoretic Analysis	322
9.5.4	Improved Conditioning	323
9.6	Inference with Structured CPDs ★	325
9.6.1	Independence of Causal Influence	325
9.6.2	Context-Specific Independence	329
9.6.3	Discussion	335
9.7	Summary and Discussion	336
9.8	Relevant Literature	337
9.9	Exercises	338

10 *Clique Trees* 345

10.1	Variable Elimination and Clique Trees	345
10.1.1	Cluster Graphs	346
10.1.2	Clique Trees	346
10.2	Message Passing: Sum Product	348
10.2.1	Variable Elimination in a Clique Tree	349
10.2.2	Clique Tree Calibration	355
10.2.3	A Calibrated Clique Tree as a Distribution	361
10.3	Message Passing: Belief Update	364
10.3.1	Message Passing with Division	364
10.3.2	Equivalence of Sum-Product and Belief Update Messages	368
10.3.3	Answering Queries	369
10.4	Constructing a Clique Tree	372
10.4.1	Clique Trees from Variable Elimination	372
10.4.2	Clique Trees from Chordal Graphs	374
10.5	Summary	376
10.6	Relevant Literature	377
10.7	Exercises	378

11 *Inference as Optimization* 381

11.1	Introduction	381
11.1.1	Exact Inference Revisited ★	382
11.1.2	The Energy Functional	384
11.1.3	Optimizing the Energy Functional	386
11.2	Exact Inference as Optimization	386
11.2.1	Fixed-Point Characterization	388
11.2.2	Inference as Optimization	390
11.3	Propagation-Based Approximation	391
11.3.1	A Simple Example	391
11.3.2	Cluster-Graph Belief Propagation	396
11.3.3	Properties of Cluster-Graph Belief Propagation	399
11.3.4	Analyzing Convergence ★	401
11.3.5	Constructing Cluster Graphs	404

11.3.6	Variational Analysis	411
11.3.7	Other Entropy Approximations ★	414
11.3.8	Discussion	428
11.4	Propagation with Approximate Messages ★	430
11.4.1	Factorized Messages	431
11.4.2	Approximate Message Computation	433
11.4.3	Inference with Approximate Messages	436
11.4.4	Expectation Propagation	442
11.4.5	Variational Analysis	445
11.4.6	Discussion	448
11.5	Structured Variational Approximations	448
11.5.1	The Mean Field Approximation	449
11.5.2	Structured Approximations	456
11.5.3	Local Variational Methods ★	469
11.6	Summary and Discussion	473
11.7	Relevant Literature	475
11.8	Exercises	477
12	<i>Particle-Based Approximate Inference</i>	487
12.1	Forward Sampling	488
12.1.1	Sampling from a Bayesian Network	488
12.1.2	Analysis of Error	490
12.1.3	Conditional Probability Queries	491
12.2	Likelihood Weighting and Importance Sampling	492
12.2.1	Likelihood Weighting: Intuition	492
12.2.2	Importance Sampling	494
12.2.3	Importance Sampling for Bayesian Networks	498
12.2.4	Importance Sampling Revisited	504
12.3	Markov Chain Monte Carlo Methods	505
12.3.1	Gibbs Sampling Algorithm	505
12.3.2	Markov Chains	507
12.3.3	Gibbs Sampling Revisited	512
12.3.4	A Broader Class of Markov Chains ★	515
12.3.5	Using a Markov Chain	518
12.4	Collapsed Particles	526
12.4.1	Collapsed Likelihood Weighting ★	527
12.4.2	Collapsed MCMC	531
12.5	Deterministic Search Methods ★	536
12.6	Summary	540
12.7	Relevant Literature	541
12.8	Exercises	544
13	<i>MAP Inference</i>	551
13.1	Overview	551
13.1.1	Computational Complexity	551

13.1.2	Overview of Solution Methods	552
13.2	Variable Elimination for (Marginal) MAP	554
13.2.1	Max-Product Variable Elimination	554
13.2.2	Finding the Most Probable Assignment	556
13.2.3	Variable Elimination for Marginal MAP ★	559
13.3	Max-Product in Clique Trees	562
13.3.1	Computing Max-Marginals	562
13.3.2	Message Passing as Reparameterization	564
13.3.3	Decoding Max-Marginals	565
13.4	Max-Product Belief Propagation in Loopy Cluster Graphs	567
13.4.1	Standard Max-Product Message Passing	567
13.4.2	Max-Product BP with Counting Numbers ★	572
13.4.3	Discussion	575
13.5	MAP as a Linear Optimization Problem ★	577
13.5.1	The Integer Program Formulation	577
13.5.2	Linear Programming Relaxation	579
13.5.3	Low-Temperature Limits	581
13.6	Using Graph Cuts for MAP	588
13.6.1	Inference Using Graph Cuts	588
13.6.2	Nonbinary Variables	592
13.7	Local Search Algorithms ★	595
13.8	Summary	597
13.9	Relevant Literature	598
13.10	Exercises	601
14	<i>Inference in Hybrid Networks</i>	605
14.1	Introduction	605
14.1.1	Challenges	605
14.1.2	Discretization	606
14.1.3	Overview	607
14.2	Variable Elimination in Gaussian Networks	608
14.2.1	Canonical Forms	609
14.2.2	Sum-Product Algorithms	611
14.2.3	Gaussian Belief Propagation	612
14.3	Hybrid Networks	615
14.3.1	The Difficulties	615
14.3.2	Factor Operations for Hybrid Gaussian Networks	618
14.3.3	EP for CLG Networks	621
14.3.4	An “Exact” CLG Algorithm ★	626
14.4	Nonlinear Dependencies	630
14.4.1	Linearization	631
14.4.2	Expectation Propagation with Gaussian Approximation	637
14.5	Particle-Based Approximation Methods	642
14.5.1	Sampling in Continuous Spaces	642
14.5.2	Forward Sampling in Bayesian Networks	643

14.5.3	MCMC Methods	644	
14.5.4	Collapsed Particles	645	
14.5.5	Nonparametric Message Passing	646	
14.6	Summary and Discussion	646	
14.7	Relevant Literature	647	
14.8	Exercises	649	
15	<i>Inference in Temporal Models</i>	651	
15.1	Inference Tasks	652	
15.2	Exact Inference	653	
15.2.1	Filtering in State-Observation Models	653	
15.2.2	Filtering as Clique Tree Propagation	654	
15.2.3	Clique Tree Inference in DBNs	655	
15.2.4	Entanglement	656	
15.3	Approximate Inference	660	
15.3.1	Key Ideas	661	
15.3.2	Factored Belief State Methods	662	
15.3.3	Particle Filtering	665	
15.3.4	Deterministic Search Techniques	675	
15.4	Hybrid DBNs	675	
15.4.1	Continuous Models	676	
15.4.2	Hybrid Models	684	
15.5	Summary	688	
15.6	Relevant Literature	690	
15.7	Exercises	692	
III	Learning	695	
16	<i>Learning Graphical Models: Overview</i>	697	
16.1	Motivation	697	
16.2	Goals of Learning	698	
16.2.1	Density Estimation	698	
16.2.2	Specific Prediction Tasks	700	
16.2.3	Knowledge Discovery	701	
16.3	Learning as Optimization	702	
16.3.1	Empirical Risk and Overfitting	703	
16.3.2	Discriminative versus Generative Training	709	
16.4	Learning Tasks	711	
16.4.1	Model Constraints	712	
16.4.2	Data Observability	712	
16.4.3	Taxonomy of Learning Tasks	714	
16.5	Relevant Literature	715	
17	<i>Parameter Estimation</i>	717	
17.1	Maximum Likelihood Estimation	717	

17.1.1	The Thumbtack Example	717	
17.1.2	The Maximum Likelihood Principle	720	
17.2	MLE for Bayesian Networks	722	
17.2.1	A Simple Example	723	
17.2.2	Global Likelihood Decomposition	724	
17.2.3	Table-CPDs	725	
17.2.4	Gaussian Bayesian Networks ★	728	
17.2.5	Maximum Likelihood Estimation as M-Projection ★	731	
17.3	Bayesian Parameter Estimation	733	
17.3.1	The Thumbtack Example Revisited	733	
17.3.2	Priors and Posteriors	737	
17.4	Bayesian Parameter Estimation in Bayesian Networks	741	
17.4.1	Parameter Independence and Global Decomposition	742	
17.4.2	Local Decomposition	746	
17.4.3	Priors for Bayesian Network Learning	748	
17.4.4	MAP Estimation ★	751	
17.5	Learning Models with Shared Parameters	754	
17.5.1	Global Parameter Sharing	755	
17.5.2	Local Parameter Sharing	760	
17.5.3	Bayesian Inference with Shared Parameters	762	
17.5.4	Hierarchical Priors ★	763	
17.6	Generalization Analysis ★	769	
17.6.1	Asymptotic Analysis	769	
17.6.2	PAC-Bounds	770	
17.7	Summary	776	
17.8	Relevant Literature	777	
17.9	Exercises	778	
18	Structure Learning in Bayesian Networks	783	
18.1	Introduction	783	
18.1.1	Problem Definition	783	
18.1.2	Overview of Methods	785	
18.2	Constraint-Based Approaches	786	
18.2.1	General Framework	786	
18.2.2	Independence Tests	787	
18.3	Structure Scores	790	
18.3.1	Likelihood Scores	791	
18.3.2	Bayesian Score	794	
18.3.3	Marginal Likelihood for a Single Variable	797	
18.3.4	Bayesian Score for Bayesian Networks	799	
18.3.5	Understanding the Bayesian Score	801	
18.3.6	Priors	804	
18.3.7	Score Equivalence ★	807	
18.4	Structure Search	807	
18.4.1	Learning Tree-Structured Networks	808	

18.4.2	Known Order	809	
18.4.3	General Graphs	811	
18.4.4	Learning with Equivalence Classes ★	821	
18.5	Bayesian Model Averaging ★	824	
18.5.1	Basic Theory	824	
18.5.2	Model Averaging Given an Order	826	
18.5.3	The General Case	828	
18.6	Learning Models with Additional Structure	832	
18.6.1	Learning with Local Structure	833	
18.6.2	Learning Template Models	837	
18.7	Summary and Discussion	838	
18.8	Relevant Literature	840	
18.9	Exercises	843	
19	<i>Partially Observed Data</i>	849	
19.1	Foundations	849	
19.1.1	Likelihood of Data and Observation Models	849	
19.1.2	Decoupling of Observation Mechanism	853	
19.1.3	The Likelihood Function	856	
19.1.4	Identifiability	860	
19.2	Parameter Estimation	862	
19.2.1	Gradient Ascent	863	
19.2.2	Expectation Maximization (EM)	868	
19.2.3	Comparison: Gradient Ascent versus EM	887	
19.2.4	Approximate Inference ★	893	
19.3	Bayesian Learning with Incomplete Data ★	897	
19.3.1	Overview	897	
19.3.2	MCMC Sampling	899	
19.3.3	Variational Bayesian Learning	904	
19.4	Structure Learning	908	
19.4.1	Scoring Structures	909	
19.4.2	Structure Search	917	
19.4.3	Structural EM	920	
19.5	Learning Models with Hidden Variables	925	
19.5.1	Information Content of Hidden Variables	926	
19.5.2	Determining the Cardinality	928	
19.5.3	Introducing Hidden Variables	930	
19.6	Summary	933	
19.7	Relevant Literature	934	
19.8	Exercises	935	
20	<i>Learning Undirected Models</i>	943	
20.1	Overview	943	
20.2	The Likelihood Function	944	
20.2.1	An Example	944	

20.2.2	Form of the Likelihood Function	946
20.2.3	Properties of the Likelihood Function	947
20.3	Maximum (Conditional) Likelihood Parameter Estimation	949
20.3.1	Maximum Likelihood Estimation	949
20.3.2	Conditionally Trained Models	950
20.3.3	Learning with Missing Data	954
20.3.4	Maximum Entropy and Maximum Likelihood ★	956
20.4	Parameter Priors and Regularization	958
20.4.1	Local Priors	958
20.4.2	Global Priors	961
20.5	Learning with Approximate Inference	961
20.5.1	Belief Propagation	962
20.5.2	MAP-Based Learning ★	967
20.6	Alternative Objectives	969
20.6.1	Pseudolikelihood and Its Generalizations	970
20.6.2	Contrastive Optimization Criteria	974
20.7	Structure Learning	978
20.7.1	Structure Learning Using Independence Tests	979
20.7.2	Score-Based Learning: Hypothesis Spaces	981
20.7.3	Objective Functions	982
20.7.4	Optimization Task	985
20.7.5	Evaluating Changes to the Model	992
20.8	Summary	996
20.9	Relevant Literature	998
20.10	Exercises	1001

IV Actions and Decisions 1007

21 Causality 1009

21.1	Motivation and Overview	1009
21.1.1	Conditioning and Intervention	1009
21.1.2	Correlation and Causation	1012
21.2	Causal Models	1014
21.3	Structural Causal Identifiability	1017
21.3.1	Query Simplification Rules	1017
21.3.2	Iterated Query Simplification	1020
21.4	Mechanisms and Response Variables ★	1026
21.5	Partial Identifiability in Functional Causal Models ★	1031
21.6	Counterfactual Queries ★	1034
21.6.1	Twinned Networks	1034
21.6.2	Bounds on Counterfactual Queries	1037
21.7	Learning Causal Models	1039
21.7.1	Learning Causal Models without Confounding Factors	1040
21.7.2	Learning from Interventional Data	1043

21.7.3	Dealing with Latent Variables ★	1047
21.7.4	Learning Functional Causal Models ★	1050
21.8	Summary	1052
21.9	Relevant Literature	1053
21.10	Exercises	1054
22	<i>Utilities and Decisions</i>	1057
22.1	Foundations: Maximizing Expected Utility	1057
22.1.1	Decision Making Under Uncertainty	1057
22.1.2	Theoretical Justification ★	1060
22.2	Utility Curves	1062
22.2.1	Utility of Money	1063
22.2.2	Attitudes Toward Risk	1064
22.2.3	Rationality	1065
22.3	Utility Elicitation	1066
22.3.1	Utility Elicitation Procedures	1066
22.3.2	Utility of Human Life	1067
22.4	Utilities of Complex Outcomes	1069
22.4.1	Preference and Utility Independence ★	1069
22.4.2	Additive Independence Properties	1072
22.5	Summary	1079
22.6	Relevant Literature	1080
22.7	Exercises	1082
23	<i>Structured Decision Problems</i>	1083
23.1	Decision Trees	1083
23.1.1	Representation	1083
23.1.2	Backward Induction Algorithm	1085
23.2	Influence Diagrams	1086
23.2.1	Basic Representation	1087
23.2.2	Decision Rules	1088
23.2.3	Time and Recall	1090
23.2.4	Semantics and Optimality Criterion	1091
23.3	Backward Induction in Influence Diagrams	1093
23.3.1	Decision Trees for Influence Diagrams	1094
23.3.2	Sum-Max-Sum Rule	1096
23.4	Computing Expected Utilities	1098
23.4.1	Simple Variable Elimination	1098
23.4.2	Multiple Utility Variables: Simple Approaches	1100
23.4.3	Generalized Variable Elimination ★	1101
23.5	Optimization in Influence Diagrams	1105
23.5.1	Optimizing a Single Decision Rule	1105
23.5.2	Iterated Optimization Algorithm	1106
23.5.3	Strategic Relevance and Global Optimality ★	1108
23.6	Ignoring Irrelevant Information ★	1117

23.7	Value of Information	1119
23.7.1	Single Observations	1120
23.7.2	Multiple Observations	1122
23.8	Summary	1124
23.9	Relevant Literature	1125
23.10	Exercises	1128

24 Epilogue 1131

A Background Material 1135

A.1	Information Theory	1135
A.1.1	Compression and Entropy	1135
A.1.2	Conditional Entropy and Information	1137
A.1.3	Relative Entropy and Distances Between Distributions	1138
A.2	Convergence Bounds	1141
A.2.1	Central Limit Theorem	1142
A.2.2	Convergence Bounds	1143
A.3	Algorithms and Algorithmic Complexity	1144
A.3.1	Basic Graph Algorithms	1144
A.3.2	Analysis of Algorithmic Complexity	1145
A.3.3	Dynamic Programming	1147
A.3.4	Complexity Theory	1148
A.4	Combinatorial Optimization and Search	1152
A.4.1	Optimization Problems	1152
A.4.2	Local Search	1152
A.4.3	Branch and Bound Search	1158
A.5	Continuous Optimization	1159
A.5.1	Characterizing Optima of a Continuous Function	1159
A.5.2	Gradient Ascent Methods	1161
A.5.3	Constrained Optimization	1165
A.5.4	Convex Duality	1169

Bibliography 1171

Notation Index 1209

Subject Index 1213