PROBABILISTIC GRAPHICAL MODELS PRINCIPLES AND TECHNIQUES



DAPHNE KOLLER AND NIR FRIEDMAN



Adaptive Computation and Machine Learning

Thomas Dietterich, Editor

Christopher Bishop, David Heckerman, Michael Jordan, and Michael Kearns, Associate Editors

Bioinformatics: The Machine Learning Approach, Pierre Baldi and Søren Brunak

Reinforcement Learning: An Introduction, Richard S. Sutton and Andrew G. Barto

Graphical Models for Machine Learning and Digital Communication, Brendan J. Frey

Learning in Graphical Models, Michael I. Jordan

Causation, Prediction, and Search, 2nd ed., Peter Spirtes, Clark Glymour, and Richard Scheines

Principles of Data Mining, David Hand, Heikki Mannila, and Padhraic Smyth

Bioinformatics: The Machine Learning Approach, 2nd ed., Pierre Baldi and Søren Brunak

Learning Kernel Classifiers: Theory and Algorithms, Ralf Herbrich

Learning with Kernels: Support Vector Machines, Regularization, Optimization, and Beyond, Bernhard Schölkopf and Alexander J. Smola

Introduction to Machine Learning, Ethem Alpaydin

Gaussian Processes for Machine Learning, Carl Edward Rasmussen and Christopher K. I. Williams

Semi-Supervised Learning, Olivier Chapelle, Bernhard Schölkopf, and Alexander Zien, eds.

The Minimum Description Length Principle, Peter D. Grünwald

Introduction to Statistical Relational Learning, Lise Getoor and Ben Taskar, eds.

Probabilistic Graphical Models: Principles and Techniques, Daphne Koller and Nir Friedman

Probabilistic Graphical Models

Principles and Techniques

Daphne Koller

Nir Friedman

The MIT Press Cambridge, Massachusetts London, England ©2009 Massachusetts Institute of Technology

All rights reserved. No part of this book may be reproduced in any form by any electronic or mechanical means (including photocopying, recording, or information storage and retrieval) without permission in writing from the publisher.

For information about special quantity discounts, please email special_sales@mitpress.mit.edu

This book was set by the authors in $\text{MT}_{E}X2_{\epsilon}$. Printed and bound in the United States of America.

Library of Congress Cataloging-in-Publication Data

Koller, Daphne.

Probabilistic Graphical Models: Principles and Techniques / Daphne Koller and Nir Friedman.

p. cm. – (Adaptive computation and machine learning)

Includes bibliographical references and index. ISBN 978-0-262-01319-2 (hardcover : alk. paper)

1. Graphical modeling (Statistics) 2. Bayesian statistical decision theory—Graphic methods. I.

Koller, Daphne. II. Friedman, Nir.

QA279.5.K65 2010 519.5'420285-dc22 2009008615

10 9 8 7 6 5

To our families

my parents Dov and Ditza my husband Dan my daughters Natalie and Maya D.K.

my parents Noga and Gad my wife Yael my children Roy and Lior N.F.

As far as the laws of mathematics refer to reality, they are not certain, as far as they are certain, they do not refer to reality.

Albert Einstein, 1921

When we try to pick out anything by itself, we find that it is bound fast by a thousand invisible cords that cannot be broken, to everything in the universe.

John Muir, 1869

The actual science of logic is conversant at present only with things either certain, impossible, or entirely doubtful ... Therefore the true logic for this world is the calculus of probabilities, which takes account of the magnitude of the probability which is, or ought to be, in a reasonable man's mind.

James Clerk Maxwell, 1850

The theory of probabilities is at bottom nothing but common sense reduced to calculus; it enables us to appreciate with exactness that which accurate minds feel with a sort of instinct for which ofttimes they are unable to account.

Pierre Simon Laplace, 1819

Misunderstanding of probability may be the greatest of all impediments to scientific literacy.

Stephen Jay Gould

Contents

Ac	knowl	edgments	xxiii	
Lis	List of Figures xxv			
Lis	st of Al	lgorithms	s xxxi	
Lis	st of Bo	oxes	xxxiii	
1	Intro	duction	1	
	1.1	Motivati	on 1	
	1.2	Structur	ed Probabilistic Models 2	
		1.2.1	Probabilistic Graphical Models 3	
		1.2.2	Representation, Inference, Learning 5	
	1.3	Overviev	v 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	Historica	al Notes 12	
2	Foun	dations	15	
	2.1	Probabil	ity 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	

X CONTENTS

36

2.2.4 Cycles and Loops Relevant Literature 39

39

2.3

2.4

Exercises

I	Rep	resentation 43
3	The E	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 79
		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	Undi	rected 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 13

CONTENTS xi

	4.6	4.5.3 Chordal Graphs 139 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	Local	Probabilistic Models 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	Тетр	late-Based Representations 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
	0.7	6.6.2 Object Uncertainty 235
	6.7	Summary 240
	6.8	Relevant Literature 242
	6.9	Exercises 243

xii *CONTENTS*

7	Gaus	sian Network Models 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 7.3	Gaussian Bayesian Networks 251 Gaussian Markov Random Fields 254
	7.3 7.4	
	7.5	,
	7.6	Exercises 258
8	The E	Exponential Family 261
	8.1	
	8.2	Exponential Families 261 8.2.1 Linear Exponential Families 263
	8.3	Factored Exponential Families 266 8.3.1 Product Distributions 266
	8.4	8.3.2 Bayesian Networks 267 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
П	Infe	erence 285
9	Exact	t Inference: Variable Elimination 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 305 9.4.1 Simple Analysis 306 9.4.2 Graph-Theoretic Analysis 306 9.4.3 Finding Elimination Orderings * 310
	9.5	Conditioning \star 315

CONTENTS xiii

	9.6 9.7 9.8 9.9	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 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 Summary and Discussion 336 Relevant Literature 337 Exercises 338
10		Inference: 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 34910.2.2 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
	10.4	10.3.3 Answering Queries 369 Constructing a Clique Tree 372
	10.4	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	Infere	nce as Optimization 381
	11.1	Introduction 381
		11.1.1 Exact Inference Revisited ★ 382
		11.1.2 The Energy Functional 384
	11 0	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
	5	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

xiv CONTENTS

		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	Parti	cle-Based Approximate Inference 487
	12.1	Forward Sampling 488
	12,1	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	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	MAP .	Inference 551
	13.1	Overview 551

CONTENTS xv

		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	Infere	ence in Hybrid Networks 605
	14.1	Introduction 605
	1111	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

xvi CONTENTS

	14.6 14.7 14.8	
15	Infere	ence in Temporal Models 651
	15.1	
	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 661
		15.3.1 Key Ideas 661
		15.3.2 Factored Belief State Methods 663
		15.3.3 Particle Filtering 665
	15.4	15.3.4 Deterministic Search Techniques 675
	15.4	Hybrid DBNs 675 15.4.1 Continuous Models 676
		15.4.2 Hybrid Models 683
	15.5	· · · · · · · · · · · · · · · · · · ·
	15.5	Relevant Literature 690
		Exercises 692
III	Lea	arning 695
16	Learn	ing Graphical Models: Overview 697
	16.1	Motivation 697
	16.2	U
		16.2.1 Density Estimation 698
		16.2.2 Specific Prediction Tasks 700
	16.2	16.2.3 Knowledge Discovery 701 Learning as Optimization 702
	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
	1011	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	Paran	neter Estimation 717
	17 1	Maximum Likelihood Estimation 717

CONTENTS xvii

		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	Struc	ture 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

xviii *CONTENTS*

		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	Parti	ally Observed Data 849
	19.1	Foundations 849
	13.1	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
	10.2	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	Learn	ning Undirected Models 943
	20.1	Overview 943
	20.2	The Likelihood Function 944
		20.2.1 An Example 944

CONTENTS

	20.3	20.2.2 20.2.3 Maximur 20.3.1 20.3.2 20.3.3	Form of the Likelihood Function 946 Properties of the Likelihood Function 947 In (Conditional) Likelihood Parameter Estimation 949 Maximum Likelihood Estimation 949 Conditionally Trained Models 950 Learning with Missing Data 954
	20.4	20.3.4 Paramete 20.4.1 20.4.2	Maximum Entropy and Maximum Likelihood ★ 956 er Priors and Regularization 958 Local Priors 958 Global Priors 961
	20.5		with Approximate Inference 961 Belief Propagation 962 MAP-Based Learning * 967
	20.6		ve Objectives 969 Pseudolikelihood and Its Generalizations 970 Contrastive Optimization Criteria 974
	20.7	Structure 20.7.1 20.7.2 20.7.3 20.7.4 20.7.5	E Learning 978 Structure Learning Using Independence Tests 979 Score-Based Learning: Hypothesis Spaces 981 Objective Functions 982 Optimization Task 985 Evaluating Changes to the Model 992
	20.8		9
	20.9		Literature 998
	20.10	Exercises	
IV	Act	ions an	d Decisions 1007
21	Cause	•	1009
	21.1	Motivatio 21.1.1 21.1.2	on and Overview 1009 Conditioning and Intervention 1009 Correlation and Causation 1012
	21.2	Causal M	Iodels 1014
	21.3	Structura 21.3.1 21.3.2	l Causal Identifiability 1017 Query Simplification Rules 1017 Iterated Query Simplification 1020
	21.4		sms and Response Variables ★ 1026
	21.5		lentifiability in Functional Causal Models ★ 1031
	21.6		actual Queries ★ 1034
		21.6.1 21.6.2	Twinned Networks 1034 Bounds on Counterfactual Queries 1037
	21.7	Learning 21.7.1 21.7.2	Causal Models 1040 Learning Causal Models without Confounding Factors 1041 Learning from Interventional Data 1044

XX CONTENTS

		21.7.3 Dealing with Latent Variables ★ 1048
		21.7.4 Learning Functional Causal Models ★ 1051
	21.8	Summary 1053
	21.9	Relevant Literature 1054
	21.10	Exercises 1055
22	Hilit	ies and Decisions 1059
22		
	22.1	Foundations: Maximizing Expected Utility 1059
		22.1.1 Decision Making Under Uncertainty 1059 22.1.2 Theoretical Justification ★ 1062
	22.2	•
	22.2	Utility Curves 1064
		22.2.1 Utility of Money 1065 22.2.2 Attitudes Toward Risk 1066
	22.2	22.2.3 Rationality 1067
	22.3	Utility Elicitation 1068
		22.3.1 Utility Elicitation Procedures 1068
	22.4	22.3.2 Utility of Human Life 1069
	22.4	Utilities of Complex Outcomes 1071
		 22.4.1 Preference and Utility Independence ★ 1071 22.4.2 Additive Independence Properties 1074
	22.5	Summary 1081
		Relevant Literature 1082
		Exercises 1084
	22.1	EXCICISES 1004
23	Struci	tured Decision Problems 1085
	23.1	Decision Trees 1085
		23.1.1 Representation 1085
		23.1.2 Backward Induction Algorithm 1087
	23.2	Influence Diagrams 1088
		23.2.1 Basic Representation 1089
		23.2.2 Decision Rules 1090
		23.2.3 Time and Recall 1092
		23.2.4 Semantics and Optimality Criterion 1093
	23.3	Backward Induction in Influence Diagrams 1095
		23.3.1 Decision Trees for Influence Diagrams 1096
		23.3.2 Sum-Max-Sum Rule 1098
	23.4	Computing Expected Utilities 1100
		23.4.1 Simple Variable Elimination 1100
		23.4.2 Multiple Utility Variables: Simple Approaches 1102
	00.5	23.4.3 Generalized Variable Elimination ★ 1103
	23.5	Optimization in Influence Diagrams 1107
		23.5.1 Optimizing a Single Decision Rule 1107
		23.5.2 Iterated Optimization Algorithm 1108
	22.0	23.5.3 Strategic Relevance and Global Optimality ★ 1110
	23.6	Ignoring Irrelevant Information ★ 1119

CONTENTS xxi

	23.7	Value of	Information 1121
		23.7.1	Single Observations 1122
		23.7.2	Multiple Observations 1124
	23.8	Summai	ry 1126
	23.9	Relevan	t Literature 1127
	23.10	Exercise	s 1130
24	Epilo	gue	1133
A	Backg	ground M	Material 1137
	A.1	Informa	tion Theory 1137
		A.1.1	Compression and Entropy 1137
		A.1.2	Conditional Entropy and Information 1139
		A.1.3	Relative Entropy and Distances Between Distributions 1140
	A.2	Converg	gence Bounds 1143
		A.2.1	Central Limit Theorem 1144
		A.2.2	Convergence Bounds 1145
	A.3	Algorith	ms and Algorithmic Complexity 1146
		A.3.1	Basic Graph Algorithms 1146
		A.3.2	Analysis of Algorithmic Complexity 1147
		A.3.3	Dynamic Programming 1149
		A.3.4	Complexity Theory 1150
	A.4	Combin	atorial Optimization and Search 1154
		A.4.1	Optimization Problems 1154
		A.4.2	Local Search 1154
		A.4.3	Branch and Bound Search 1160
	A.5	Continu	ous Optimization 1161
		A.5.1	Characterizing Optima of a Continuous Function 1161
		A.5.2	Gradient Ascent Methods 1163
		A.5.3	Constrained Optimization 1167
		A.5.4	Convex Duality 1171
Bil	bliogra	phy	1173
No	tation	Index	1211
Subject Index		ndex	1215

Acknowledgments

This book owes a considerable debt of gratitude to the many people who contributed to its creation, and to those who have influenced our work and our thinking over the years.

First and foremost, we want to thank our students, who, by asking the right questions, and forcing us to formulate clear and precise answers, were directly responsible for the inception of this book and for any clarity of presentation.

We have been fortunate to share the same mentors, who have had a significant impact on our development as researchers and as teachers: Joe Halpern, Stuart Russell. Much of our core views on probabilistic models have been influenced by Judea Pearl. Judea through his persuasive writing and vivid presentations inspired us, and many other researchers of our generation, to plunge into research in this field.

There are many people whose conversations with us have helped us in thinking through some of the more difficult concepts in the book: Nando de Freitas, Gal Elidan, Dan Geiger, Amir Globerson, Uri Lerner, Chris Meek, David Sontag, Yair Weiss, and Ramin Zabih. Others, in conversations and collaborations over the year, have also influenced our thinking and the presentation of the material: Pieter Abbeel, Jeff Bilmes, Craig Boutilier, Moises Goldszmidt, Carlos Guestrin, David Heckerman, Eric Horvitz, Tommi Jaakkola, Michael Jordan, Kevin Murphy, Andrew Ng, Ben Taskar, and Sebastian Thrun.

We especially want to acknowledge Gal Elidan for constant encouragement, valuable feedback, and logistic support at many critical junctions, throughout the long years of writing this book.

Over the course of the years of work on this book, many people have contributed to it by providing insights, engaging in enlightening discussions, and giving valuable feedback. It is impossible to individually acknowledge all of the people who made such contributions. However, we specifically wish to express our gratitude to those people who read large parts of the book and gave detailed feedback: Rahul Biswas, James Cussens, James Diebel, Yoni Donner, Tal El-Hay, Gal Elidan, Stanislav Funiak, Amir Globerson, Russ Greiner, Carlos Guestrin, Tim Heilman, Geremy Heitz, Maureen Hillenmeyer, Ariel Jaimovich, Tommy Kaplan, Jonathan Laserson, Ken Levine, Brian Milch, Kevin Murphy, Ben Packer, Ronald Parr, Dana Pe'er, and Christian Shelton.

We are deeply grateful to the following people, who contributed specific text and/or figures, mostly to the case studies and concept boxes without which this book would be far less interesting: Gal Elidan, to chapter 11, chapter 18, and chapter 19; Stephen Gould, to chapter 4 and chapter 13; Vladimir Jojic, to chapter 12; Jonathan Laserson, to chapter 19; Uri Lerner, to chapter 14; Andrew McCallum and Charles Sutton, to chapter 4; Brian Milch, to chapter 6; Kevin

xxiv Acknowledgments

Murphy, to chapter 15; and Benjamin Packer, to many of the exercises used throughout the book. In addition, we are very grateful to Amir Globerson, David Sontag and Yair Weiss whose insights on chapter 13 played a key role in the development of the material in that chapter.

Special thanks are due to Bob Prior at MIT Press who convinced us to go ahead with this project and was constantly supportive, enthusiastic and patient in the face of the recurring delays and missed deadlines. We thank Greg McNamee, our copy editor, and Mary Reilly, our artist, for their help in improving this book considerably. We thank Chris Manning, for allowing us to use his MEX macros for typesetting this book, and for providing useful advice on how to use them. And we thank Miles Davis for invaluable technical support.

We also wish to thank the many colleagues who used drafts of this book in teaching provided enthusiastic feedback that encouraged us to continue this project at times where it seemed unending. Sebastian Thrun deserves a special note of thanks, for forcing us to set a deadline for completion of this book and to stick to it.

We also want to thank the past and present members of the DAGS group at Stanford, and the Computational Biology group at the Hebrew University, many of whom also contributed ideas, insights, and useful comments. We specifically want to thank them for bearing with us while we devoted far too much of our time to working on this book.

Finally, noone deserves our thanks more than our long-suffering families — Natalie Anna Koller Avida, Maya Rika Koller Avida, and Dan Avida; Lior, Roy, and Yael Friedman — for their continued love, support, and patience, as they watched us work evenings and weekends to complete this book. We could never have done this without you.

List of Figures

1.1	Different perspectives on probabilistic graphical models	4
1.2	A reader's guide to the structure and dependencies in this book	10
2.1	Example of a joint distribution $P(Intelligence, Grade)$	22
2.2	Example PDF of three Gaussian distributions	29
2.3	An example of a partially directed graph ${\cal K}$	35
2.4	Induced graphs and their upward closure	35
2.5	An example of a polytree	38
3.1	Simple Bayesian networks for the student example	48
3.2	The Bayesian network graph for a naive Bayes model	50
3.3	The Bayesian Network graph for the Student example	52
3.4	Student Bayesian network $\mathcal{B}^{student}$ with CPDs	53
3.5	The four possible two-edge trails	70
3.6	A simple example for the d-separation algorithm	76
3.7	Skeletons and v-structures in a network	7
3.8	Three minimal I-maps for $P_{\mathcal{B}^{student}}$, induced by different orderings	80
3.9	Network for the OneLetter example	82
3.10	Attempted Bayesian network models for the Misconception example	83
3.11	Simple example of compelled edges in an equivalence class.	88
3.12	Rules for orienting edges in PDAG	89
3.13	More complex example of compelled edges in an equivalence class	90
3.14	A Bayesian network with qualitative influences	97
3.15	A simple network for a burglary alarm domain	98
3.16	Illustration of the concept of a self-contained set	10
4.1	Factors for the Misconception example	104
4.2	Joint distribution for the Misconception example	105
4.3	An example of factor product	107
4.4	The cliques in two simple Markov networks	109
4.5	An example of factor reduction	11
4.6	Markov networks for the factors in an extended Student example	112

xxvi LIST OF FIGURES

4.7	An attempt at an I-map for a nonpositive distribution P	122
4.8	Different factor graphs for the same Markov network	123
4.9	Energy functions for the Misconception example	124
4.10	Alternative but equivalent energy functions	128
4.11	Canonical energy function for the Misconception example	130
4.12	Example of alternative definition of d-separation based on Markov networks	137
4.13	Minimal I-map Bayesian networks for a nonchordal Markov network	138
4.14	Different linear-chain graphical models	143
4.15	A chain graph K and its moralized version	149
4.16	Example for definition of c-separation in a chain graph	150
5.1	Example of a network with a deterministic CPD	160
5.2	A slightly more complex example with deterministic CPDs	161
5.3	The Student example augmented with a <i>Job</i> variable	162
5.4	A tree-CPD for $P(J \mid A, S, L)$	163
5.5	The OneLetter example of a multiplexer dependency	165
5.6	tree-CPD for a rule-based CPD	169
5.7	Example of removal of spurious edges	173
5.8	Two reduced CPDs for the OneLetter example	174
5.9	Decomposition of the noisy-or model for <i>Letter</i>	176
5.10	The behavior of the noisy-or model	177
5.11	The behavior of the sigmoid CPD	180
5.12	Example of the multinomial logistic CPD	181
5.13	Independence of causal influence	182
5.14	Generalized linear model for a thermostat	191
5.15	Example of encapsulated CPDs for a computer system model	193
6.1	A highly simplified DBN for monitoring a vehicle	203
6.2	HMM as a DBN	203
6.3	Two classes of DBNs constructed from HMMs	205
6.4	A simple 4-state HMM	208
6.5	One possible world for the University example	215
6.6	Plate model for a set of coin tosses sampled from a single coin	217
6.7	Plate models and ground Bayesian networks for a simplified Student example	219
6.8	Illustration of probabilistic interactions in the University domain	220
6.9	Examples of dependency graphs	227
7.1	Examples of 2-dimensional Gaussians	249
8.1	Example of M- and I-projections into the family of Gaussian distributions	275
8.2	Example of M- and I-projections for a discrete distribution	276
8.3	Relationship between parameters, distributions, and expected sufficient statistics	279
9.1	Network used to prove \mathcal{NP} -hardness of exact inference	289
9.2	Computing $P(D)$ by summing out the joint distribution	294
9.3	The first transformation on the sum of figure 9.2	295

LIST OF FIGURES xxvii

9.4	The second transformation on the sum of figure 9.2	295
9.5	The third transformation on the sum of figure 9.2	295
9.6	The fourth transformation on the sum of figure 9.2	295
9.7	Example of factor marginalization	297
9.8	The Extended-Student Bayesian network	300
9.9	Understanding intermediate factors in variable elimination	303
9.10	Variable elimination as graph transformation in the Student example	308
9.11	Induced graph and clique tree for the Student example	309
9.12	Networks where conditioning performs unnecessary computation	321
9.13	Induced graph for the Student example using both conditioning and elimination	323
9.14	Different decompositions for a noisy-or CPD	326
9.15	Example Bayesian network with rule-based structure	329
9.16	Conditioning in a network with CSI	334
10.1	Cluster tree for the VE execution in table 9.1	346
10.2	Simplified clique tree ${\mathcal T}$ for the Extended Student network	349
10.3	Message propagations with different root cliques in the Student clique tree	350
10.4	An abstract clique tree that is not chain-structured	352
10.5	Two steps in a downward pass in the Student network	356
10.6	Final beliefs for the Misconception example	362
10.7	An example of factor division	365
10.8	A modified Student BN with an unambitious student	373
10.9	A clique tree for the modified Student BN of figure 10.8	373
10.10	Example of clique tree construction algorithm	375
11.1	An example of a cluster graph versus a clique tree	391
11.2	An example run of loopy belief propagation	392
11.3	Two examples of generalized cluster graph for an MRF	393
11.4	An example of a 4×4 two-dimensional grid network	398
11.5	An example of generalized cluster graph for a 3×3 grid network	399
11.6	A generalized cluster graph for the 3×3 grid when viewed as pairwise MRF	405
11.7	Examples of generalized cluster graphs for network with potentials $\{A, B, C\}$, $\{B, C, D\}$, $\{B, D, F\}$, $\{B, E\}$ and $\{D, E\}$	406
11.8	Examples of generalized cluster graphs for networks with potentials $\{A,B,C\}$,	
11.0	$\{B,C,D\}$, and $\{A,C,D\}$	407
11.9	An example of simple region graph	420
11.10	The region graph corresponding to the Bethe cluster graph of figure 11.7a	421
11.11	The messages participating in different region graph computations	425
11.12	A cluster for a 4 × 4 grid network	430
11.13	Effect of different message factorizations on the beliefs in the receiving factor	431
11.14	Example of propagation in cluster tree with factorized messages	433
11.15	Markov network used to demonstrate approximate message passing	438
11.16	An example of a multimodal mean field energy functional landscape	456
11.17	Two structures for variational approximation of a 4×4 grid network	457
11.18	A diamond network and three possible approximating structures	462

xxviii LIST OF FIGURES

11.19	Simplification of approximating structure in cluster mean field	468
11.20	Illustration of the variational bound $-\ln(x) \ge -\lambda x + \ln(\lambda) + 1$	469
12.1	The Student network $\mathcal{B}^{student}$ revisited	488
12.2	The mutilated network $\mathcal{B}^{ ext{student}}_{I=i^1,G=g^2}$ used for likelihood weighting	499
12.3	The Grasshopper Markov chain	507
12.4	A simple Markov chain	509
12.5	A Bayesian network with four students, two courses, and five grades	514
12.6	Visualization of a Markov chain with low conductance	520
12.7	Networks illustrating collapsed importance sampling	528
13.1	Example of the max-marginalization factor operation for variable B	555
13.2	A network where a marginal MAP query requires exponential time	561
13.3	The max-marginals for the Misconception example	564
13.4	Two induced subgraphs derived from figure 11.3a	570
13.5	Example graph construction for applying min-cut to the binary MAP problem	590
14.1	Gaussian MRF illustrating convergence properties of Gaussian belief propagation	615
14.2	CLG network used to demonstrate hardness of inference	615
14.3	Joint marginal distribution $p(X_1, X_2)$ for a network as in figure 14.2	616
14.4	Summing and collapsing a Gaussian mixture	619
14.5	Example of unnormalizable potentials in a CLG clique tree	623
14.6	A simple CLG and possible clique trees with different correctness properties	624
14.7	Different Gaussian approximation methods for a nonlinear dependency	636
15.1	Clique tree for HMM	654
15.2	Different clique trees for the Car DBN of figure 6.1	659
15.3	Nonpersistent 2-TBN and different possible clique trees	660
15.4	Performance of likelihood weighting over time	667
15.5	Illustration of the particle filtering algorithm	669
15.6	Likelihood weighting and particle filtering over time	670
15.7	Three collapsing strategies for CLG DBNs, and their EP perspective	687
16.1	The effect of ignoring hidden variables	714
17.1	A simple thumbtack tossing experiment	718
17.2	The likelihood function for the sequence of tosses H, T, T, H, H	718
17.3	Meta-network for IID samples of a random variable	734
17.4	Examples of Beta distributions for different choices of hyperparameters	736
17.5	The effect of the Beta prior on our posterior estimates	741
17.6	The effect of different priors on smoothing our parameter estimates	742
17.7	Meta-network for IID samples from $X \to Y$ with global parameter independence	743
17.8	Meta-network for IID samples from $X \to Y$ with local parameter independence	746
17.9	Two plate models for the University example, with explicit parameter variables	758
17.10	Example meta-network for a model with shared parameters	763
17.11	Independent and hierarchical priors	765

LIST OF FIGURES xxix

18.1	Marginal training likelihood versus expected likelihood on underlying distribution	796
18.2	Maximal likelihood score versus marginal likelihood for the data $\langle H, T, T, H, H \rangle$.	797
18.3	The effect of correlation on the Bayesian score	801
18.4	The Bayesian scores of three structures for the ICU-Alarm domain	802
18.5	Example of a search problem requiring edge deletion	813
18.6	Example of a search problem requiring edge reversal	814
18.7	Performance of structure and parameter learning for instances from ICU-Alarm	
1011	network	820
18.8	MCMC structure search using 500 instances from ICU-Alarm network	830
18.9	MCMC structure search using 1,000 instances from ICU-Alarm network	831
18.10	MCMC order search using 1,000 instances from ICU-Alarm network	833
18.11	A simple module network	847
19.1	Observation models in two variants of the thumbtack example	851
19.2	An example satisfying MAR but not MCAR	853
19.3	A visualization of a multimodal likelihood function with incomplete data	857
19.4	The meta-network for parameter estimation for $X \to Y$	858
19.5	Contour plots for the likelihood function for $X \to Y$	858
19.6	A simple network used to illustrate learning algorithms for missing data	864
19.7	The naive Bayes clustering model	875
19.8	The hill-climbing process performed by the EM algorithm	882
19.9	Plate model for Bayesian clustering	902
19.10	Nondecomposability of structure scores in the case of missing data	918
19.11	An example of a network with a hierarchy of hidden variables	931
19.12	An example of a network with overlapping hidden variables	931
20.1	Log-likelihood surface for the Markov network $A{-}B{-}C$	945
20.2	A highly connected CRF that allows simple inference when conditioned	952
20.3	Laplacian distribution ($\beta = 1$) and Gaussian distribution ($\sigma^2 = 1$)	959
21.1	Mutilated Student networks representing interventions	1015
21.2	Causal network for Simpson's paradox	1016
21.3	Models where $P(Y \mid do(X))$ is identifiable	1025
21.4	Models where $P(Y \mid do(X))$ is not identifiable	1025
21.5	A simple functional causal model for a clinical trial	1030
21.6	Twinned counterfactual network with an intervention	1036
21.7	Models corresponding to the equivalence class of the Student network	1043
21.8	Example PAG and members of its equivalence class	1050
21.9	Learned causal network for exercise 21.12	1057
22.1	Example curve for the utility of money	1066
22.2	Utility curve and its consequences to an agent's attitude toward risk	1067
23.1	Decision trees for the Entrepreneur example	1086
23.2	Influence diagram \mathcal{I}_F for the basic Entrepreneur example	1089
23.3	Influence diagram $\mathcal{I}_{F,C}$ for Entrepreneur example with market survey	1091

XXX LIST OF FIGURES

23.4	Decision tree for the influence diagram $\mathcal{I}_{F,C}$ in the Entrepreneur example	1096
23.5	Iterated optimization versus variable elimination	1099
23.6	An influence diagram with multiple utility variables	1101
23.7	Influence diagrams, augmented to test for s-reachability	1112
23.8	Influence diagrams and their relevance graphs	1114
23.9	Clique tree for the imperfect-recall influence diagram of figure 23.5.	1116
23.10	More complex influence diagram \mathcal{I}_S for the Student scenario	1120
23.11	Example for computing value of information using an influence diagram	1123
A.1	Illustration of asymptotic complexity	1149
A.2	Illustration of line search with Brent's method	1165
A.3	Two examples of the convergence problem with line search	1166

List of Algorithms

3.1	Algorithm for finding nodes reachable from X given Z via active trails	75
3.2	Procedure to build a minimal I-map given an ordering	80
3.3	Recovering the undirected skeleton for a distribution P that has a P-map	85
3.4	Marking immoralities in the construction of a perfect map	86
3.5	Finding the class PDAG characterizing the P-map of a distribution P	89
5.1	Computing d-separation in the presence of deterministic CPDs	160
5.2	Computing d-separation in the presence of context-specific CPDs	173
9.1	Sum-product variable elimination algorithm	298
9.2	Using Sum-Product-VE for computing conditional probabilities	304
9.3	Maximum cardinality search for constructing an elimination ordering	312
9.4	Greedy search for constructing an elimination ordering	314
9.5	Conditioning algorithm	317
9.6	Rule splitting algorithm	332
9.7	Sum-product variable elimination for sets of rules	333
10.1	Upward pass of variable elimination in clique tree	353
10.2	Calibration using sum-product message passing in a clique tree	357
10.3	Calibration using belief propagation in clique tree	367
10.4	Out-of-clique inference in clique tree	371
11.1	Calibration using sum-product belief propagation in a cluster graph	397
11.2	Convergent message passing for Bethe cluster graph with convex counting	
	numbers	418
11.3	Algorithm to construct a saturated region graph	423
11.4	Projecting a factor set to produce a set of marginals over a given set of scopes	434
11.5	Modified version of BU-Message that incorporates message projection	44]
11.6	Message passing step in the expectation propagation algorithm	443
11.7	The Mean-Field approximation algorithm	455
12.1	Forward Sampling in a Bayesian network	489
12.2	Likelihood-weighted particle generation	493
12.3	Likelihood weighting with a data-dependent stopping rule	502
12.4	Generating a Gibbs chain trajectory	506
12.5	Generating a Markov chain trajectory	509
13.1	Variable elimination algorithm for MAP	557

xxxii LIST OF ALGORITHMS

13.2	Max-product message computation for MAP	562
13.3	Calibration using max-product BP in a Bethe-structured cluster graph	573
13.4	Graph-cut algorithm for MAP in pairwise binary MRFs with submodular	
	potentials	591
13.5	Alpha-expansion algorithm	593
13.6	Efficient min-sum message passing for untruncated 1-norm energies	603
14.1	Expectation propagation message passing for CLG networks	622
15.1	Filtering in a DBN using a template clique tree	657
15.2	Likelihood-weighted particle generation for a 2-TBN	666
15.3	Likelihood weighting for filtering in DBNs	666
15.4	Particle filtering for DBNs	670
18.1	Data perturbation search	817
19.1	Computing the gradient in a network with table-CPDs	867
19.2	Expectation-maximization algorithm for BN with table-CPDs	873
19.3	The structural EM algorithm for structure learning	922
19.4	The incremental EM algorithm for network with table-CPDs	939
19.5	Proposal distribution for collapsed Metropolis-Hastings over data completions	941
19.6	Proposal distribution over partitions in the Dirichlet process priof	942
20.1	Greedy score-based structure search algorithm for log-linear models	986
23.1	Finding the MEU strategy in a decision tree	1088
23.2	Generalized variable elimination for joint factors in influence diagrams	1105
23.3	Iterated optimization for influence diagrams with acyclic relevance graphs	1116
A.1	Topological sort of a graph	1146
A.2	Maximum weight spanning tree in an undirected graph	1147
A.3	Recursive algorithm for computing Fibonacci numbers	1150
A.4	Dynamic programming algorithm for computing Fibonacci numbers	1150
A.5	Greedy local search algorithm with search operators	1155
A.6	Local search with tabu list	1157
A.7	Beam search	1158
A.8	Greedy hill-climbing search with random restarts	1159
A.9	Branch and bound algorithm	1161
A.10	Simple gradient ascent algorithm	1164
A.11	Conjugate gradient ascent	1167

List of Boxes

Box 3.A	Concept: The Naive Bayes Model	50
Box 3.B	Case Study: The Genetics Example	. 58
Figure	3.B.1 Modeling Genetic Inheritance	58
Box 3.C	Skill: Knowledge Engineering	64
Box 3.D	Case Study: Medical Diagnosis Systems	67
	Concept: Pairwise Markov Networks	
Figure	4.A.1 A pairwise Markov network (MRF) structured as a grid	. 110
Box 4.B	Case Study: Markov Networks for Computer Vision	112
Figure	4.B.1 Two examples of image segmentation results	114
Box 4.C	Concept: Ising Models and Boltzmann Machines	. 126
Box 4.D	Concept: Metric MRFs	. 127
	Case Study: CRFs for Text Analysis	
	4.E.1 Two models for text analysis based on a linear chain CRF	
	Case Study: Context-Specificity in Diagnostic Networks	
	5.A.1 Context-specific independencies for diagnostic networks	
	Concept: Multinets and Similarity Networks	
	Concept: BN2O Networks	
Figure	5.C.1 A two-layer noisy-or network	. 178
	Case Study: Noisy Rule Models for Medical Diagnosis	
	Case Study: Robot Motion and Sensors	
	5.E.1 Probabilistic model for robot localization track	
	Case Study: HMMs and Phylo-HMMs for Gene Finding	
	Case Study: HMMs for Speech Recognition	
	6.B.1 A phoneme-level HMM for a fairly complex phoneme	
	Case Study: Collective Classification of Web Pages	
	Case Study: Object Uncertainty and Citation Matching	
	6.D.1 Two template models for citation-matching	
	Concept: The Network Polynomial	
	Concept: Polytrees	
	Case Study: Variable Elimination Orderings	
Figure	9.C.1 Comparison of algorithms for selecting variable elimination ordering	. 316

xxxiv List of Boxes

Box 9.D	Case Study: Inference with Local Structure	335
Box 10.A	Skill: Efficient Implementation of Factor Manipulation Algorithms	358
Algorit	hm 10.A.1 Efficient implementation of a factor product operation	359
Box 11.A	Case Study: Turbocodes and loopy belief propagation	393
Figure	11.A.1 Two examples of codes	394
Box 11.B	Skill: Making loopy belief propagation work in practice	407
	Case Study: BP in practice	
Figure	11.C.1 Example of behavior of BP in practice on an 11×11 Ising grid	410
Box 12.A	Skill: Sampling from a Discrete Distribution	489
Box 12.B		
	Case Study: The Bugs System	
	12.C.1 Example of Bugs model specification	
	Concept: Correspondence and Data Association	
Figure	12.D.1 Results of a correspondence algorithm for 3D human body scans	535
Box 13.A	Concept: Tree-Reweighted Belief Propagation	576
Box 13.B	Case Study: Energy Minimization in Computer Vision	593
Figure	13.B.1 MAP inference for stereo reconstruction	594
Box 15.A	Case Study: Tracking, Localization, and Mapping	679
	15.A.1 Illustration of Kalman filtering for tracking	
Figure	15.A.2 Sample trajectory of particle filtering for robot localization	681
Figure	15.A.3 Kalman filters for the SLAM problem	682
Figure	15.A.4 Collapsed particle filtering for SLAM	684
Box 16.A	Skill: Design and Evaluation of Learning Procedures	705
Algorit	hm 16.A.1 Algorithms for holdout and cross-validation tests	707
Box 16.B	Concept: PAC-bounds	708
Box 17.A	Concept: Naive Bayes Classifier	727
Box 17.B	Concept: Nonparametric Models	730
Box 17.C	Case Study: Learning the ICU-Alarm Network	749
Figure	17.C.1 The ICU-Alarm Bayesian network	750
Figure	17.C.2 Learning curve for parameter estimation for the ICU-Alarm network	751
Box 17.D	Concept: Representation Independence	752
Box 17.E	Concept: Bag-of-Word Models for Text Classification	766
Figure	17.E.1 Different plate models for text	768
Box 18.A	Skill: Practical Collection of Sufficient Statistics	819
Box 18.B	Concept: Dependency Networks	822
Box 18.C	Case Study: Bayesian Networks for Collaborative Filtering	823
Figure	18.C.1 Learned Bayesian network for collaborative filtering	823
Box 19.A	Case Study: Discovering User Clusters	877
Figure	19.A.1 Application of Bayesian clustering to collaborative filtering	878
	Case Study: EM in Practice	
	19.B.1 Convergence of EM run on the ICU Alarm network	
	19.B.2 Local maxima in likelihood surface	
	Skill: Practical Considerations in Parameter Learning	
	Case Study: EM for Robot Mapping	
	19.D.1 Sample results from EM-based 3D plane mapping	

List of Boxes xxxv

Box 19.E	Skill:	Sampling from a Dirichlet distribution	900
Box 19.F	Conc	ept: Laplace Approximation	909
Box 19.G	Case	Study: Evaluating Structure Scores	915
Figure	19.G.1	Evaluation of structure scores for a naive Bayes clustering model.	916
Box 20.A	Con	cept: Generative and Discriminative Models for Sequence Labeling.	952
Figure	20.A.1	Different models for sequence labeling: HMM, MEMM, and CRF	953
Box 20.B	Case	Study: CRFs for Protein Structure Prediction	$\dots\dots968$
Box 21.A	Case	Study: Identifying the Effect of Smoking on Cancer	1021
Figure	21.A.1	Three candidate models for smoking and cancer	1022
		Determining causality between smoking and cancer	
Box 21.B	Case	Study: The Effect of Cholestyramine	1033
Box 21.C	Case	Study: Persistence Networks for Diagnosis	1037
		Study: Learning Cellular Networks from Intervention Data	
Box 22.A	Case	Study: Prenatal Diagnosis	1079
Figure	22.A.1	Typical utility function decomposition for prenatal diagnosis	$\dots 1080$
Box 22.B	Case	Study: Utility Elicitation in Medical Diagnosis	1080
Box 23.A	Case	Study: Decision Making for Prenatal Testing	1094
Box 23.B	Case	Study: Coordination Graphs for Robot Soccer	1117
Box 23.C	Case	Study: Decision Making for Troubleshooting	1125

Introduction

1.1 Motivation

Most tasks require a person or an automated system to *reason*: to take the available information and reach conclusions, both about what might be true in the world and about how to act. For example, a doctor needs to take information about a patient — his symptoms, test results, personal characteristics (gender, weight) — and reach conclusions about what diseases he may have and what course of treatment to undertake. A mobile robot needs to synthesize data from its sonars, cameras, and other sensors to conclude where in the environment it is and how to move so as to reach its goal without hitting anything. A speech-recognition system needs to take a noisy acoustic signal and infer the words spoken that gave rise to it.

In this book, we describe a general framework that can be used to allow a computer system to answer questions of this type. In principle, one could write a special-purpose computer program for every domain one encounters and every type of question that one may wish to answer. The resulting system, although possibly quite successful at its particular task, is often very brittle: If our application changes, significant changes may be required to the program. Moreover, this general approach is quite limiting, in that it is hard to extract lessons from one successful solution and apply it to one which is very different.

We focus on a different approach, based on the concept of a *declarative representation*. In this approach, we construct, within the computer, a *model* of the system about which we would like to reason. This model encodes our knowledge of how the system works in a computer-readable form. This representation can be manipulated by various algorithms that can answer questions based on the model. For example, a model for medical diagnosis might represent our knowledge about different diseases and how they relate to a variety of symptoms and test results. A reasoning algorithm can take this model, as well as observations relating to a particular patient, and answer questions relating to the patient's diagnosis. The key property of a declarative representation is the separation of knowledge and reasoning. The representation has its own clear semantics, separate from the algorithms that one can apply to it. Thus, we can develop a general suite of algorithms that apply any model within a broad class, whether in the domain of medical diagnosis or speech recognition. Conversely, we can improve our model for a specific application domain without having to modify our reasoning algorithms constantly.

Declarative representations, or model-based methods, are a fundamental component in many fields, and models come in many flavors. Our focus in this book is on models for complex sys-

declarative representation

model



uncertainty

tems that involve a significant amount of *uncertainty*. Uncertainty appears to be an inescapable aspect of most real-world applications. It is a consequence of several factors. We are often uncertain about the true state of the system because our observations about it are partial: only some aspects of the world are observed; for example, the patient's true disease is often not directly observable, and his future prognosis is never observed. Our observations are also noisy — even those aspects that are observed are often observed with some error. The true state of the world is rarely determined with certainty by our limited observations, as most relationships are simply not deterministic, at least relative to our ability to model them. For example, there are few (if any) diseases where we have a clear, universally true relationship between the disease and its symptoms, and even fewer such relationships between the disease and its prognosis. Indeed, while it is not clear whether the universe (quantum mechanics aside) is deterministic when modeled at a sufficiently fine level of granularity, it is quite clear that it is not deterministic relative to our current understanding of it. To summarize, uncertainty arises because of limitations in our ability to observe the world, limitations in our ability to model it, and possibly even because of innate nondeterminism.

Because of this ubiquitous and fundamental uncertainty about the true state of world, we need to allow our reasoning system to consider different possibilities. One approach is simply to consider any state of the world that is possible. Unfortunately, it is only rarely the case that we can completely eliminate a state as being impossible given our observations. In our medical diagnosis example, there is usually a huge number of diseases that are *possible* given a particular set of observations. Most of them, however, are highly unlikely. If we simply list all of the possibilities, our answers will often be vacuous of meaningful content (e.g., "the patient can have any of the following 573 diseases"). **Thus, to obtain meaningful conclusions, we need to reason not just about what is possible, but also about what is probable.**

probability theory

The calculus of *probability theory* (see section 2.1) provides us with a formal framework for considering multiple possible outcomes and their likelihood. It defines a set of mutually exclusive and exhaustive possibilities, and associates each of them with a *probability* — a number between 0 and 1, so that the total probability of all possibilities is 1. This framework allows us to consider options that are unlikely, yet not impossible, without reducing our conclusions to content-free lists of every possibility.



Furthermore, one finds that probabilistic models are very liberating. Where in a more rigid formalism we might find it necessary to enumerate every possibility, here we can often sweep a multitude of annoying exceptions and special cases under the "probabilistic rug," by introducing outcomes that roughly correspond to "something unusual happens." In fact, as we discussed, this type of approximation is often inevitable, as we can only rarely (if ever) provide a deterministic specification of the behavior of a complex system. Probabilistic models allow us to make this fact explicit, and therefore often provide a model which is more faithful to reality.

1.2 Structured Probabilistic Models

This book describes a general-purpose framework for constructing and using probabilistic models of complex systems. We begin by providing some intuition for the principles underlying this framework, and for the models it encompasses. This section requires some knowledge of

basic concepts in probability theory; a reader unfamiliar with these concepts might wish to read section 2.1 first.

Complex systems are characterized by the presence of multiple interrelated aspects, many of which relate to the reasoning task. For example, in our medical diagnosis application, there are multiple possible diseases that the patient might have, dozens or hundreds of symptoms and diagnostic tests, personal characteristics that often form predisposing factors for disease, and many more matters to consider. These domains can be characterized in terms of a set of *random variables*, where the value of each variable defines an important property of the world. For example, a particular disease, such as *Flu*, may be one variable in our domain, which takes on two values, for example, *present* or *absent*; a symptom, such as *Fever*, may be a variable in our domain, one that perhaps takes on continuous values. The set of possible variables and their values is an important design decision, and it depends strongly on the questions we may wish to answer about the domain.

random variable

joint probability distribution

posterior distribution

Example 1.1

Our task is to reason probabilistically about the values of one or more of the variables, possibly given observations about some others. In order to do so using principled probabilistic reasoning, we need to construct a *joint distribution* over the space of possible assignments to some set of random variables \mathcal{X} . This type of model allows us to answer a broad range of interesting queries. For example, we can make the observation that a variable X_i takes on the specific value x_i , and ask, in the resulting *posterior distribution*, what the probability distribution is over values of another variable X_i .

Consider a very simple medical diagnosis setting, where we focus on two diseases — flu and hayfever; these are not mutually exclusive, as a patient can have either, both, or none. Thus, we might have two binary-valued random variables, Flu and Hayfever. We also have a 4-valued random variable Season, which is correlated both with flu and hayfever. We may also have two symptoms, Congestion and Muscle Pain, each of which is also binary-valued. Overall, our probability space has $2 \times 2 \times 4 \times 2 \times 2 = 64$ values, corresponding to the possible assignments to these five variables. Given a joint distribution over this space, we can, for example, ask questions such as how likely the patient is to have the flu given that it is fall, and that she has sinus congestion but no muscle pain; as a probability expression, this query would be denoted

$$P(Flu = true \mid Season = fall, Congestion = true, Muscle Pain = false).$$

1.2.1 Probabilistic Graphical Models

Specifying a joint distribution over 64 possible values, as in example 1.1, already seems fairly daunting. When we consider the fact that a typical medical- diagnosis problem has dozens or even hundreds of relevant attributes, the problem appears completely intractable. This book describes the framework of probabilistic graphical models, which provides a mechanism for exploiting structure in complex distributions to describe them compactly, and in a way that allows them to be constructed and utilized effectively.

Probabilistic graphical models use a graph-based representation as the basis for compactly encoding a complex distribution over a high-dimensional space. In this graphical representation, illustrated in figure 1.1, the nodes (or ovals) correspond to the variables in our domain, and the edges correspond to direct probabilistic interactions between them. For example, figure 1.1a (top)

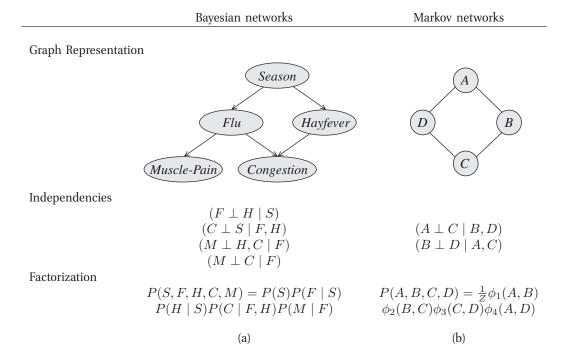


Figure 1.1 Different perspectives on probabilistic graphical models: top — the graphical representation; middle — the independencies induced by the graph structure; bottom — the factorization induced by the graph structure. (a) A sample Bayesian network. (b) A sample Markov network.

illustrates one possible graph structure for our flu example. In this graph, we see that there is no direct interaction between *Muscle Pain* and *Season*, but both interact directly with *Flu*.

There is a dual perspective that one can use to interpret the structure of this graph. From one perspective, the graph is a compact representation of a set of *independencies* that hold in the distribution; these properties take the form X is independent of Y given Z, denoted $(X \perp Y \mid Z)$, for some subsets of variables X, Y, Z. For example, our "target" distribution P for the preceding example — the distribution encoding our beliefs about this particular situation — may satisfy the conditional independence ($Congestion \perp Season \mid Flu, Hayfever$). This statement asserts that

$$P(Congestion \mid Flu, Hayfever, Season) = P(Congestion \mid Flu, Hayfever);$$

that is, if we are interested in the distribution over the patient having congestion, and we know whether he has the flu and whether he has hayfever, the season is no longer informative. Note that this assertion does *not* imply that *Season* is independent of *Congestion*; only that all of the information we may obtain from the season on the chances of having congestion we already obtain by knowing whether the patient has the flu and has hayfever. Figure 1.1a (middle) shows the set of independence assumptions associated with the graph in figure 1.1a (top).

factor

The other perspective is that the graph defines a skeleton for compactly representing a high-dimensional distribution: Rather than encode the probability of every possible assignment to all of the variables in our domain, we can "break up" the distribution into smaller factors, each over a much smaller space of possibilities. We can then define the overall joint distribution as a product of these factors. For example, figure 1.1(a-bottom) shows the factorization of the distribution associated with the graph in figure 1.1 (top). It asserts, for example, that the probability of the event "spring, no flu, hayfever, sinus congestion, muscle pain" can be obtained by multiplying five numbers: P(Season = spring), $P(Flu = false \mid Season = spring)$, $P(Hayfever = true \mid Season = spring)$, $P(Congestion = true \mid Hayfever = true, Flu = false)$, and $P(Muscle\ Pain = true \mid Flu = false)$. This parameterization is significantly more compact, requiring only 3+4+4+4+2=17 nonredundant parameters, as opposed to 63 nonredundant parameters for the original joint distribution (the 64th parameter is fully determined by the others, as the sum over all entries in the joint distribution must sum to 1). The graph structure defines the factorization of a distribution P associated with it — the set of factors and the variables that they encompass.



It turns out that these two perspectives — the graph as a representation of a set of independencies, and the graph as a skeleton for factorizing a distribution — are, in a deep sense, equivalent. The independence properties of the distribution are precisely what allow it to be represented compactly in a factorized form. Conversely, a particular factorization of the distribution guarantees that certain independencies hold.

Bayesian network

Markov network

We describe two families of graphical representations of distributions. One, called *Bayesian networks*, uses a directed graph (where the edges have a source and a target), as shown in figure 1.1a (top). The second, called *Markov networks*, uses an undirected graph, as illustrated in figure 1.1b (top). It too can be viewed as defining a set of independence assertions (figure 1.1b [middle] or as encoding a compact factorization of the distribution (figure 1.1b [bottom]). Both representations provide the duality of independencies and factorization, but they differ in the set of independencies they can encode and in the factorization of the distribution that they induce.

1.2.2 Representation, Inference, Learning

The graphical language exploits structure that appears present in many distributions that we want to encode in practice: the property that variables tend to interact *directly* only with very few others. Distributions that exhibit this type of structure can generally be encoded naturally and compactly using a graphical model.

This framework has many advantages. First, it often allows the distribution to be written down tractably, even in cases where the explicit representation of the joint distribution is astronomically large. Importantly, the type of representation provided by this framework is *transparent*, in that a human expert can understand and evaluate its semantics and properties. This property is important for constructing models that provide an accurate reflection of our understanding of a domain. Models that are opaque can easily give rise to unexplained, and even undesirable, answers.

Second, as we show, the same structure often also allows the distribution to be used effectively for *inference* — answering queries using the distribution as our model of the world. In particular, we provide algorithms for computing the posterior probability of some variables given evidence

inference

on others. For example, we might observe that it is spring and the patient has muscle pain, and we wish to know how likely he is to have the flu, a query that can formally be written as $P(Flu = true \mid Season = spring, Muscle Pain = true)$. These inference algorithms work directly on the graph structure and are generally orders of magnitude faster than manipulating the joint distribution explicitly.

Third, this framework facilitates the effective construction of these models, whether by a human expert or automatically, by *learning* from data a model that provides a good approximation to our past experience. For example, we may have a set of patient records from a doctor's office and wish to learn a probabilistic model encoding a distribution consistent with our aggregate experience. Probabilistic graphical models support a *data-driven approach* to model construction that is very effective in practice. In this approach, a human expert provides some rough guidelines on how to model a given domain. For example, the human usually specifies the attributes that the model should contain, often some of the main dependencies that it should encode, and perhaps other aspects. The details, however, are usually filled in automatically, by fitting the model to data. The models produced by this process are usually much better reflections of the domain than models that are purely hand-constructed. Moreover, they can sometimes reveal surprising connections between variables and provide novel insights about a domain.

data-driven approach



These three components — representation, inference, and learning — are critical components in constructing an intelligent system. We need a declarative representation that is a reasonable encoding of our world model. We need to be able to use this representation effectively to answer a broad range of questions that are of interest. And we need to be able to acquire this distribution, combining expert knowledge and accumulated data. Probabilistic graphical models are one of a small handful of frameworks that support all three capabilities for a broad range of problems.

1.3 Overview and Roadmap

1.3.1 Overview of Chapters

The framework of probabilistic graphical models is quite broad, and it encompasses both a variety of different types of models and a range of methods relating to them. This book describes several types of models. For each one, we describe the three fundamental cornerstones: representation, inference, and learning.

We begin in part I, by describing the most basic type of graphical models, which are the focus of most of the book. These models encode distributions over a fixed set \mathcal{X} of random variables. We describe how graphs can be used to encode distributions over such spaces, and what the properties of such distributions are.

Specifically, in chapter 3, we describe the Bayesian network representation, based on directed graphs. We describe how a Bayesian network can encode a probability distribution. We also analyze the independence properties induced by the graph structure.

In chapter 4, we move to Markov networks, the other main category of probabilistic graphical models. Here also we describe the independencies defined by the graph and the induced factorization of the distribution. We also discuss the relationship between Markov networks and Bayesian networks, and briefly describe a framework that unifies both.

In chapter 5, we delve a little deeper into the representation of the parameters in probabilistic

models, focusing mostly on Bayesian networks, whose parameterization is more constrained. We describe representations that capture some of the finer-grained structure of the distribution, and show that, here also, capturing structure can provide significant gains.

In chapter 6, we turn to formalisms that extend the basic framework of probabilistic graphical models to settings where the set of variables is no longer rigidly circumscribed in advance. One such setting is a *temporal* one, where we wish to model a system whose state evolves over time, requiring us to consider distributions over entire trajectories, We describe a compact representation — a *dynamic Bayesian network* — that allows us to represent structured systems that evolve over time. We then describe a family of extensions that introduce various forms of higher level structure into the framework of probabilistic graphical models. Specifically, we focus on domains containing *objects* (whether concrete or abstract), characterized by attributes, and related to each other in various ways. Such domains can include repeated structure, since different objects of the same type share the same probabilistic model. These languages provide a significant extension to the expressive power of the standard graphical models.

In chapter 7, we take a deeper look at models that include continuous variables. Specifically, we explore the properties of the multivariate Gaussian distribution and the representation of such distributions as both directed and undirected graphical models. Although the class of Gaussian distributions is a limited one and not suitable for all applications, it turns out to play a critical role even when dealing with distributions that are not Gaussian.

In chapter 8, we take a deeper, more technical look at probabilistic models, defining a general framework called the *exponential family*, that encompasses a broad range of distributions. This chapter provides some basic concepts and tools that will turn out to play an important role in later development.

We then turn, in part II, to a discussion of the inference task. In chapter 9, we describe the basic ideas underlying exact inference in probabilistic graphical models. We first analyze the fundamental difficulty of the exact inference task, separately from any particular inference algorithm we might develop. We then present two basic algorithms for exact inference — variable elimination and conditioning — both of which are equally applicable to both directed and undirected models. Both of these algorithms can be viewed as operating over the graph structure defined by the probabilistic model. They build on basic concepts, such as graph properties and dynamic programming algorithms, to provide efficient solutions to the inference task. We also provide an analysis of their computational cost in terms of the graph structure, and we discuss where exact inference is feasible.

In chapter 10, we describe an alternative view of exact inference, leading to a somewhat different algorithm. The benefit of this alternative algorithm is twofold. First, it uses dynamic programming to avoid repeated computations in settings where we wish to answer more than a single query using the same network. Second, it defines a natural algorithm that uses message passing on a graph structure; this algorithm forms the basis for approximate inference algorithms developed in later chapters.

Because exact inference is computationally intractable for many models of interest, we then proceed to describe approximate inference algorithms, which trade off accuracy with computational cost. We present two main classes of such algorithms. In chapter 11, we describe a class of methods that can be viewed from two very different perspectives: On one hand, they are direct generalizations of the graph-based message-passing approach developed for the case of exact inference in chapter 10. On the other hand, they can be viewed as solving an optimization

problem: one where we approximate the distribution of interest using a simpler representation that allows for feasible inference. The equivalence of these views provides important insights and suggests a broad family of algorithms that one can apply to approximate inference.

In chapter 12, we describe a very different class of methods: *particle-based methods*, which approximate a complex joint distribution by considering samples from it (also known as particles). We describe several methods from this general family. These methods are generally based on core techniques from statistics, such as importance sampling and Markov-chain Monte Carlo methods. Once again, the connection to this general class of methods suggests multiple opportunities for new algorithms.

While the representation of probabilistic graphical models applies, to a great extent, to models including both discrete and continuous-valued random variables, inference in models involving continuous variables is significantly more challenging than the purely discrete case. In chapter 14, we consider the task of inference in continuous and *hybrid* (continuous/discrete) networks, and we discuss whether and how the exact and approximate inference methods developed in earlier chapters can be applied in this setting.

The representation that we discussed in chapter 6 allows a compact encoding of networks whose size can be unboundedly large. Such networks pose particular challenges to inference algorithms. In this chapter, we discuss some special-purpose methods that have been developed for the particular settings of networks that model dynamical systems.

We then turn, in part III, to the third of our main topics — learning probabilistic models from data. We begin in chapter 16 by reviewing some of the fundamental concepts underlying the general task of learning models from data. We then present the spectrum of learning problems that we address in this part of the book. These problems vary along two main axes: the extent to which we are given prior knowledge specifying the model, and whether the data from which we learn contain complete observations of all of the relevant variables. In contrast to the inference task, where the same algorithms apply equally to Bayesian networks and Markov networks, the learning task is quite different for these two classes of models. We begin with studying the learning task for Bayesian networks.

In chapter 17, we focus on the most basic learning task: learning parameters for a Bayesian network with a given structure, from fully observable data. Although this setting may appear somewhat restrictive, it turns out to form the basis for our entire development of Bayesian network learning. As we show, the factorization of the distribution, which was central both to representation and to inference, also plays a key role in making inference feasible.

We then move, in chapter 18, to the harder problem of learning both Bayesian network structure and the parameters, still from fully observed data. The learning algorithms we present trade off the accuracy with which the learned network represents the empirical distribution for the complexity of the resulting structure. As we show, the type of independence assumptions underlying the Bayesian network representation often hold, at least approximately, in real-world distributions. Thus, these learning algorithms often result in reasonably compact structures that capture much of the signal in the distribution.

In chapter 19, we address the Bayesian network learning task in a setting where we have access only to partial observations of the relevant variables (for example, when the available patient records have missing entries). This type of situation occurs often in real-world settings. Unfortunately, the resulting learning task is considerably harder, and the resulting algorithms are both more complex and less satisfactory in terms of their performance.

We conclude the discussion of learning in chapter 20 by considering the problem of learning Markov networks from data. It turns out that the learning tasks for Markov networks are significantly harder than the corresponding problem for Bayesian networks. We explain the difficulties and discuss the existing solutions.

Finally, in part IV, we turn to a different type of extension, where we consider the use of this framework for other forms of reasoning. Specifically, we consider cases where we can act, or intervene, in the world.

In chapter 21, we focus on the semantics of intervention and its relation to causality. We present the notion of a *causal model*, which allows us to answer not only queries of the form "if I observe X, what do I learn about Y," but also *intervention queries*, of the form "if I manipulate X, what effect does it have on Y."

We then turn to the task of *decision making* under uncertainty. Here, we must consider not only the distribution over different states of the world, but also the preferences of the agent regarding these outcomes. In chapter 22, we discuss the notion of *utility functions* and how they can encode an agent's preferences about complex situations involving multiple variables. As we show, the same ideas that we used to provide compact representations of probability distribution can also be used for utility functions.

In chapter 23, we describe a unified representation for decision making, called *influence diagrams*. Influence diagrams extend Bayesian networks by introducing actions and utilities. We present algorithms that use influence diagrams for making decisions that optimize the agent's expected utility. These algorithms utilize many of the same ideas that formed the basis for exact inference in Bayesian networks.

We conclude with a high-level synthesis of the techniques covered in this book, and with some guidance on how to use them in tackling a new problem.

1.3.2 Reader's Guide

As we mentioned, the topics described in this book relate to multiple fields, and techniques from other disciplines — probability theory, computer science, information theory, optimization, statistics, and more — are used in various places throughout it. While it is impossible to present all of the relevant material within the scope of this book, we have attempted to make the book somewhat self-contained by providing a very brief review of the key concepts from these related disciplines in chapter 2.

Some of this material, specifically the review of probability theory and of graph-related concepts, is very basic yet central to most of the development in this book. Readers who are less familiar with these topics may wish to read these sections carefully, and even knowledgeable readers may wish to briefly review them to gain familiarity with the notations used. Other background material, covering such topics as information theory, optimization, and algorithmic concepts, can be found in the appendix.

The chapters in the book are structured as follows. The main text in each chapter provides the detailed technical development of the key ideas. Beyond the main text, most chapters contain boxes that contain interesting material that augments these ideas. These boxes come in three types: *Skill boxes* describe "hands-on" tricks and techniques, which, while often heuristic in nature, are important for getting the basic algorithms described in the text to work in practice. *Case study boxes* describe empirical case studies relating to the techniques described in the text.

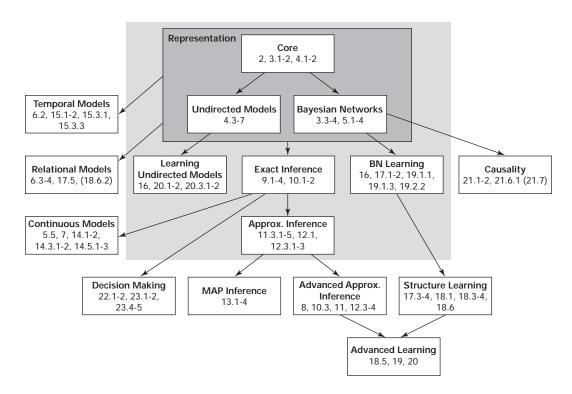


Figure 1.2 A reader's guide to the structure and dependencies in this book

These case studies include both empirical results on how the algorithms perform in practice and descriptions of applications of these algorithms to interesting domains, illustrating some of the issues encountered in practice. Finally, *concept boxes* present particular instantiations of the material described in the text, which have had significant impact in their own right.

This textbook is clearly too long to be used in its entirety in a one-semester class. Figure 1.2 tries to delineate some coherent subsets of the book that can be used for teaching and other purposes. The small, labeled boxes represent "units" of material on particular topics. Arrows between the boxes represent dependencies between these units. The first enclosing box (solid line) represents material that is fundamental to everything else, and that should be read by anyone using this book. One can then use the dependencies between the boxes to expand or reduce the depth of the coverage on any given topic. The material in the larger box (dashed line) forms a good basis for a one-semester (or even one-quarter) overview class. Some of the sections in the book are marked with an asterisk, denoting the fact that they contain more technically advanced material. In most cases, these sections are self-contained, and they can be skipped without harming the reader's ability to understand the rest of the text.

We have attempted in this book to present a synthesis of ideas, most of which have been developed over many years by multiple researchers. To avoid futile attempts to divide up the credit precisely, we have omitted all bibliographical references from the technical presentation

in the chapters. Rather, each chapter ends with a section called "Relevant Literature," which describes the historical evolution of the material in the chapter, acknowledges the papers and books that developed the key concepts, and provides some additional readings on material relevant to the chapter. We encourage the reader who is interested in a topic to follow up on some of these additional readings, since there are many interesting developments that we could not cover in this book.

Finally, each chapter includes a set of exercises that explore in additional depth some of the material described in the text and present some extensions to it. The exercises are annotated with an asterisk for exercises that are somewhat more difficult, and with two asterisks for ones that are truly challenging.

Additional material related to this book, including slides and figures, solutions to some of the exercises, and errata, can be found online at http://pgm.stanford.edu.

1.3.3 Connection to Other Disciplines

The ideas we describe in this book are connected to many fields. From probability theory, we inherit the basic concept of a probability distribution, as well as many of the operations we can use to manipulate it. From computer science, we exploit the key idea of using a graph as a data structure, as well as a variety of algorithms for manipulating graphs and other data structures. These algorithmic ideas and the ability to manipulate probability distributions using discrete data structures are some of the key elements that make the probabilistic manipulations tractable. Decision theory extends these basic ideas to the task of decision making under uncertainty and provides the formal foundation for this task.

From computer science, and specifically from artificial intelligence, these models inherit the idea of using a declarative representation of the world to separate procedural reasoning from our domain knowledge. This idea is of key importance to the generality of this framework and its applicability to such a broad range of tasks.

Various ideas from other disciplines also arise in this field. Statistics plays an important role both in certain aspects of the representation and in some of the work on learning models from data. Optimization plays a role in providing algorithms both for approximate inference and for learning models from data. Bayesian networks first arose, albeit in a restricted way, in the setting of modeling genetic inheritance in human family trees; in fact, restricted version of some of the exact inference algorithms we discuss were first developed in this context. Similarly, undirected graphical models first arose in physics as a model for systems of electrons, and some of the basic concepts that underlie recent work on approximate inference developed from that setting.

Information theory plays a dual role in its interaction with this field. Information-theoretic concepts such as entropy and information arise naturally in various settings in this framework, such as evaluating the quality of a learned model. Thus, tools from this discipline are a key component in our analytic toolkit. On the other side, the recent successes in coding theory, based on the relationship between inference in probabilistic models and the task of decoding messages sent over a noisy channel, have led to a resurgence of work on approximate inference in graphical models. The resulting developments have revolutionized both the development of error-correcting codes and the theory and practice of approximate message-passing algorithms in graphical models.

1.3.3.1 What Have We Gained?

Although the framework we describe here shares common elements with a broad range of other topics, it has a coherent common core: the use of structure to allow a compact representation, effective reasoning, and feasible learning of general-purpose, factored, probabilistic models. These elements provide us with a general infrastructure for reasoning and learning about complex domains.

As we discussed earlier, by using a declarative representation, we essentially separate out the description of the model for the particular application, and the general-purpose algorithms used for inference and learning. Thus, this framework provides a general algorithmic toolkit that can be applied to many different domains.

Indeed, probabilistic graphical models have made a significant impact on a broad spectrum of real-world applications. For example, these models have been used for medical and fault diagnosis, for modeling human genetic inheritance of disease, for segmenting and denoising images, for decoding messages sent over a noisy channel, for revealing genetic regulatory processes, for robot localization and mapping, and more. Throughout this book, we will describe how probabilistic graphical models were used to address these applications and what issues arise in the application of these models in practice.

In addition to practical applications, these models provide a formal framework for a variety of fundamental problems. For example, the notion of conditional independence and its explicit graph-based representation provide a clear formal semantics for irrelevance of information. This framework also provides a general methodology for handling data fusion — we can introduce sensor variables that are noisy versions of the true measured quantity, and use Bayesian conditioning to combine the different measurements. The use of a probabilistic model allows us to provide a formal measure for model quality, in terms of a numerical fit of the model to observed data; this measure underlies much of our work on learning models from data. The temporal models we define provide a formal framework for defining a general trend toward persistence of state over time, in a way that does not raise inconsistencies when change does occur.

In general, part of the rich development in this field is due to the close and continuous interaction between theory and practice. In this field, unlike many others, the distance between theory and practice is quite small, and there is a constant flow of ideas and problems between them. Problems or ideas arise in practical applications and are analyzed and subsequently developed in more theoretical papers. Algorithms for which no theoretical analysis exists are tried out in practice, and the profile of where they succeed and fail often provides the basis for subsequent analysis. This rich synergy leads to a continuous and vibrant development, and it is a key factor in the success of this area.

1.4 Historical Notes

The foundations of probability theory go back to the sixteenth century, when Gerolamo Cardano began a formal analysis of games of chance, followed by additional key developments by Pierre de Fermat and Blaise Pascal in the seventeenth century. The initial development involved only discrete probability spaces, and the analysis methods were purely combinatorial. The foundations of modern probability theory, with its measure-theoretic underpinnings, were laid by Andrey Kolmogorov in the 1930s.

1.4. Historical Notes

Particularly central to the topics of this book is the so-called *Bayes theorem*, shown in the eighteenth century by the Reverend Thomas Bayes (Bayes 1763). This theorem allows us to use a model that tells us the conditional probability of event a given event b (say, a symptom given a disease) in order to compute the contrapositive: the conditional probability of event b given event a (the disease given the symptom). This type of reasoning is central to the use of graphical models, and it explains the choice of the name *Bayesian network*.

The notion of representing the interactions between variables in a multidimensional distribution using a graph structure originates in several communities, with very different motivations. In the area of statistical physics, this idea can be traced back to Gibbs (1902), who used an undirected graph to represent the distribution over a system of interacting particles. In the area of genetics, this idea dates back to the work on path analysis of Sewal Wright (Wright 1921, 1934). Wright proposed the use of a directed graph to study inheritance in natural species. This idea, although largely rejected by statisticians at the time, was subsequently adopted by economists and social scientists (Wold 1954; Blalock, Jr. 1971). In the field of statistics, the idea of analyzing interactions between variables was first proposed by Bartlett (1935), in the study of *contingency tables*, also known as *log-linear models*. This idea became more accepted by the statistics community in the 1960s and 70s (Vorobev 1962; Goodman 1970; Haberman 1974).

In the field of computer science, probabilistic methods lie primarily in the realm of Artificial Intelligence (AI). The AI community first encountered these methods in the endeavor of building *expert systems*, computerized systems designed to perform difficult tasks, such as oil-well location or medical diagnosis, at an expert level. Researchers in this field quickly realized the need for methods that allow the integration of multiple pieces of evidence, and that provide support for making decisions under uncertainty. Some early systems (de Bombal et al. 1972; Gorry and Barnett 1968; Warner et al. 1961) used probabilistic methods, based on the very restricted *naive Bayes model*. This model restricts itself to a small set of possible hypotheses (e.g., diseases) and assumes that the different evidence variables (e.g., symptoms or test results) are independent given each hypothesis. These systems were surprisingly successful, performing (within their area of expertise) at a level comparable to or better than that of experts. For example, the system of de Bombal et al. (1972) averaged over 90 percent correct diagnoses of acute abdominal pain, whereas expert physicians were averaging around 65 percent.

Despite these successes, this approach fell into disfavor in the AI community, owing to a combination of several factors. One was the belief, prevalent at the time, that artificial intelligence should be based on similar methods to human intelligence, combined with a strong impression that people do not manipulate numbers when reasoning. A second issue was the belief that the strong independence assumptions made in the existing expert systems were fundamental to the approach. Thus, the lack of a flexible, scalable mechanism to represent interactions between variables in a distribution was a key factor in the rejection of the probabilistic framework.

The rejection of probabilistic methods was accompanied by the invention of a range of alternative formalisms for reasoning under uncertainty, and the construction of expert systems based on these formalisms (notably Prospector by Duda, Gaschnig, and Hart 1979 and Mycin by Buchanan and Shortliffe 1984). Most of these formalisms used the production rule framework, where each rule is augmented with some number(s) defining a measure of "confidence" in its validity. These frameworks largely lacked formal semantics, and many exhibited significant problems in key reasoning patterns. Other frameworks for handling uncertainty proposed at the time included fuzzy logic, possibility theory, and Dempster-Shafer belief functions. For a

expert systems