Probabilistic Graphical Models

SummaryFabian Damken
February 18, 2022



Contents

1	Intro	duction												ξ
	1.1	Examp	ples	 										8
	1.2	Funda	amental Questions	 										8
2	Four	ndation	ns.											ç
_			bility Theory											_
	2.1	2.1.1												
			Inference											10
	0.0		Potentials											
	2.2		ine Learning											
		2.2.1	(Document) Classification	 	• •		•	 ٠	 ٠	•	 •	٠	•	10
3	Baye	esian N	letworks											12
	3.1	The Na	aive Bayes Model	 										13
		3.1.1	Classification	 										13
		3.1.2	Maximum Likelihood Parameter Estimation											
		3.1.3	Application											
	3.2		tion and Independence Assumptions											
	·-		Local Markov Assumption											
		3.2.2	"Explaining Away" / Berkson's Paradox											13
		3.2.3	Representation Theorem											13
		3.2.4	•											13
	3.3		led Independencies											13
	5.5	3.3.1	Dependency Structures											13
		3.3.2	<u>. </u>											
		3.3.2	d-Separation											
			Faithful Distributions											
		3.3.4	Context-Specific Independence (CSI)											
		3.3.5	The Bayes' Ball Algorithm	 	• •		٠	 ٠	 ٠	•	 ٠	•	•	13
4	Infe	rence												14
	4.1	Chain	Models	 										14
	4.2	Variab	ole Elimination	 										14
		4.2.1	Evidence	 										14
		4.2.2	Complexity	 										14
			VE for Potentials											
	4.3		ctive Inference											14
		4.3.1	Consistency											14
		4.3.2	Finding Most Probable Explanations (MPEs)											14
	4.4		lexity of Conditional Queries											14
		Morali		 • •		• •	•	 •	 •	•	 •	•		14

	4.6	Variabl	Elimination in Moral Graphs	14
		4.6.1	Perfect Elimination Sequences	14
		4.6.2	Complexity	14
		4.6.3	Induced Graph	14
		4.6.4	Induced Treewidth	
		4.6.5	Elimination on Trees	
		4.6.6	General Networks	
		1.0.0	General Networks	
5	Mar	kov Ran	dom Fields	15
	5.1	Bavesia	n Networks as MRFs	15
	5.2	•	ılated Graphs	
	5.3	U	ees	
	5.4		n Trees	15
	J.¬		Collecting Evidence	15
			Distributing Evidence	
			iangulated Graphs	
	5.5	NOII-11	langurated Graphs	19
6	Lear	rning		16
U		_	ete and Incomplete Data Sets	
	0.1	_	Hidden Variables	
	()			
	6.2		ter Estimation	16
		6.2.1	Known Structure, Complete Data	16
			Known Structure, Incomplete Data (Expectation-Maximization)	16
		6.2.3	Gradient Ascent	16
		6.2.4	Bayesian Parameter Estimation	
		6.2.5	Summary	
	6.3	Structu	re Learning / Model Selection	17
		6.3.1	Minimal I-Maps	17
		6.3.2	Perfect Maps (P-Maps)	17
		6.3.3	I-Equivalence	17
		6.3.4	Obtaining a P-Map	
		6.3.5	Accurate Structures	
		6.3.6	Learning	
		6.3.7	Structure Search as Optimization	
		6.3.8	Structural EM	
		6.3.9	Summary	
		0.5.7	ounniary	11
7	Dyna	amic Ba	yesian Networks	18
	7.1		Markov Models	19
	–	Inferer		19
	/	7.2.1	Decoding	19
		7.2.1	Best State Sequence	19
		7.2.2	Parameter Estimation	19
	7.0			
	7.3		stimation (Kalman Filter)	19
		7.3.1	Recursive Bayesian Updating	19
		7.3.2	(Modeling) Actions	19
		7.3.3	Bayes Filter	19
		7.3.4	Discrete-Time Kalman Filter	19

	7.4	General Dynamic Bayesian Networks	19
		7.4.1 Exact Inference	19
		7.4.2 Tractable, Approximate Inference	19
8	App	proximate Inference	20
	8.1		20
		8.1.1 Sum-Product Belief Propagation	
		8.1.2 (Acyclic) Belief Propagation as Dynamic Programming	
		8.1.3 Loopy Belief Propagation	
	8.2	Sampling	
		8.2.1 Forward Sampling (Without Evidence)	
		8.2.2 Forward Sampling (With Evidence)	
		8.2.3 Gibbs Sampling	
		8.2.4 Likelihood Weighting	
9	Trac	ctable Probabilistic Models	21
ד	9.1	Deep Learning	
		Probabilistic Circuits	
	9.2	Sum-Product Networks	
	9.3	9.3.1 Inference	
		,	
		9.3.3 Inference on Devices	Z 1
10	Dee	p Generative Models	22
	10.1	Likelihood-Based	22
		10.1.1 Autoregressive Generatie Models	22
		10.1.2 Variational Auto-Encoders	
		10.1.3 Normalizing Flows	
	10.2	2 Likelihood-Free	
		10.2.1 Generative Adversarial Networks	
	10.3	3 Applications in Scientific Discovery	

List of Figures

2.1	Comparison of a CPT (left) and the corresponding potential (right). The rightmost column in	
	the potential $\tilde{\phi}$ is equivalent to ϕ as it can be normalized accordingly.	11

List of Tables

List of Algorithms

1 Introduction

- 1.1 Examples
- 1.2 Fundamental Questions

2 Foundations

This chapter covers fundamental concepts of probability theory and machine learning that are required for the later chapters. Note that not all relevant concepts of probability theory are covered.

2.1 Probability Theory

This section covers some very important concepts of probability theory, however, one should already be familiar with some basics like probability measures, density functions, joint distributions, marginalization, etc.¹

One note on notation: whenever a sum represents a marginalization over some random variable X, it is written as

$$P(Y) = \sum_{X}^{\text{marg.}} P(X,Y) \coloneqq \sum_{x \in \text{val}(X)} P(X = x,Y)$$

for brevity.

2.1.1 (Conditional) Independence

The most important concept leveraged in probabilistic graphical models is (conditional) independence of random variables. Two random variables X and Y are *statistically independent* if knowing either does not change the belief/probability of the other, i.e.,

$$P(X | Y) = P(X)$$
 and $P(Y | X) = P(Y)$.

This is equivalent to the definition of independence, P(X,Y) = P(X) P(Y). Independence is denoted $X \perp Y$ and is a symmetric properties. A milder property is *conditional* independence, i.e., two random variables X and Y are independent if Z is given:

$$P(X | Y, Z) = P(X | Z)$$
 and $P(Y | X, Z) = P(Y | Z)$.

Again, this property can be written as $P(X,Y \mid Z) = P(X \mid Z) P(Y \mid Z)$ by the chain rule. Conditional independency is denoted $X \perp Y \mid Z$.

The following properties hold and can be useful for some proofs later on:

Take a look the chapter of statistics fundamentals of https://fabian.damken.net/summaries/cs/elective/vc/statml/statml-summary.pdf.

Monty Hall Problem

2.1.2 Inference

Information Theory

Information theory is trying to quantify how much information is encoded in some distribution P(X). The central measure is *entropy*:

$$H_P(X) = \mathbb{E}\big[\log(1/P(X))\big] = \sum_{x \in \operatorname{val}(X)} P(X) \, \log \frac{1}{\log P(X)} = -\sum_{x \in \operatorname{val}(X)} P(X) \, \log P(X)$$

If the logarithm is of base two, the entropy encodes how much bits are required *on average* to encode X when X follows the distribution P(X). Similarly, *conditional entropy* can be defined as

$$H_P(X | Y) = \mathbb{E}[\log(1/P(X | Y))] = H_P(X, Y) - H_P(X)$$

where $H_P(X,Y)$ is the joint entropy over X and Y. Like for probabilities, a chain rule of entropies is derivable:

$$H_P(X, Y, Z) = H_P(X) + H_P(Y \mid X) + H_P(Z \mid X, Y).$$

To quantify (in)dependency between two variables *X* and *Y*, the mutual information

$$I_P(X;Y) = H_P(X) - H_P(X \mid Y)$$

can be used. This quantity is symmetric and is zero if and only if X and Y are independent.

2.1.3 Potentials

A potential is an alternative way of representing (conditional) probabilities aside from conditional probability tables (CPTs). A potential $\phi_{X,Y,Z}$ is is a function that maps each configuration $(x,y,z) \in \operatorname{val}(X) \times \operatorname{val}(Y) \times \operatorname{val}(Z)$ to a non-negative real number. The set of random variables targeted by a potential is its *domain*, i.e., dom $f_{X,Y,Z} = \{X,Y,Z\}$. Note that a (conditional) probability distribution is a special case of potentials where the potential is normalized. Vice versa, a potential can always be normalized into a CPT. This is illustrated in Figure 2.1.

Similar to CPTs, potentials can be multiplied by pairing up the entries and marginalized by summing up the corresponding entries. Compared to CPTs, it is not necessary to normalize a potential into a probability distribution afterwards, easing some calculations.

Potentials will come in handy later on when covering inference in junction trees (section 5.4).

2.2 Machine Learning

2.2.1 (Document) Classification

Figure 2.1: Comparison of a CPT (left) and the corresponding potential (right). The rightmost column in the potential $\tilde{\phi}$ is equivalent to ϕ as it can be normalized accordingly.

3 Bayesian Networks

3.1 The Naive Bayes Model
3.1.1 Classification
3.1.2 Maximum Likelihood Parameter Estimation
3.1.3 Application
3.2 Definition and Independence Assumptions
<u></u>
3.2.1 Local Markov Assumption
·
3.2.2 "Explaining Away" / Berkson's Paradox
3.2.3 Representation Theorem
3.2.4 Building a Bayesian Network
2.2 Encoded Independencies
3.3 Encoded Independencies
3.3.1 Dependency Structures
3.3.2 d-Separation
/a .: \= !!
(Active) Trails

Independencies
Soundness
Completeness
2.2.2 Faithful Diatributions
3.3.3 Faithful Distributions
3.3.4 Context-Specific Independence (CSI)
5.5.4 Context-Specific independence (CSI)
Tree CPD
Determinism
3.3.5 The Bayes' Ball Algorithm

4 Inference

4.1 Chain Models
4.2 Variable Elimination
4.2.1 Evidence
4.2.2 Complexity
4.2.3 VE for Potentials
4.3 Abductive Inference
4.3.1 Consistency
4.3.2 Finding Most Probable Explanations (MPEs)
4.4 Complexity of Conditional Queries
4.5 Moralizing
4.6 Variable Elimination in Moral Graphs
4.6.1 Perfect Elimination Sequences
4.6.2 Complexity
4.6.3 Induced Graph
'
4.6.4 Induced Treewidth
4.6.5 Elimination on Trees
Dalistus as
Polytrees
4.6.6 General Networks
TION CONCINING

5 Markov Random Fields

5.1 Bayesian Networks as MRFs
5.2 Triangulated Graphs
5.3 Join Trees
5.4 Junction Trees
5.4.1 Collecting Evidence
5.4.2 Distributing Evidence
5.5 Non-Triangulated Graphs

6 Learning

6.1 Complete and Incomplete Data Sets
6.1.1 Hidden Variables
6.2 Parameter Estimation
6.2.1 Known Structure, Complete Data
Maximum Likelihood
Decomposability of the Likelihood
Likelihood for (Conditional) Bi- and Multinomials
COOK Otherstone Incomplete Date (Francische Marini-stick)
6.2.2 Known Structure, Incomplete Data (Expectation-Maximization)
EM Idea
Complete-Data Likelihood
- The state of the
EM for (Conditional) Multinomials
Monotonicity
6.2.3 Gradient Ascent
6.2.4 Bayesian Parameter Estimation
•
Laplace Estimation
Bayesian Prediction
Bayesian Frediction
Conjugate Priors
Binomial Prior
Dirichlet Prior

Bayesian Networks and Bayesian Prediction				
6.2.5 Summary				
6.3 Structure Learning / Model Selection				
6.3.1 Minimal I-Maps				
6.3.2 Perfect Maps (P-Maps)				
6.3.3 I-Equivalence				
Skeleton and Immoralities				
6.3.4 Obtaining a P-Map				
Identifying the Skeleton				
Identifying Immoralities				
From Immoralities to Structures				
6.3.5 Accurate Structures				
6.3.6 Learning				
Constrained-Based				
Score-Based				
Likelihood Score				
Bayesian Score and Bayesian Information Criterion				
6.3.7 Structure Search as Optimization				
Learning Trees (Complete Data)				
Heuristic (Local) Search				
6.3.8 Structural EM				
6.3.9 Summary				

7 Dynamic Bayesian Networks

7.1 Hidden Markov Models
7.2 Inference
7.2.1 Decoding
Forward Pass
Backward Pass
7.2.2 Best State Sequence
Viterbi Algorithm
7.2.3 Parameter Estimation
7.3 State Estimation (Kalman Filter)
7.3.1 Recursive Bayesian Updating
7.3.2 (Modeling) Actions
7.3.3 Bayes Filter
7.3.4 Discrete-Time Kalman Filter
Dynamics and Observations
Belief Update: Prediction
Belief Update: Correction
7.4 General Dynamic Bayesian Networks
7.4.1 Exact Inference
7.4.2 Tractable, Approximate Inference
Assumed Density Filtering

8 Approximate Inference

8.1 Message Passing
8.1.1 Sum-Product Belief Propagation
0.4.0 (A
8.1.2 (Acyclic) Belief Propagation as Dynamic Programming
8.1.3 Loopy Belief Propagation
8.2 Sampling
8.2.1 Forward Sampling (Without Evidence)
8.2.2 Forward Sampling (With Evidence)
8.2.3 Gibbs Sampling
Burn-In
Irreducibility, Aperiodicity, and Ergodicity
Treducibility, Aperiodicity, and Ergodicity
Convergence
Performance
Speeding Convergence
Skipping Samples
Dendender d Westelde Onden
Randomized Variable Order
Blocking
Rao-Blackwellization
Multiple Chains
8.2.4 Likelihood Weighting

9 Tractable Probabilistic Models

9.1 Deep Learning	
9.2 Probabilistic Circuits	
9.3 Sum-Product Networks	
9.3.1 Inference	
9.3.2 Learning	
Directly Learning SPNs	
9.3.3 Inference on Devices	

10 Deep Generative Models

10.1 Likelihood-Based
10.1.1 Autoregressive Generatie Models
Learning and Inference
Parametrization
10.1.2 Variational Auto-Encoders
Inference as Optimization
Variational Bayes
Learning and Inference
Open Questions
10.1.3 Normalizing Flows
Learning and Inference
10.2 Likelihood-Free
10.2.1 Generative Adversarial Networks
Inference
10.3 Applications in Scientific Discovery