Probabilistic Graphical Models

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Contents

1		oduction 8
		Examples
	1.2	Fundamental Questions
2	Four	ndations 9
_	2.1	Probability Theory
	2.1	J J
		2.1.2 Inference
		2.1.3 Potentials
	2.2	Machine Learning
		2.2.1 (Document) Classification 10
3	Bave	esian Networks 12
	3.1	The Naive Bayes Model
	0.1	3.1.1 Maximum Likelihood Parameter Estimation 13
		3.1.2 Application
	3.2	Definition and Independence Assumptions
	3.2	3.2.1 "Explaining Away" / Berkson's Paradox
		3.2.2 Representation Theorem
	0.0	3.2.3 "Adding Edges Does Not Hurt"
	3.3	Encoded Independencies
		3.3.1 Dependency Structures
		3.3.2 d-Separation
		3.3.3 Context-Specific Independence (CSI)
		3.3.4 The Bayes' Ball Algorithm
	3.4	SOTA Modal
4	Infe	rence 19
•	4.1	Chain Models
	4.2	Variable Elimination
	7.4	4.2.1 Evidence
		4.2.2 Complexity
		4.2.3 VE for Potentials
	4.0	
	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			 	 	 	 	 		 	19
		4.6.3	Induced Graph			 	 	 	 	 		 	19
		4.6.4	Induced Treewidth			 	 	 	 	 		 	19
		4.6.5	Elimination on Trees			 	 	 	 	 			19
		4.6.6	General Networks										
5	Mar	kov Rar	ndom Fields										20
	5.1	Bayesi	ian Networks as MRFs			 	 	 	 	 			20
	5.2	Triang	gulated Graphs			 	 	 	 	 		 	20
	5.3	Join T	rees			 	 	 	 	 		 	20
	5.4	Juncti	ion Trees			 	 	 	 	 		 	20
			Collecting Evidence										
			Distributing Evidence										
	5.5		riangulated Graphs										
	0.0	11011 1	Transarated Graphs			 	 	 	 	 	•	 	_0
6	Lear	ning											21
			lete and Incomplete Data Sets .			 	 	 	 	 			21
			Hidden Variables										
	6.2		neter Estimation										
	0.2	6.2.1	Known Structure, Complete D										
		6.2.2	Known Structure, Incomplete										
		6.2.3	Gradient Ascent		_								
		6.2.4	Bayesian Parameter Estimatio										
		6.2.5	Summary										
	()		•										
	6.3		ture Learning / Model Selection										
		6.3.1	Minimal I-Maps										
		6.3.2	Perfect Maps (P-Maps)										
		6.3.3	I-Equivalence										
		6.3.4	Obtaining a P-Map										
		6.3.5	Accurate Structures										
		6.3.6	Learning										
		6.3.7	Structure Search as Optimizat	ion		 	 	 	 	 		 	22
		6.3.8	Structural EM			 	 	 	 	 		 	22
		6.3.9	Summary			 	 	 	 	 		 	22
7	•		ayesian Networks										23
	7.1		n Markov Models										24
	7.2	Infere	nce			 	 	 	 	 		 	24
		7.2.1	Decoding			 	 	 	 	 		 	24
		7.2.2	Best State Sequence			 	 	 	 	 			24
		7.2.3	Parameter Estimation			 	 	 	 	 			24
	7.3	State 1	Estimation (Kalman Filter)			 	 	 	 	 			24
		7.3.1	Recursive Bayesian Updating										24
		7.3.2	(Modeling) Actions										24
		7.3.3	Bayes Filter										$\frac{1}{24}$
		7.3.4	Discrete-Time Kalman Filter										24
	7.4	,	al Dynamic Bayesian Networks										
	/ · I	7.4.1	Exact Inference										
		/ • 1• ±	Litact Hillerence			 	 	 	 	 		 	∠ T

		7.4.2	Tractable, Approximate Inference	24
8	Аррі	roximat	te Inference	25
			ige Passing	25
			Sum-Product Belief Propagation	
		8.1.2	(Acyclic) Belief Propagation as Dynamic Programming	
		8.1.3	Loopy Belief Propagation	
	8.2		ling	
		8.2.1	Forward Sampling (Without Evidence)	
		8.2.2	Forward Sampling (With Evidence)	
		8.2.3	Gibbs Sampling	
			Likelihood Weighting	
9	Trac	table P	Probabilistic Models	26
	9.1	Deep l	Learning	26
	9.2	Probal	bilistic Circuits	26
	9.3	Sum-F	Product Networks	26
		9.3.1	Inference	26
		9.3.2	Learning	26
			Inference on Devices	
10	Daai	n Cana	rativa Madala	27
10			rative Models	
	10.1		hood-Based	
			Autoregressive Generatie Models	
			2 Variational Auto-Encoders	
			3 Normalizing Flows	
	10.2		hood-Free	
			Generative Adversarial Networks	
	10.3	Applic	cations in Scientific Discovery	27

List of Figures

2.1	Comparison of CPT and Potential	11
	Naive Bayes Bayesian Network	
3.2	A Bayesian Network Captures More than Local Independencies	15
3.3	Illustration of Independency Capturing	16

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

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

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

Bayesian networks provide a compact representation for exponentially-large distribution by exploiting conditional independencies. When representing a joint distribution $P(X_1, X_2, \ldots, X_n)$ with $|\text{val}(X_i)| = k$ for simplicity, the CPT has $k^n - 1$ entries¹! But lots of information is redundant in the joint if some of the variables exhibit independencies. Assume, for instance, that all subsets $\mathcal{X}, \mathcal{Y} \subseteq \{X_1, X_2, \ldots, X_n\}$ are independent $(\mathcal{X} \perp \mathcal{Y})$. Then the joint can be written as

$$P(X_1, X_2, \dots, X_n) = \prod_{i=1}^n P(X_i),$$

requiring only $n(k-1) \in \mathcal{O}(n)$ parameters! This is linear in the number of random variables! While this assumption seems rather simplistic, it is used with success in practice: this is the assumption of the naive Bayed classifier covered in section 3.1.

3.1 The Naive Bayes Model

In the *naive Bayes model*, it is assumed that some feature random variables $\{X_1, X_2, \dots, X_n\}$ are all conditionally independent given the class C; $\forall \mathcal{X}, \mathcal{Y} \subseteq \{X_1, X_2, \dots, X_n\} : \mathcal{X} \perp \mathcal{Y} \mid C$. The joint distribution is therefore simply

$$P(X_1, X_2, \dots, X_n, C) = P(X) \prod_{i=1}^n P(X_i).$$
(3.1)

Using Bayesian networks, the independencies are represented using a graph as shown in Figure 3.1.

To classify a new instance x (a vector composed of the individual instances of X_1, X_2, \dots, X_n), the class $c \in \text{val}(C)$ with the highest posterior probability is selected:

$$c_{\operatorname{MAP}} = \underset{c \in \operatorname{val}(C)}{\operatorname{arg}} \max \ P(c \,|\, \boldsymbol{x}) = \underset{c \in \operatorname{val}(C)}{\operatorname{arg}} \max \ \frac{P(\boldsymbol{x} \,|\, c) \, P(c)}{P(\boldsymbol{x})} = \underset{c \in \operatorname{val}(C)}{\operatorname{arg}} \max \ P(\boldsymbol{x} \,|\, c) \, P(c) = \underset{c \in \operatorname{val}(C)}{\operatorname{arg}} \max \ P(X) \prod_{i=1}^n P(X_i).$$

 $^{^{1}}$ The -1 comes from the requirement of the probability being normalized, hence the probability of the "last" configuration is implicit.

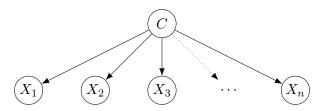


Figure 3.1: Bayesian network for the naive Bayes classifier.

3.1.1 Maximum Likelihood Parameter Estimation

To learn the probabilities required to perform classification using the naive Bayes model, the straightforward approach is to use maximum likelihood estimates, i.e., the frequencies in the data:

$$\hat{P}(C = c_j) = \frac{N(C = c_j)}{N} \qquad \qquad \hat{P}(X_i = x_{ik} \mid c_j) = \frac{N(X_i = x_{ik}, C = C_j)}{N(C = c_j)}.$$

here, $N(C=c_j)$ is the number of data points where the class is c_j and $N(X_i=x_{ik},C=C_j)$ is the number of data points with class c_j and value x_{ik} in the i-th feature. Using the identity function $\mathbb{1}[\psi]$ that is one iff ψ is true and zero otherwise, these quantities can be expressed as

$$N(C = c_j) = \sum_{((x_1, x_2, \dots, x_n), c) \in \mathcal{D}} \mathbb{1}[c = c_j] \qquad N(X_i = x_{ik}, C = C_j) = \sum_{(x_1, x_2, \dots, x_n, c) \in \mathcal{D}} \mathbb{1}[x_i = x_{ik}, c = c_j]$$

where $\mathcal{D} \subseteq \operatorname{val}(X_1) \times \operatorname{val}(X_2) \times \cdots \times \operatorname{val}(X_n) \times \operatorname{val}(C)$ is the data set. Note that the formality of the data set and values is quite rigorous in this section. From now on, the notation will be abused from time to time for brevity.

This estimation method poses a major challenge: if no instances have been observed of a given feature/class-configuration, the evidence is zero and no matter how high other evidence is in the joint (3.1), the joint will be zero. This problem can be reducing by *smoothing* the distributions to avoid overfitting,

$$\hat{P}(X_i = x_{ik} \mid c_j) = \frac{N(X_i = x_{ik}, C = C_j) + m(N(X_i = x_{ik})/N)}{N(C = c_j) + m},$$

where m controls the extend of smoothing and is a hyper-parameter.

3.1.2 Application

Even though the assumption of all features being conditionally independent is often false, the naive Bayes classifier turns out to be quite effective in practice. While not being the best classification method, is usually serves as a good and dependable baseline. *If* the assumption holds, the Bayes classifier is optimal (and can be tuned for different misclassification costs, for example).

Also, it is very fast: learning is done in a single pass over the data (by counting) and testing is linear in the number of attributes and data size. For the same reason (small CPTs), it requires very little storage, making it suitable for on-device classification.

3.2 Definition and Independence Assumptions

After some introductory treatment of the naive Bayes classifier and its associated Bayesian network, this section now focuses on a more rigorous treatment of the independencies that are actually encoded in a Bayesian network and a formal definition of what a Bayesian network is.

The key idea for Bayesian networks is the incorporation of independence assumptions into their structure. A formal Bayesian network consists of the following components:

- Set of random variables $\{X_1, X_2, \dots, X_n\}$.
- Directed acyclic graph (DAG) encoding the (in-) dependencies.

• Conditional probability table for each random variable, $P(X_i | Pa(X_i))$. $Pa(X_i)$ contains all parents of the random variable in the given DAG.

Then, the joint distribution is given by

$$P(X_1, X_2, \dots, X_n) = \prod_{i=1}^{n} P(X_i \mid Pa(X_i))$$
(3.2)

and the local Markov assumption holds. The local Markov assumption states that a random variable X_i is independent of all its non-descendants $ND(X_i)$ given its parents $Pa(X_i)$:

$$X_i \perp ND(X_i) \mid Pa(X_i)$$
.

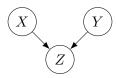
Let $Ch(X_i)$ be the children of X_i , then X_i 's non-descendants are all random variables that are not in $Des(X_i)$, X_i 's descendants:

$$\operatorname{ND}(X_i) = \{X_1, X_2, \dots, X_n\} \setminus \operatorname{Des}(X_i), \qquad \qquad \operatorname{Des}(X_i) = \operatorname{Ch}(X_i) \cup \bigcup_{X_j \in \operatorname{Ch}(X_i)} \operatorname{Des}(X_j).$$

This is a recursive definition for which $Des(X_i) = \emptyset$ holds iff X_i does not have children.

3.2.1 "Explaining Away" / Berkson's Paradox

Berkson's paradox describe the phenomenon that, by the local Markov assumption, for a network like



the independence $X \perp Y$ holds but $X \perp Y \mid Z$ does not. This implies that information can flow from X to Y iff Z is given, i.e., having evidence on either X or Y is already sufficient to explain the evidence on Z:

$$P(X = x | Z = z, Y = y) \le P(X = x | Z = z).$$

3.2.2 Representation Theorem

All this work on independencies raise the question of whether it is actually worth it: what distributions can be represented using a Bayesian network? And what networks are required to represent a distribution? Also, what other independencies apart from the local Markov assumption are encoded in a network? Some independencies can certainly be derived using the relations presented in subsection 2.1.1. Let P be the real distribution and let I(P) be the independencies encoded in the true distribution. Similarly, let $I_{\ell}(G)$ be the local independencies (induces by the local Markov assumption) encoded in a graph G. Then the key assumption of Bayesian networks is that

$$I_{\ell}(G) \subseteq I(P)$$
.

That is, the local independencies only capture such that are actual present in the true distribution. If this relation holds, G is said to be an I-map (independency map) of P.

Theorem The *representation theorem* states that G if an I-map of P if and only if P factorizes according to G via (3.2).



Figure 3.2: Illustration of a Bayesian network capturing more independencies than induced by the local Markov assumption. In this BN, the local Markov assumption encodes $I_{\ell}(G) = \{B \perp A \,|\, A, C \perp (A,B) \,|\, B, D \perp (A,B,C) \,|\, C\}$. However, also $A \perp D \,|\, C$ is a captured independency, for example.

Proof The proof is split into proofing "if" and "only if". "if".

"only if": Assume, w.l.o.g., a topological ordering X_1, X_2, \ldots, X_n where j < i for all children X_j of some random variable X_i . Applying the chain rule to the joint yields $P(X_1, X_2, \ldots, X_n) = \prod_{i=1}^n P(X_1 \mid X_1, X_2, \ldots, X_{i-1})$. By the topological ordering, $Pa(X_1) \subseteq \{X_1, X_2, \ldots, X_{i-1}\}$ and hence, using the local Markov assumption, $P(X_i \mid X_1, X_2, \ldots, X_{i-1}) = P(X_1 \mid Pa(X_i))$. Therefore, P factorized according to (3.2).

3.2.3 "Adding Edges Does Not Hurt"

Theorem Let G be an I-map for P. Then any DAG G' having the same directed edges as G, then G' is also an I-map of P.

From this theorem it follows that

- G' is strictly more expressive than G by capturing more independencies, and
- adding edges to *G* still results in an I-map.

Proof Idea Let $I_{\ell}(G) \subseteq I(P)$. To show that $I_{\ell}(G') \subseteq I(P)$ holds, it is enough to show $I_{\ell}(G') \subseteq I_{\ell}(G)$. Note that is enough to show that this property holds if a single edge is added as adding two edges can be understood as two modifications, resulting in a third graph G''. It therefore follows from $I_{\ell}(G'') \subseteq I_{\ell}(G') \subseteq I_{\ell}(G)$ that also $I_{\ell}(G'') \subseteq I_{\ell}(G)$.

Let X and Y be some random variables of G such that $Y \notin Pa_G(X)$. Then adding an edge $Y \to X$ only removes local independencies, but does not induce new ones.

3.3 Encoded Independencies

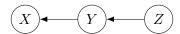
So far, only local independencies have been considered. However, a Bayesian network encodes even more dependencies by applying the algebra of conditional independencies (subsection 2.1.1; see Figure 3.2 for an example).

The findings of this section are summarized in Figure 3.3 which gives an overview of the different variants to getting the set of independencies (read this section first before inspecting the figure).

3.3.1 Dependency Structures

In a three-node BN, four types of structures are possible. The first, second, and third are indirect causal and evidential effects and a common cause, respectively:







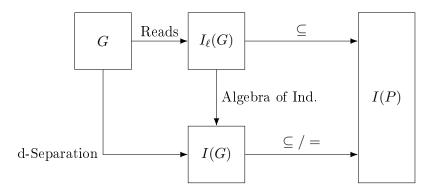


Figure 3.3: Illustration of different methods to capture the independencies of a distribution. Note that I(G) and I(P) are equal (i.e., P is faithful to G) for almost all P that factor over G.

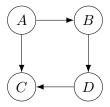
In both cases, the conditional independence $X \perp Y \mid Z$ holds, but *not* the simple independence $X \perp Y$. The last and most special structure is a v-structure, where two variables have a common effect:

$$X$$
 Y

In this case, the independencies are inverted: the simple independence $X \perp Y$ holds, but $X \perp Y \mid Z$ does not. This is the same effect as the "explain away" phenomenon / Berkson's paradox (subsection 3.2.1).

3.3.2 d-Separation

d-Separation (dependence separation) is a principled way of finding all independencies modeled by a Bayesian network. The main component are trails. A *trail* is a non-cyclic path $X_1' \leftrightarrow X_2' \leftrightarrow \cdots \leftrightarrow X_k'$ from one random variable X_1' to another X_k' . Note that a trail can also be along an edge in opposite order (i.e., the trail itself is undirected) and that every edge and note can only be visited once. For example, the network



has the following trails:

- $A \rightarrow B$, $A \rightarrow C \leftarrow D \leftarrow B$; $A \rightarrow C$, $A \rightarrow B \rightarrow D \rightarrow C$; $A \rightarrow B \rightarrow D$, $A \rightarrow C \leftarrow D$
- $B \leftarrow A, \ B \rightarrow D \rightarrow C \leftarrow A; \ B \leftarrow A \rightarrow C, \ B \rightarrow D \rightarrow C; \ B \rightarrow D, \ B \leftarrow A \rightarrow C \leftarrow D$
- $C \leftarrow A$, $C \leftarrow D \leftarrow B \leftarrow A$; $C \leftarrow A \rightarrow B$, $C \leftarrow D \leftarrow B$; $C \leftarrow D$, $C \leftarrow A \rightarrow B \rightarrow D$
- $D \leftarrow B \leftarrow A$, $D \rightarrow C \leftarrow A$; $D \leftarrow B$, $D \rightarrow C \leftarrow A \rightarrow B$; $D \rightarrow C$, $D \leftarrow B \leftarrow A \rightarrow C$

Note that as trails are themselves undirected, the graph itself really has half as many trails, but they are kept for consistency.

d-Separation now uses these trails to extract independencies. Consider any trail $X'_1 \leftrightarrow X'_2 \leftrightarrow \cdots \leftrightarrow X'_k$ between two variables X'_1 and X'_k this trail is *active* if for each triplet $X'_{i-1} \leftrightarrow X'_i \leftrightarrow X'_{i+1}$, the following holds:

- for $X_{i-1} \to X_i \to X_{i+1}$, X_i is not observed.
- for $X_{i-1} \leftarrow X_i \leftarrow X_{i+1}$, X_i is not observed.
- for $X_{i-1} \leftarrow X_i \rightarrow X_{i+1}$, X_i is not observed.
- for $X_{i-1} \to X_i \leftarrow X_{i+1}$, X_i or one of its descendants is observed.

Theorem Two variables X and Y are independent given a set of variables \mathcal{Z} if there is no active trail between X and Y if \mathcal{Z} are observed. They are said to be *d-separated*. The set of independencies obtained via d-separation is called I(G).

Soundness

Theorem d-Separation is *sound*. That is, if P factorizes over G, then $I(G) \subseteq I(P)$. This means that d-separation only captured independencies that the true distributions exhibits.

Proof

Completeness

A distribution P is said to be *faithful* if it does not have independencies that cannot be read from G.

Theorem For almost all distributions P that factorize over G, I(G) = I(P). "Almost all" means that the possible distributions are a set of measure zero parametrizations of the CPTs.

Hence, the Bayesian network is usually sufficient for capturing all independence properties of the distribution! But this only holds for complete independence, but there might be context-specific independencies that are not captured.

Proof

3.3.3 Context-Specific Independence (CSI)

As already said, d-separation only captures complete independencies, i.e., once for which

$$\forall x \in \operatorname{val}(X), y \in \operatorname{val}(Y), z \in (Z) : (X = x \perp Y = y \mid Z = z)$$

holds but context-specific independencies,

$$\exists x, \in \operatorname{val}(X), y \in \operatorname{val}(Y), z \in (Z) : (X = x \perp Y = y \mid Z = z),$$

are not captured.

One option for representing CSIs are Tree CPDs. Tree CPDs encode a distribution $P(X \mid Pa(X))$ using a decision-tree like structure, where the paths are an assignment of (a subset of) Pa(X) and leaves represent the distributions given the assignments on the path. This way, representation size can be drastically reduced when CSIs are present.

Another variant where CSIs occur is determinism. While determinism already makes the CPT sparse, it has even greater influences on inference as propagating the zeros often leads to a bunch of new zeros.

3.3.4 The Bayes' Ball Algorithm

The Bayes' ball algorithm is a algorithmic approach to applying d-separation.

3.4 SOTA Modal

Current state-of-the-art (SOTA) models are often characterized by richness in their local structures (determinism, CSI), massive sizes (thousand of variables), and high connectivity (treewidth, see subsection 4.6.4). These developments are enabled by high-level modeling tools (relational and first-order logic), the overall advancement in machine learning, and new application areas (e.g., bioinformatics and sensor networks).

In these big models, it is a must to exploit local and relational structure!

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)
440 1 1 60 101 10 1
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
Delutrose
Polytrees
4.6.6 General Networks
T.U.U GEHEIGH MELWUINS

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
6.2.2 Known Structure, Incomplete Data (Expectation-Maximization)
EM Idea
Complete-Data Likelihood
FAA for (Oor distance) NAvisin on interest
EM for (Conditional) Multinomials
Monotonicity
(0 2 Our Hant Assent
6.2.3 Gradient Ascent
6.2.4 Payasian Darameter Estimation
6.2.4 Bayesian Parameter Estimation
Laplace Estimation
Bayesian Prediction
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

74 1011 14 1 14 11
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
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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
Troubliney, 7 periodicity, and Engodicity
Convergence
Performance
Speeding Convergence
Skipping Samples
Randomized Variable Order
Blocking
Rao-Blackwellization
Multiple Chains
8.2.4 Likelihood Weighting
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9 Tractable Probabilistic Models

9.1 Deep Learning	
<u> </u>	
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