

52935 - Probabilistic Methods in Artificial Intelligence

Lecturer: Prof. Gal Elidan
Teaching Assistant: Ela Falik

Hadar Tal

Hebrew University of Jerusalem, Israel

May 24, 2024

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1 Probability Review

Definition 1.1 (Probability Space)

A probability space is a triple (Ω, \mathcal{F}, P) where:

1. Ω is the sample space
2. \mathcal{F} is a σ -algebra of subsets of Ω
3. P is a probability measure on \mathcal{F} such that $P(\Omega) = 1$

Definition 1.2 (Joint Probability)

The joint probability of two events A and B is:

$$P(A, B) := P(A \cap B)$$

Definition 1.3 (Random Variable)

A random variable X is a function $X : \Omega \rightarrow \mathbb{R}$.

$$\text{Val}(X) = \text{Image}(X) = \{x \in \mathbb{R} : \exists \omega \in \Omega \text{ s.t. } X(\omega) = x\}$$

Definition 1.4 (Probability Mass Function (PMF))

The probability mass function of a random variable X is:

$$P(X = x) := P(\{\omega \in \Omega : X(\omega) = x\})$$

Definition 1.5 (Joint Distribution)

A joint distribution over a set of RVs $\mathcal{X} = \{X_1, X_2, \dots, X_n\}$ is a probability distribution $P_{\mathcal{X}} : \text{Val}(X_1) \times \text{Val}(X_2) \times \dots \times \text{Val}(X_n) \rightarrow [0, 1]$ defined by:

$$\forall x_1, \dots, x_n : x_i \in \text{Val}(X_i) \quad P_{\mathcal{X}}(x_1, x_2, \dots, x_n) := P(X_1 = x_1, X_2 = x_2, \dots, X_n = x_n)$$

Proposition 1.1 (Law of Total Probability)

For X, Y random variables, we can write:

$$P(X) = \sum_{y \in \text{Val}(Y)} P(X, Y = y)$$

Definition 1.6 (Conditional distribution)

For X, Y RVs, and for any $y \in \text{Val}(Y)$ where $P(Y = y) > 0$ the conditional distribution of X given $Y=y$ is:

$$P(X|y) := \frac{P_{X,Y}(X = x, Y = y)}{P_Y(Y = y)}$$

Proposition 1.2 (Chain Rule)

For any set of random variables X_1, X_2, \dots, X_n :

$$P(X_1, X_2, \dots, X_n) = P(X_1)P(X_2|X_1)P(X_3|X_1, X_2) \dots P(X_n|X_1, X_2, \dots, X_{n-1})$$

Proposition 1.3 (Bayes' Rule)

For any two random variables H, E :

$$P(H = h|E = e) = \frac{P(E = e|H = h)P(H = h)}{P(E = e)}$$

where we often call:

- $P(H = h)$ the **prior** probability

- $P(H = h|E = e)$ the **posterior** probability in light of evidence $E = e$
- $P(E = e|H = h)$ the **likelihood** of the evidence $E = e$ given the hypothesis $H = h$

Definition 1.7 (Marginal Independence)

Let P be a probability distribution over a set of random variables \mathcal{X} and let $X, Y \in \mathcal{X}$. We say that X is independent of Y , denoted $P \models X \perp Y$, if

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

Definition 1.8 (Conditional Independence)

Let P be a probability distribution over a set of random variables \mathcal{X} and let $X, Y, Z \in \mathcal{X}$. We say that X is independent of Y given Z , denoted $P \models X \perp Y|Z$, if

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

Lemma 1.1 (Equivalent Definitions of Conditional Independence)

Let P be a probability distribution over a set of random variables \mathcal{X} and let $X, Y, Z \in \mathcal{X}$. The following are equivalent:

1. $P \models X \perp Y|Z$
2. $P(X, Y|Z) = P(X|Z)P(Y|Z)$
3. $P(X, Y, Z) = P(X|Z)P(Y, Z)$
4. $\exists f, g : P(X, Y, Z) = f(X, Z)g(Y, Z)$

Theorem 1.1 (Properties of Conditional Independence)

Let P be a probability distribution over a set of random variables \mathcal{X} and let $X, Y, Z, W \in \mathcal{X}$. The following hold:

1. **Symmetry** - $(X \perp Y|Z) \implies (Y \perp X|Z)$
2. **Decomposition** - $(X \perp Y, W|Z) \implies (X \perp Y|Z) \wedge (X \perp W|Z)$
3. **Weak Union** - $(X \perp Y, W|Z) \implies (X \perp Y|W, Z)$
4. **Contraction** - $(X \perp Y|Z) \wedge (X \perp W|Y, Z) \implies (X \perp Y, W|Z)$
5. **Intersection** - For strictly positive distributions,

$$(X \perp Y|W, Z) \wedge (X \perp W|Y, Z) \implies (X \perp Y, W|Z)$$

2 Bayesian Networks

2.1 Bayesian Networks Basics

Definition 2.1 (Probabilistic Graphical Model (PGM))

A probabilistic graphical model is a pair (\mathcal{G}, P) where:

1. \mathcal{G} is a graph
2. P is a probability distribution

Definition 2.2 (Bayesian Network)

A Bayesian Network \mathcal{B} is:

1. **Bayesian Network Structure** - A directed acyclic graph (DAG) $\mathcal{G} = (\mathcal{X}, E)$ ($|\mathcal{X}| = n$)
2. **Set of CPDs** - $\{P_i(X_i | Pa(X_i))\}_{i=1}^n$

the network defines a probability distribution:

$$P_{\mathcal{B}}(X_1, X_2, \dots, X_n) = \prod_{i=1}^n P_i(X_i | Pa(X_i))$$

A Bayesian Network is the tuple $\mathcal{B} = (\mathcal{G}, P_{\mathcal{B}})$.

Theorem 2.1 (Bayesian Network defines a probability distribution)

For any Bayesian Network \mathcal{B} , $P_{\mathcal{B}}(X_1, X_2, \dots, X_n)$ is a joint probability distribution over the variables X_1, X_2, \dots, X_n .

Definition 2.3 (Descendants of a node)

Let $G = (V, E)$ be a directed graph and let $X_i \in V$. The descendants of X_i are:

$$D(X_i) = \{X_j \in \mathcal{X} : \exists \text{ directed path } X_i \rightarrow \dots \rightarrow X_j\}$$

Definition 2.4 (Naive Bayes Model)

A Naive Bayes Model is a Bayesian Network where all the features are non adjacent children of the class node.

Definition 2.5 (Naive Bayes Classifier)

A Naive Bayes Classifier is a classifier that uses the Naive Bayes Model to classify instances.

$$\hat{c} = \operatorname{argmax}_{c \in C} P(c | x_1, x_2, \dots, x_n) = \operatorname{argmax}_{c \in C} P(c, x_1, x_2, \dots, x_n) = \operatorname{argmax}_{c \in C} P(c) \prod_{i=1}^n P(x_i | c)$$

2.2 Independencies and Factorization in Bayesian Networks

Definition 2.6 ($I_{LM}(\mathcal{G})$)

The **Local Markov Independencies Set** of a Bayesian Network \mathcal{B} is the set of all independencies that hold in the network:

$$I_{LM}(\mathcal{G}) = \{(X_i \perp ND(X_i) | Pa(X_i))\}_{i=1}^{|\mathcal{X}|}$$

Definition 2.7 (I(P))

The set of independencies that hold in a distribution P over \mathcal{X} is:

$$I(P) = \{(X \perp Y | Z) : (X, Y, Z) \subseteq \mathcal{X}, \quad P \models (X \perp Y | Z)\}$$

Definition 2.8 (I-map)

A DAG \mathcal{G} is an I-map of a distribution P if all independencies assumptions of \mathcal{G} hold in P :

$$I_{LM}(\mathcal{G}) \subseteq I(P)$$

Theorem 2.2 (Factorization)

If \mathcal{G} is an I-map of P , then we can write:

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

Definition 2.9 (Factorization)

We say that P factorizes over \mathcal{G} if there exist CPDs $\{P_i\}_{i=1}^n$ such that:

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

Corollary 2.1 (Independencies implies Factorization)

If \mathcal{G} is an I-map of P ($P \models I_{LM}(\mathcal{G})$), then P factorizes over \mathcal{G} .

Corollary 2.2 (Independencies implies Factorization (2))

If \mathcal{G} is an I-map of P ($P \models I_{LM}(\mathcal{G})$), then (\mathcal{G}, P) is a Bayesian Network.

Theorem 2.3 (Independencies in P_B)

For P_B it holds for all i that

1. $X_i \perp ND(X_i) | Pa(X_i) \quad (I_{LM}(\mathcal{G}))$
2. $P_B(X_i | ND(X_i)) = P_i(X_i | Pa(X_i))$

Corollary 2.3 (Factorization implies Independencies)

If P factorizes over \mathcal{G} , then \mathcal{G} is an I-map of P ($P \models I_{LM}(\mathcal{G})$).

Theorem 2.4 (Fundamental Theorem of Bayesian Networks)

Let \mathcal{G} be a BN structure over $\mathcal{X} = X_1, X_2, \dots, X_n$ and let P be a joint distribution over \mathcal{X} . Then \mathcal{G} is an I-map of $P \Leftrightarrow P$ factorizes over \mathcal{G} .

Definition 2.10 (Minimal I-map)

A DAG \mathcal{G} is a minimal I-map of a distribution P if

1. \mathcal{G} is an I-map of P
2. If $\mathcal{G}' \subset \mathcal{G}$ then \mathcal{G}' is not an I-map of P

2.3 Reasoning Patterns in Bayesian Networks**Definition 2.11 (Reasoning Patterns in Bayesian Networks)**

There are 4 main reasoning patterns in Bayesian Networks:

- **Downstream (causal) reasoning** - $X \rightarrow Z \rightarrow Y$
- **Upstream (evidential) reasoning** - $X \leftarrow Z \leftarrow Y$
- **Common Causal reasoning** - $X \leftarrow Z \rightarrow Y$
- **Common Effect reasoning** - $X \rightarrow Z \leftarrow Y$

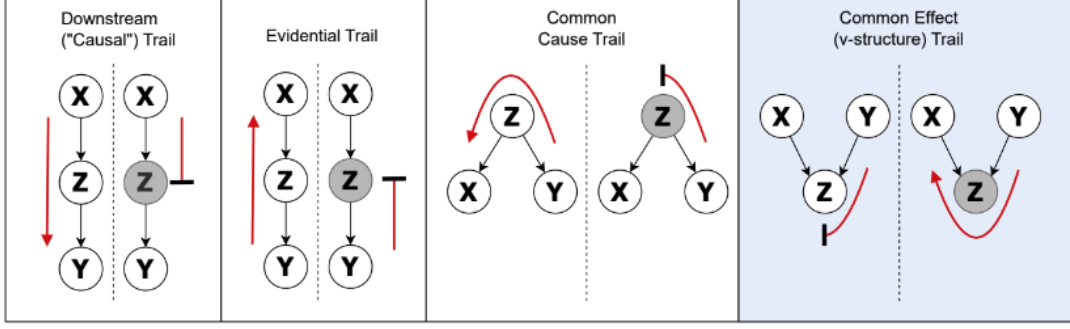


Figure 1: Reasoning Patterns in Bayesian Networks

2.4 D-separation and Global Markov Independencies

Question 2.1

If P factorizes over \mathcal{G} , then \mathcal{G} is an I-map of P ($P \models I_{LM}(\mathcal{G})$).

Can p satisfy more independencies than those implied by \mathcal{G} ? Yes.

Given $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \in \mathcal{X}$, we would like to characterize when does $P \models I_{LM}(\mathcal{G}) \implies P \models X \perp Y | Z$.

Or characterize the complement - Can we find P that factorizes over \mathcal{G} but $P \not\models X \perp Y | Z$?

Definition 2.12 (Active Trail)

A trail $X = X_1 - X_2 - \dots - X_n$ between X and Y in a BN is active given a set of observed RVs Z , if whenever there is a v-structure along the trail $X_{i-1} \rightarrow X_i \leftarrow X_{i+1}$, then X_i or one of its descendants is in Z , and all other nodes along the trail are not in Z .

Definition 2.13 (d-separation)

The sets \mathbf{X} and \mathbf{Y} are d-separated given \mathbf{Z} in \mathcal{G} , denoted $d\text{-sep}_{\mathcal{G}}(\mathbf{X}; \mathbf{Y} | \mathbf{Z})$, if there is no active trail between any node in \mathbf{X} and any node in \mathbf{Y} given \mathbf{Z} .

Definition 2.14 (Global Markov Independencies)

The set of global Markov Independencies of a BN structure \mathcal{G} is the set of all independencies that correspond to d-separation:

$$I(\mathcal{G}) := I_{GM}(\mathcal{G}) := \{(X \perp Y | Z) : d\text{-sep}_{\mathcal{G}}(X; Y | Z)\}$$

d-separation characterizes precisely the full set of independencies that a BN structure encodes.

Theorem 2.5 (Soundness)

If a distribution P factorizes over a BN structure \mathcal{G} , then $I(\mathcal{G}) \subseteq I(P)$.

Note - the other direction is not true. If a distribution P factorizes over \mathcal{G} , then it is not necessarily true that $I(P) \subseteq I(\mathcal{G})$.

Theorem 2.6 (Completeness)

If $(X \perp Y | Z) \notin I(\mathcal{G})$, then there exists a distribution P that factorizes over \mathcal{G} in which $P \not\models (X \perp Y | Z)$.

2.5 The relationship between Local and Global Markov Independencies

Proposition 2.1 ($I_{LM}(\mathcal{G}) \subseteq I_{GM}(\mathcal{G})$)

For any BN structure \mathcal{G} , it holds that $I_{LM}(\mathcal{G}) \subseteq I_{GM}(\mathcal{G})$.

Proposition 2.2

For a DAG \mathcal{G} and distribution P , it holds that $P \models I_{LM}(\mathcal{G}) \iff P \models I_{GM}(\mathcal{G})$.

Definition 2.15 (Perfect Map (P-map))

A graph \mathcal{G} is a P-map of a distribution P if $I(\mathcal{G}) = I(P)$.

2.6 Markov Blanket in Bayesian Networks

Definition 2.16 (Markov Blanket in a Bayesian Network Structure)

The Markov Blanket of a node X_i in a BN structure \mathcal{G} is the minimal set of nodes that renders X_i independent of all other nodes in the graph

$$MB(X_i) := \underset{\mathbf{Z} \in \mathcal{X}}{\operatorname{argmin}} \{ |\mathbf{Z}| : X_i \perp \mathcal{X} / (X_i \cup \mathbf{Z}) | \mathbf{Z} \}$$

Definition 2.17 (Spouses of a node)

The spouses of a node X_i in a BN structure \mathcal{G} are the parents of the children of X_i

$$Sp(X_i) := \{X_j \in \mathcal{X} : X_j \text{ is a parent of a child of } X_i\}$$

Theorem 2.7 (Markov Blanket Theorem (in Bayesian Networks))

For any node X_i in a BN structure \mathcal{G} , it holds that:

$$MB(X_i) = Pa(X_i) \cup Ch(X_i) \cup Sp(X_i)$$

Lemma 2.1 (Markov Blanket is not unique)

Let P be a distribution over \mathcal{X} and let $X_i \in \mathcal{X}$. $MB(X_i)$ is not unique.

3 Markov Chains

3.1 Markov Chains Basics

Definition 3.1 (Markov Property)

Given a random process $\{X^{(t)}\}_{t \in \mathbb{N}}$, over a state space \mathcal{S} , we say it possess the Markov property, if $\forall t \geq 1$,

$$X^{(t+1)} \perp X^{(1)}, \dots, X^{(t-1)} | X^{(t)}$$

that is,

$$\forall t \in \mathbb{N} \quad P_t(X^{(t+1)} | X^{(1)}, \dots, X^{(t)}) = P(X^{(t+1)} | X^{(t)})$$

Definition 3.2 (Time-invariant assumption)

$$\forall t \in \mathbb{N} \quad P_t(X^{(t+1)} | X^{(t)}) = P(X^{(t+1)} | X^{(t)})$$

Definition 3.3 (Markov Chain)

A Markov Chain is a random process $\{X^{(t)}\}_{t \in \mathbb{N}}$ that possess the Markov property.

Note: Markov Chains are often represented as a directed graph, where each node is a state in the state space, and each edge is a transition between states. The transition diagram is a very different entity from the graph encoding the structure of a Bayesian Network.

3.2 Hidden Markov Models (HMMs)

Definition 3.4 (Hidden Markov Model)

A pair of random processes $(\{X^{(t)}\}_{t \in \mathbb{N}} \text{ and } \{O^{(t)}\}_{t \in \mathbb{N}})$ is a Hidden Markov Model if:

1. $X^{(t)}$ is a Markov process whose behavior is not directly observable (hidden).
2. For each t ,

$$O^{(t)} \perp X^{(1:t-1)}, X^{(t+1:T)} | X^{(t)}$$

that is,

$$P(O^{(t)} | X^{(1:t-1)}, X^{(t+1:T)}) = P(O^{(t)} | X^{(t)})$$

We call:

- $X^{(t)}$ the **hidden states**,
- $O^{(t)}$ the **observed states**,
- $P(X^{(t+1)} | X^{(t)})$ the **transition probability**
- $P(O^{(t)} | X^{(t)})$ the **emission probability**

4 Markov Networks

4.1 Markov Networks Basics

Definition 4.1 (Gibbs Distribution)

A Gibbs distribution over a set of random variables \mathcal{X} is a probability distribution of the form:

$$P_{\mathcal{X}}(x_1, x_2, \dots, x_n) = \frac{1}{\mathcal{Z}} \prod_j \phi_j(X_{c_j})$$

where

- $\mathcal{C} = \{c_1, c_2, \dots, c_m\}$ is a set of cliques in the graph.
- X_{c_j} is the set of random variables in clique c_j
- $\phi_j : \text{Val}(X_{c_j}) \rightarrow \mathbb{R}^+$ is a potential function / factor over the clique c_j
- \mathcal{Z} is the normalization constant (partition function)

Definition 4.2 (Markov Network)

A Markov Network \mathcal{M} is:

1. **Markov Network Structure** - An undirected graph $\mathcal{H} = (\mathcal{X}, E)$ ($|\mathcal{X}| = n$)
2. **Set of Factors** - $\Phi = \{\phi_j(X_{c_j})\}_j$ such that every X_{c_j} is a clique in \mathcal{H}

the network defines a probability distribution:

$$P_{\Phi}(X_1, X_2, \dots, X_n) = \frac{1}{\mathcal{Z}} \prod_j \phi_j(X_{c_j})$$

A Markov Network is the tuple $\mathcal{M} = (\mathcal{H}, P_{\Phi})$.

4.2 Independencies and Factorization in Markov Networks

Definition 4.3 (Separating Set)

A set of nodes Z separates X and Y in an undirected graph \mathcal{H} if every path between X and Y passes through Z , denoted $\text{sep}_{\mathcal{H}}(X; Y|Z)$.

Definition 4.4 (I(\mathcal{H}))

The set of independencies that hold in a MN structure \mathcal{H} is

$$I(\mathcal{H}) = \{(X \perp Y|Z) : \text{sep}_{\mathcal{H}}(X; Y|Z)\}$$

Lemma 4.1 (Monotonicity of separation)

If $Z \subseteq Z'$, then $\text{sep}_{\mathcal{H}}(X; Y|Z) \subseteq \text{sep}_{\mathcal{H}}(X; Y|Z')$.

Definition 4.5 (Factorization)

We say that P factorizes over \mathcal{H} if there exist factors $\{\phi_j\}_j$ and a normalization constant \mathcal{Z} such that:

$$P(X_1, X_2, \dots, X_n) = \frac{1}{\mathcal{Z}} \prod_j \phi_j(X_{c_j})$$

such that every c_j is a clique in \mathcal{H} .

Theorem 4.1 (Soundness)

If a distribution P factorizes over \mathcal{H} , then \mathcal{H} is an I-map of P ($P \models I(\mathcal{H})$).

Theorem 4.2 (Completeness)

Let \mathcal{H} be a MN structure. If X, Y are not separated by Z in \mathcal{H} , then there exists a distribution P that factorizes over \mathcal{H} in which $P \models X \perp Y | Z$.

Definition 4.6 ($I_{pair}(\mathcal{H})$)

The **Pairwise Independencies Set** of a \mathcal{H} is defined as:

$$I_{pair}(\mathcal{H}) = \{(X \perp Y | \mathcal{X} / \{X, Y\}) : X - Y \notin \mathcal{H}\}$$

(i.e., X and Y are independent given all other nodes)

Definition 4.7 (Neighbors of a node ($Ne(X_i)$))

The neighbors of a node X_i in a MN structure \mathcal{H} are the nodes that are connected to X_i in the graph

$$Ne(X_i) := \{X_j \in \mathcal{X} : X_i - X_j \in \mathcal{H}\}$$

Definition 4.8 ($I_{local}(\mathcal{H})$)

The **Local Independencies Set** of a \mathcal{H} is defined as:

$$I_{local}(\mathcal{H}) = \{(X_i \perp (\mathcal{X} / (\{X_i\} \cup Ne(X_i))) | Ne(X_i))\}$$

(i.e., X_i is independent of all other nodes given its neighbors)

Lemma 4.2 (Independence implies pairwise independence)

$$P \models I(\mathcal{H}) \implies P \models I_{local}(\mathcal{H}) \implies I_{pair}(\mathcal{H})$$

Theorem 4.3 (For positive P , pairwise independence implies independence)

If P is a strictly positive distribution, then

$$P \models I_{pair}(\mathcal{H}) \Leftrightarrow P \models I(\mathcal{H})$$

4.3 Markov Blanket in Markov Networks**Definition 4.9 (Markov Blanket in a Markov Network Structure)**

The Markov Blanket of a node X_i in a MN structure \mathcal{H} is the minimal set of nodes that renders X_i independent of all other nodes in the graph

$$MB(X_i) := \operatorname{argmin}_{\mathbf{Z} \in \mathcal{X}} \{|\mathbf{Z}| : X_i \perp \mathcal{X} / (X_i \cup \mathbf{Z}) | \mathbf{Z}\} = \operatorname{argmin}_{\mathbf{Z} \in \mathcal{X}} \{|\mathbf{Z}| : \operatorname{sep}_{\mathcal{H}}(X_i; \mathcal{X} / (X_i \cup \mathbf{Z}) | \mathbf{Z})\}$$

Theorem 4.4 (Markov Blanket Theorem (in Markov Networks))

For strictly positive MN (\mathcal{H}, P_{Φ}) , for any node X_i in \mathcal{H} , it holds that:

$$MB(X_i) = Ne(X_i)$$

4.4 Building a minimal I-map \mathcal{H} for P **Definition 4.10 (I-map)**

An undirected graph \mathcal{H} is an I-map of a distribution P if all independencies assumptions of \mathcal{H} hold in P :

$$I(\mathcal{H}) \subseteq I(P)$$

Algorithm 1: Building a minimal I-map \mathcal{H} for P

Input: An oracle that returns $\forall X, Y, Z \subseteq \mathcal{X}$ if $P \models X \perp Y | Z$

Output: \mathcal{H} - a minimal I-map of P

```
foreach  $X_i \in X_1, \dots, X_n$  do
  foreach  $X_j \in \{X_1, \dots, X_n\} / \{X_i\}$  do
    if  $P \not\models X_i \perp X_j | \mathcal{X} / \{X_i, X_j\}$  then
       $\mathcal{H}_e \leftarrow \mathcal{H}_e \cup \{X_i - X_j\}$ 
    end
  end
end
end
```

Theorem 4.5 (Uniqueness of minimal I-map)

There exists a unique undirected minimal I-map \mathcal{H} of a distribution P .

4.5 The transitions between Bayesian Networks and Markov Networks

4.5.1 BM \rightarrow MN

Definition 4.11 (Immortality)

An immortality in a BN structure \mathcal{G} is a pair of nodes X_i, X_j that have a common child X_k but are not connected by an edge.

Definition 4.12 (The Moral Graph $M(\mathcal{G})$)

The moral graph of a BN structure \mathcal{G} is the undirected graph that is created in the following way:

1. $M(\mathcal{G})$ contains all the nodes of \mathcal{G}
2. $M(\mathcal{G})$ contains all the edges in \mathcal{G} undirected
3. For every pair of nodes X_i, X_j that have a common child in \mathcal{G} , add an edge between X_i and X_j in $M(\mathcal{G})$

Theorem 4.6 ($M(\mathcal{G})$ is a minimal I-map of G)

The moral graph $M(\mathcal{G})$ is a minimal I-map of the distribution P that has exactly the same independencies as \mathcal{G} .

Theorem 4.7

If \mathcal{G} is a moral graph, then $M[\mathcal{G}]$ is a P-map of G ; i.e.,

$$I(\mathcal{G}) = I(M[\mathcal{G}])$$

4.5.2 MN \rightarrow BM

Definition 4.13 (Triangulated Graph)

A graph \mathcal{H} is triangulated if every cycle of length ≥ 4 has a chord.

Definition 4.14 (Skeleton of a Bayesian Network)

The skeleton of a Bayesian Network \mathcal{G} is the undirected graph that is created by removing the directions of the edges in \mathcal{G} .

Theorem 4.8

If \mathcal{G} is an I-map of \mathcal{H} , then the skeleton of \mathcal{G} is a triangulation of \mathcal{H} .

Lemma 4.3

If \mathcal{G} is a moral graph, then the skeleton of \mathcal{G} is a triangulated graph.