## Probabilistic Graphical Models: Principles and Applications

# Chapter 7: BAYESIAN NETWORKS: REPRESENTATION AND INFERENCE (Part I) 

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## Introduction

- Bayesian networks are directed graphical models that represent the joint distribution of a set of random variables
- In this graphs, the nodes represent random variables and the arcs direct dependencies between variables
- The structure of the graph encodes a set of conditional independence relations between the variables


## Example



- Fever is independent of Body ache given Flu (common cause)
- Fever is independent of Unhealthy food given Typhoid (indirect cause)
- Typhoid is independent of Flu when Fever is NOT known (common effect). Knowing Fever makes Typhoid and Flu dependent


## Introduction

- In addition to the structure, a Bayesian network considers a set of local parameters, which are the conditional probabilities for each variable given its parents in the graph
- The joint probability of all the variables in the network can be represented based on these local parameters; this usually implies an important saving in the number of required parameters
- Given a Bayesian network we can answer several probabilistic queries. For instance, for the previous example: What is the probability of Fever given Flu? Which is more probable, Typhoid or Flu, given Fever and Unhealthy food?


## Bayesian Networks

- A Bayesian network (BN) represents the joint distribution of a set of $n$ (discrete) variables, $X_{1}, X_{2}, \ldots, X_{n}$, as a directed acyclic graph (DAG) and a set of conditional probability tables (CPTs)
- Each node, that corresponds to a variable, has an associated CPT that contains the probability of each state of the variable given its parents in the graph
- The structure of the network implies a set of conditional independence assertions, which give power to this representation


## An example



- Joint distribution:

$$
\begin{aligned}
& P(C, T, G, R, F, D)= \\
& P(C) P(G) P(T \mid C) P(R \mid T) P(F \mid T, G) P(D \mid T, G)
\end{aligned}
$$

## Conditional Independence Assertions

- The conditional independence assertions implied by the structure of a BN should correspond to the conditional independence relations of the joint probability distribution, and vice versa
- If $X$ is conditionally independent of $Z$ given $Y$ :
- In the probability distribution: $P(X \mid Y, Z)=P(X \mid Y)$.
- In the graph: $I\langle X| Y|Z\rangle$.


## D-Separation

- Conditional independence assertions can be verified directly from the structure of a BN using a criteria called D-separation
- 3 basic BN structures for 3 variables and 2 arcs:
- Sequential: $X \rightarrow Y \rightarrow Z$.
- Divergent: $X \leftarrow Y \rightarrow Z$.
- Convergent: $X \rightarrow Y \leftarrow Z$.
- In the first two cases, $X$ and $Z$ are conditionally independent given $Y$, however in the third case this is not true


## D-Separation

- Given a graph $G$, a set of variables $A$ is conditionally independent of a set $B$ given a set $C$, if there is no trajectory in $G$ between $A$ and $B$ such that:
(1) All convergent nodes are or have descendants in $C$.
(2) All other nodes are outside $C$.


## Bayes Ball

- Consider that we have a path from node $X$ to $Z$ with $Y$ in the middle $-Y$ is shaded if it is known (instantiated), otherwise it is not shaded
- We throw a ball from $X$ to $Z$, if the ball arrives to $Z$ then $X$ and $Z$ are NOT independent given $Y$ :
(1) If $Y$ is sequential or divergent and is not shaded, the ball goes through.
(2) If $Y$ is sequential or divergent and it is shaded, the ball is blocked.
(3) If $Y$ is convergent and not shaded, the ball is blocked.
(4) If $Y$ is convergent and shaded, the ball goes through.


## Bayes Ball



## Contours

- Markov assumption: any node $X$ is conditionally independent of all nodes in $G$ that are not descendants of $X$ given its parents in the graph, $\operatorname{Pa}(X)$
- The structure of a BN can be specified by the parents of each variable; thus the set of parents of a variable $X$ is known as the contour of $X$
- Given this condition and using the chain rule, we can specify the joint probability distribution of the set of variables in a BN as the product of the conditional probability of each variable given its parents


## Markov Blanket

- The Markov Blanket of a node $X, M B(X)$, is the set of nodes that make it independent of all the other nodes in $G$, that is $P(X \mid G-X)=P(X \mid M B(X))$
- For a BN, the Markov blanket of $X$ is:
- the parents of $X$,
- the sons of $X$,
- and other parents of the sons of $X$.


## Mappings

- Given a probability distribution $P$ of $\mathbf{X}$, and its graphical representation $G$, there must be a correspondence between the conditional independence in $P$ and in $G$ mappings:

D-Map: all the conditional independence relations in $P$ are satisfied (by D-Separation) in $G$.
I-Map: all the conditional independence relations in $G$ are true in $P$.
P-Map: or perfect map, it is a D-Map and an I-Map.

- It is not always possible to have a perfect mapping of the independence relations between the graph $(G)$ and the distribution $(P)$, so we settle for what is called a Minimal I-Map: all the conditional independence relations implied by $G$ are true in $P$, and if any arc is deleted in $G$ this condition is lost


## Independence Axioms

- Given some conditional independence relations between subsets of random variables, we can derive other conditional independence relations axiomatically
- Independence axioms:

Symmetry: $I(X, Z, Y) \rightarrow I(Y, Z, X)$
Decomposition:

$$
I(X, Z, Y \cup W) \rightarrow I(X, Z, Y) \wedge I(X, Z, W)
$$

Weak Union: $I(X, Z, Y \cup W) \rightarrow I(X, Z \cup W, Y)$
Contraction:

$$
I(X, Z, Y) \wedge I(X, Z \cup Y, W) \rightarrow I(X, Z, Y \cup W)
$$

Intersection: $I(X, Z \cup W, Y) \wedge I(X, Z \cup Y, W) \rightarrow$

$$
I(X, Z, Y \cup W)
$$

## Graphically

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(c)

(d)


## CPTs

- In the case of a BN, the parameters are the conditional probabilities of each node given its parents in the graph
- If we consider discrete variables:
- Root nodes: vector of marginal probabilities.
- Other nodes: conditional probability table (CPT) of the variable given its parents in the graph.


## Example



## Canonical Models

- Canonical models represent the relations between a set of random variables for particular interactions using few parameters
- There are several classes of canonical models, the most common are the Noisy OR and Noisy AND for binary variables, and their extensions for multivalued variables, Noisy Max and Noisy Min, respectively
- For example, consider a variable that represents a disease, $D$. In the case of the binary canonical models it has two values, True and False. For a multivalued model, it could be defined as
$D \in\{$ False, Mild, Intermediate, Severe $\}$, such that these values follow a predefined order


## Noisy-OR

- The Noisy OR model is applied when several variables or causes can produce an effect if any one of them is True, and as more of the causes are true, the probability of the effect increases



## Conditions

- The following two conditions must be satisfied for a Noisy OR canonical model to be applicable:
Responsibility: the effect is false if all the possible causes are false.
Independence of exceptions: if an effect is the manifestation of several causes, the mechanisms that inhibit the occurrence of the effect under one cause are independent of the mechanisms that inhibit it under the other causes.
- The probability that the effect $E$ is inhibited (it does not occur) under cause $C_{i}$ is defined as:

$$
\begin{equation*}
q_{i}=P\left(E=\text { False } \mid C_{i}=\text { True }\right) \tag{1}
\end{equation*}
$$

## Parameters

- The parameters in the CPT for a Noisy OR model can be obtained using the following expressions when all the $m$ causes are True:

$$
\begin{align*}
& P\left(E=\text { False } \mid C_{1}=\operatorname{True}, \ldots C_{m}=\operatorname{True}\right)=\prod_{i=i}^{m} q_{i}  \tag{2}\\
& P\left(E=\text { True } \mid C_{1}=\operatorname{True}, \ldots C_{m}=\operatorname{True}\right)=1-\prod_{i=i}^{m} q_{i} \tag{3}
\end{align*}
$$

- If $k$ of $m$ causes are True, then
$P\left(E=\right.$ False $\left.\mid C_{1}=\operatorname{True}, \ldots C_{k}=\operatorname{True}\right)=\prod_{i=i}^{k} q_{i}$, so that if all the causes are False then the effect is False with a probability of one


## Example

- Three causes, $C_{1}, C_{2}, C_{3}$
- $q_{1}=q_{2}=q_{3}=0.1$


## CPT:

| $C_{1}$ | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 1 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $C_{2}$ | 0 | 0 | 1 | 1 | 0 | 0 | 1 | 1 |
| $C_{3}$ | 0 | 1 | 0 | 1 | 0 | 1 | 0 | 1 |
| $P(E=0)$ | 1 | 0.1 | 0.1 | 0.01 | 0.1 | 0.01 | 0.01 | 0.001 |
| $P(E=1)$ | 0 | 0.9 | 0.9 | 0.99 | 0.9 | 0.99 | 0.99 | 0.999 |

## Decision Trees

- An alternative representation is based on the observation that in the probability tables for many domains, the same probability values tend to be repeated several times in the same table
- A decision tree (DT) could be used for representing a CPT in a compact way:
Each internal node corresponds to a variable in the CPT, and the branches from a node correspond to the different values a variable can take. The leaf nodes in the tree represent the different probability values. A trajectory from the root to a leaf, specifies a probability value for the corresponding variables-values in the trajectory


## Example - CPT

| Fepresenara. | A | B | C | D | E | F | G | X |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Mion | T | T/F | T/F | T/F | T/F | T/F | T/F | 0.9 |
| Semes | F | T | T/F | T | T/F | T | T | 0.9 |
| Ineerence natec | F | T | T/F | T | T/F | T | F | 0.0 |
| References | F | T | T/F | T | T/F | F | T/F | 0.0 |
|  | F | T | T | F | T | T/F | T | 0.9 |
|  | F | T | T | F | T | T/F | F | 0.0 |
|  | F | T | T | F | F | T/F | T/F | 0.0 |
|  | F | T | F | F | T/F | T/F | T/F | 0.0 |
|  | F | F | T | T/F | T | T/F | T | 0.9 |
|  | F | F | T | T/F | T | T/F | F | 0.0 |
|  | F | F | T | T/F | F | T/F | T/F | 0.0 |
|  | F | F | F | T/F | T/F | T/F | T/F | 0.0 |

## Example - DT



## Decision Diagram

- A decision diagram (DD) extends a DT by considering a directed acyclic graph structure, such that it is not restricted to a tree
- This avoids the need to duplicate repeated probability values in the leaf nodes, and in some cases provides an even more compact representation


## Example - DD



## Probabilistic inference

- Probabilistic inference consists in propagating the effects of certain evidence in a Bayesian network to estimate its effect on the unknown variables
- There are basically two variants of the inference problem in BNs:
- Single query inference: obtaining the posterior probability of a single variable, $H$, given a subset of known (instantiated) variables, E, that is, $P(H \mid \mathbf{E})$
- Conjunctive query inference: consists in calculating the posterior probability of a set of variables, $\mathbf{H}$ given the evidence, $\mathbf{E}$, that is, $P(\mathbf{H} \mid \mathbf{E})$


## Inference algorithms:

(1) Probability propagation (Pearl's algorithm)
(2) Variable elimination
(3) Conditioning
(4) Junction tree
(5) Stochastic simulation

## Complexity

- In the worst case the inference problem is NP-hard for Bayesian networks
- There are efficient (polynomial) algorithms for certain types of structures (singly connected networks)
- For other structures it depends on the connectivity of the graph.
- In many applications, the graphs are sparse and in this case there are inference algorithms which are very efficient


## Probability propagation in trees

- Given that the BN has a tree structure, any node divides the network into two independent subtrees



## Basic equations

- Given certain evidence, E (subset of instantiated variables), the posterior probability for a value $i$ of any variable $B$, can be obtained by applying the Bayes rule:

$$
\begin{equation*}
P(B i \mid \mathbf{E})=P(B i) P(\mathbf{E} \mid B i) / P(\mathbf{E}) \tag{4}
\end{equation*}
$$

- We can separate the evidence into:

E-: Evidence in the tree rooted in $B$.
$E_{+}$: All other evidence.

- Then:

$$
\begin{equation*}
P(B i \mid \mathbf{E})=P(B i) P(\mathbf{E}-, \mathbf{E}+\mid B i) / P(\mathbf{E}) \tag{5}
\end{equation*}
$$

## Basic equations

- Given that $\mathbf{E}+$ and $\mathbf{E}$ - are independent, by applying the Bayes rule again, we obtain:

$$
\begin{equation*}
P(B i \mid \mathbf{E})=\alpha P(B i \mid \mathbf{E}+) P(\mathbf{E}-\mid B i) \tag{6}
\end{equation*}
$$

Where $\alpha$ is a normalization constant.

- We define the following terms:

$$
\begin{gather*}
\lambda(B i)=P(\mathbf{E}-\mid B i)  \tag{7}\\
\pi(B i)=P(B i \mid \mathbf{E}+) \tag{8}
\end{gather*}
$$

- Then:

$$
\begin{equation*}
P(B i \mid \mathbf{E})=\alpha \pi(B i) \lambda(B i) \tag{9}
\end{equation*}
$$

## Propagation algorithm

- The computation of the posterior probability of any node $B$ is decomposed into two parts: (i) the evidence coming from the sons of $B$ in the tree $(\lambda)$, and the evidence coming from the parent of $B,(\pi)$
- We can think of each node $B$ in the tree as a simple processor that stores its vectors $\pi(B)$ and $\lambda(B)$, and its conditional probability table, $P(B \mid A)$
- The evidence is propagated via a message passing mechanism, in which each node sends the corresponding messages to its parent and sons in the tree


## Messages

- A message sent from node $B$ to its parent $A$ :


## Inference

$$
\begin{equation*}
\lambda_{B}(A i)=\sum_{j} P\left(B_{j} \mid A_{i}\right) \lambda\left(B_{j}\right) \tag{10}
\end{equation*}
$$

- A message sent from node $B$ to its son $S_{k}$ :

$$
\begin{equation*}
\pi_{k}(B i)=\alpha \pi\left(B_{j}\right) \prod_{l \neq k} \lambda_{l}\left(B_{j}\right) \tag{11}
\end{equation*}
$$

where / refers to each one of the sons of $B$

## Combination and Propagation

- Each node can receive several $\lambda$ messages, which are combined via a term by term multiplication for the $\lambda$ messages received from each son:

$$
\begin{equation*}
\lambda(A i)=\prod_{j=1}^{m} \lambda_{S j}(A i) \tag{12}
\end{equation*}
$$

- The propagation algorithm starts by assigning the evidence to the known variables, and then propagating it through the message passing mechanism until the root of the tree is reached for the $\lambda$ messages, and the leaves are reached for the $\pi$ messages


## Bottom-up propagation



## Top-down propagation



## Initial Conditions

Leaf nodes: If not known, $\lambda=[1,1, \ldots, 1]$ (a uniform distribution). If known, $\lambda=[0,0, \ldots, 1, \ldots, 0]$ (one for the assigned value and zero for all other values).
Root node: If not known, $\pi=P(A)$ (prior marginal probability vector). If known, $\pi=[0,0, \ldots, 1, \ldots, 0]$ (one for the assigned value and zero for all other values).

## Propagation - example



- Consider that the only evidence is $F=$ false - initial conditions for the leaf nodes are: $\lambda_{F}=[1,0]$ and $\lambda_{D}=[1,1]$ (no evidence)


## Example - $\lambda$ propagation

- Multiplying the $\lambda$ vectors by the corresponding CPTs:

$$
\begin{gathered}
\lambda_{F}(E)=[1,0]\left[\begin{array}{l}
0.9,0.5 \\
0.1,0.5
\end{array}\right]=[0.9,0.5] \\
\lambda_{D}(E)=[1,1]\left[\begin{array}{l}
0.7,0.4 \\
0.3,0.6
\end{array}\right]=[1,1]
\end{gathered}
$$

- Then, $\lambda(E)$ is obtained by combining the messages from its two sons:

$$
\lambda(E)=[0.9,0.5] \times[1,1]=[0.9,0.5]
$$

- Propagation to its parent, $C$ :

$$
\lambda_{E}(C)=[0.9,0.5]\left[\begin{array}{l}
0.9,0.7 \\
0.1,0.3
\end{array}\right]=[0.86,0.78]
$$

## Example - $\pi$ propagation

- Given that $C$ is not instantiated, $\pi(C)=[0.8,0.2]$
- Propagate to its son, $E$, which also corresponds to multiplying the $\pi$ vector by the corresponding CPT:

$$
\pi(E)=[0.8,0.2]\left[\begin{array}{c}
0.9,0.7 \\
0.1,0.3
\end{array}\right]=[0.86,0.14]
$$

- We now propagate to its son $D$; however, given that $E$ has another son, $F$, we also need to consider the $\lambda$ message from this other son, thus:

$$
\pi(D)=[0.86,0.14] \times[0.9,0.5]\left[\begin{array}{l}
0.7,0.4 \\
0.3,0.6
\end{array}\right]=[0.57,0.27]
$$

## Example - posterior probabilities

- Given the $\lambda$ and $\pi$ vectors for each unknown variable, we just multiply them term by term and then normalize to obtain the posterior probabilities:

$$
\begin{gathered}
P(C)=[0.86,0.2] \times[0.86,0.78]=\alpha[0.69,0.16] \\
=[0.815,0.185] \\
P(E)=[0.86,0.14] \times[0.9,0.5]=\alpha[0.77,0.07] \\
=[0.917,0.083] \\
P(D)=[0.57,0.27] \times[1,1]=\alpha[0.57,0.27]=[0.67,0.33]
\end{gathered}
$$

## Analysis

- The time complexity to obtain the posterior probability of all the variables in the tree is proportional to the diameter of the network (the number of arcs in the trajectory from the root to the most distant leaf).
- The message passing mechanism can be directly extended to polytrees, as these are also singly connected networks. In this case, a node can have multiple parents, so the $\lambda$ messages should be sent from a node to all its parents
- The propagation algorithm only applies to singly connected network


## Book

## Sucar, L. E, Probabilistic Graphical Models, Springer 2015 Chapter 7

## Additional Reading

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