## Advanced Data Analysis and Modelling Summerschool

## Inference in Bayesian Networks

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## Inference

- By inference in BNs we refer to the task of computing a-posteriori probabilities.
■ This task can be found under different names: probability propagation, belief updating, belief revision, ...
- Most of queries involve observations or evidence

Evidence on a variable is a statement of the certainties of its states, i.e., (flu=yes).

- Hard evidence. An evidence function that assigns a zero probability to all but one state is said to provide hard evidence. Hard evidence e over a set of variables $E$ is often referred to as instantiation.
temperature=high, headache=no
- Soft evidence. An evidence function that assigns a probability distribution over $\operatorname{dom}\left(E_{i}\right)$ for each $E_{i} \in E$ is said to provide soft evidence.
- Example. If dom(temperature) = (no, ligth, high, very-high) and dom(headache)=(yes,no), the we can have the following soft evidence:
- $\operatorname{se}($ temperature $)=(0,0,2,1)$ and se(headache $)=(2,1)$


## Type of queries

- The simplest query: to compute the evidence probability:

$$
P(\mathbf{e})=\sum_{X_{i} \notin} P\left(X_{1}, \ldots, X_{n}, \mathbf{e}\right)
$$

- The most frequent query: compute the a-posteriori probability for a given target or interest variable.

$$
P(X \mid \mathbf{e})=\frac{P(X, \mathbf{e})}{P(\mathbf{e})}
$$

To do this we only need to compute $P(X, \mathbf{e})$, because

$$
P(\mathbf{e})=\sum_{x \in \operatorname{dom}(X)} P(X=x, \mathbf{e})
$$

In general, we are not only interested in a single variable but in a set of them, usually all the unobserved ones.

- Computing the a-posteriori probability of a given variable is useful in different situations:
- Predictive or deductive reasoning: What is the probability of observing a sympton knowing the presence of a given desease?
In this case the target variable usually is a descendant of the evidence.
- Diagnostic or abductive reasoning: What is the probability of desease $D$ being the correct diagnosis given some symptoms? In this case the target variable usually is an ancestor of the evidence.
- That is, in the BNs framework the direction of the links between the variables does not constraint the type of query to be posed.


## Type of queries (III)

Queries about sets of variables:
■ A-posteriori probability of a subset of variables: $P(X, Y, \ldots \mid \mathbf{e})$

- Searching for the most probable explanation, the configuration of maximal probabiity, belief revision or abductive inference:
- Total abduction or MPE: If $X_{1}, \ldots, X_{n}$ are the unobserved variables, then the goal is to identify the configuration $\left(x_{1}, \ldots, x_{n}\right)$ that maximises $P\left(X_{1}, \ldots, X_{n} \mid \mathbf{e}\right)$.
- Partial abduction or MAP: Given a subset $\left\{X_{1}, \ldots, X_{l}\right\}$ of the unobserved variables, then the goal is to identify the configuration $\left(x_{1}, \ldots, x_{l}\right)$ that maximises $P\left(X_{1}, \ldots, X_{l} \mid \mathbf{e}\right)$.
- In general, the goal is to look for the $K$ most probable explanations.


## Basic operations

To get answers for the previous queries we only need a few operations:
■ Projection. Given two sets of variables $\mathbf{X}$ and $\mathbf{Y}$, such that, $\mathbf{X} \cap \mathbf{Y} \neq 0$, then

$$
\mathbf{Z}=\mathbf{X}^{\downarrow \mathbf{Y}}
$$

contains the variables of $\mathbf{X}$ that also are in $\mathbf{Y}$.

- Projection also applies to configurations, thus, if $\mathbf{x}$ and $\mathbf{y}$ are configurations of $\mathbf{X}$ and $\mathbf{Y}$, then

$$
z=x^{\downarrow y}
$$

contains the sub-configuration of $\mathbf{x}$ restricted to the variables in $\mathbf{X}$ that also are in $\mathbf{Y}$.

- Combination. Given two pieces of information defined over $\mathbf{X}$ and $\mathbf{Y}$, the goal of the combination is to obtain a new information defined over the $\mathbf{X} \cup \mathbf{Y}$.
- In our case the piece of information are probability functions or potentials, and the result is a new probability function or potential obtained by point-wise multiplication:


## Basic Operations (II)

- Combination Example: Assuming all variables are binary, then from $f_{1}(A, B)$ and $f_{2}(A, C)$ we get:

$$
\begin{gathered}
f(A, B, C)=f_{1}(A, B) \times f_{2}(A, C) \\
\left(\begin{array}{lll} 
& b & \bar{b} \\
a & 0.5 & 0.8 \\
\bar{a} & 0.5 & 0.2
\end{array}\right) \times\left(\begin{array}{lll} 
& c & \bar{c} \\
a & 1.0 & 0.4 \\
\bar{a} & 0.0 & 0.6
\end{array}\right)=\left(\begin{array}{lllll} 
& b, c & b, \bar{c} & \bar{b}, c & \bar{b}, \bar{c} \\
a & 0.50 & 0.20 & 0.80 & 0.32 \\
\bar{a} & 0.00 & 0.30 & 0.00 & 0.12
\end{array}\right)
\end{gathered}
$$

■ Division. Point-wise division is used.
However, we distinguish two cases in order to take care with division by zero, thus

$$
(\phi / \psi)(\mathbf{z})=\left\{\begin{array}{cc}
0 & \text { if } \psi\left(x^{\downarrow Z}\right)=0 \\
\phi\left(x^{\mid Z}\right) / \psi\left(y^{\mid Z}\right) & \text { if } \psi\left(y^{\mid Z}\right) \neq 0
\end{array}\right.
$$

- In fact in the operations involved in probabilistic networks, $\psi\left(x^{\downarrow Z}\right)=0$ implies $\psi\left(y^{\downarrow Z}\right)=0$ upon division of $\phi$ by $\psi$, and thus defining $0 / 0=0$, the division operator is always defined.


## Basic Operations (III)

- Marginalization. Given an information defined over a set of variables $X_{I}$, marginalization restricts that information over a subset of $X_{J} \subseteq X_{I}$.
In Belief revision variables not included in the interest set are marginalised out by addition, while in belief revision or abduction they are marginalised out by maximum.
Example:

$$
\begin{gathered}
f_{1}(A)=\sum_{B, C} f(A, B, C)=\sum_{B, C}\left(\begin{array}{lllll} 
& b, c & b, \bar{c} & \bar{b}, c & \bar{b}, \bar{c} \\
a & 0.50 & 0.20 & 0.80 & 0.32 \\
\bar{a} & 0.00 & 0.30 & 0.00 & 0.12
\end{array}\right)=\left(\begin{array}{ll}
a & 1.82 \\
\bar{a} & 0.42
\end{array}\right) \\
f_{1}(A)=\max _{B, C} f(A, B, C)=\max _{B, C}\left(\begin{array}{lllll} 
& b, c & b, \bar{c} & \bar{b}, c & \bar{b}, \bar{c} \\
a & 0.50 & 0.20 & 0.80 & 0.32 \\
\bar{a} & 0.00 & 0.30 & 0.00 & 0.12
\end{array}\right)=\left(\begin{array}{ll}
a & 0.80 \\
\bar{a} & 0.30
\end{array}\right)
\end{gathered}
$$

## Computing $P\left(X_{i} \mid \mathbf{e}\right)$ : Brute-force approach

- We focus on the computation of $P(X \mid \mathbf{e})$.
- By the moment we suppose that no evidence has been entered $\rightarrow$ to compute $P(X)$.

■ Given a BN with $n$ variables $\left\{X_{1}, \ldots, X_{n}\right\}$ and their probability families $f_{i}, i=1, \ldots, n$, then to compute $P\left(X_{i}\right)$ (or $P\left(X_{i} \mid \mathbf{e}\right)$ is:

> Conceptually easy
> Computationally complex

■ Brute-force approach:

$$
P\left(X_{i}\right)=\sum_{X_{1}, \ldots, X_{i-1}, X_{i+1}, \ldots, X_{n}}\left(\prod_{j=1}^{n} f_{j}\right),
$$

Problem: this is the same to compute the j.p.d. $\Rightarrow$ computationally very inneficient and even intractable in most of cases.

## Improving brute-force approach

In order to improve the brute-force approach we will take advantage from two sources:

- The factorisation encoded by the BN
- The distributive law


## Distributive Law.

Let $f$ and $g$ to be potentials or probability fucntions defined over $\operatorname{dom}(\mathbf{X})=\left\{\mathbf{x}_{\mathbf{1}}, \ldots, \mathbf{x}_{\mathbf{m}}\right\}$ and $\operatorname{dom}(\mathbf{Y})=\left\{\mathbf{y}_{\mathbf{1}}, \ldots, \mathbf{y}_{\mathbf{n}}\right\}$, where $\mathbf{X} \cap \mathbf{Y}=0$, and given $\mathbf{X}^{\prime} \subseteq \mathbf{X}$ and $\mathbf{Y}^{\prime} \subseteq \mathbf{Y}$, then we get

$$
\begin{aligned}
\sum_{\mathbf{X} \backslash \mathbf{X}^{\prime}} \sum_{\mathbf{Y} \backslash \mathbf{Y}^{\prime}}(f \times g)= & \sum_{\mathbf{x} \in \operatorname{dom}\left(\mathbf{X} \backslash \mathbf{X}^{\prime}\right)} \sum_{\mathbf{y} \in \operatorname{dom}\left(\mathbf{Y} \backslash \mathbf{Y}^{\prime}\right)}(f(\mathbf{x}) \times g(\mathbf{y})) \\
= & f\left(\mathbf{x}_{1}\right) g\left(\mathbf{y}_{1}\right)+\cdots+f\left(\mathbf{x}_{1}\right) g\left(\mathbf{y}_{\mathbf{n}}\right)+\cdots+ \\
& f\left(\mathbf{x}_{\mathbf{m}}\right) g\left(\mathbf{y}_{\mathbf{1}}\right)+\cdots+f\left(\mathbf{x}_{\mathbf{m}}\right) g\left(\mathbf{y}_{\mathbf{n}}\right) \\
= & f\left(\mathbf{x}_{1}\right)\left[g\left(\mathbf{y}_{\mathbf{1}}\right)+\cdots+g\left(\mathbf{y}_{\mathbf{n}}\right)\right]+\cdots+ \\
= & f\left(\mathbf{x}_{\mathbf{m}}\right)\left[g\left(\mathbf{y}_{\mathbf{1}}\right)+\cdots+g\left(\mathbf{y}_{\mathbf{n}}\right)\right] \\
= & \sum_{\mathbf{x} \in \operatorname{dom}\left(\mathbf{X} \backslash \mathbf{X}^{\prime}\right)} f(\mathbf{x}) \sum_{\mathbf{y} \in \operatorname{dom}\left(\mathbf{Y} \backslash \mathbf{Y}^{\prime}\right)} g(\mathbf{y}) \\
= & \sum_{\mathbf{x} \backslash \mathbf{X}^{\prime}} f \sum_{\mathbf{Y} \backslash \mathbf{Y}^{\prime}} g
\end{aligned}
$$

## Ordering the computations effectively

As we will see with the following example, the use of the distributive law can help a lot in terms of reducing computations:


$$
\begin{aligned}
& \mathrm{f} 1=\mathrm{P}(\mathrm{X} 1) \\
& \mathrm{f} 2=\mathrm{P}(\mathrm{X} 2 \mid \mathrm{X} 1) \\
& \mathrm{f} 3=\mathrm{P}(\mathrm{X} 3 \mid \mathrm{X} 2, \mathrm{X} 4) \\
& \mathrm{f} 4=\mathrm{P}(\mathrm{X} 4) \\
& \mathrm{f} 5=\mathrm{P}(\mathrm{X} 5 \mid \mathrm{X} 1)
\end{aligned}
$$

As commented before we suppose that any evidence has been observed. Our goal is to compute $P\left(X_{2}\right)$. Thus, be brute-force approach we have:

$$
P\left(X_{2}\right)=\sum_{X_{1}, X_{3}, X_{4}, X_{5}}\left(\prod_{j=1}^{5} f_{j}\right)=
$$

## Ordering the computations effectively (II)

$$
\sum_{X_{1}, X_{3}, X_{4}, X_{5}}\left\{P\left(X_{1}\right) \cdot P\left(X_{2} \mid X_{1}\right) \cdot P\left(X_{3} \mid X_{2}, X_{4}\right) \cdot P\left(X_{4}\right) \cdot P\left(X_{5} \mid X_{1}\right)\right\}
$$

If $|\operatorname{dom}(X)|=2$ for all the variables, then this expression implies to construct a probability table with 32 entries (i.e. the j.p.d.).

However, from the factorisation and the distributive law we can simplify the process by moving in some additions:

$$
P\left(X_{2}\right)=
$$

Moving the summation over $X_{5}$.

$$
=\sum_{X_{1}, X_{3}, X_{4}}\{(\underbrace{\sum_{X_{5}} P\left(X_{5} \mid X_{1}\right)}_{f_{1}\left(X_{1}\right)}) \cdot P\left(X_{1}\right) \cdot P\left(X_{2} \mid X_{1}\right) \cdot P\left(X_{3} \mid X_{2}, X_{4}\right) \cdot P\left(X_{4}\right)\}
$$

## Ordering the computations effectively (III)

Moving the summation over $X_{3}$.

$$
=\sum_{X_{1}, X_{4}}\{(\underbrace{\sum_{X_{5}} P\left(X_{5} \mid X_{1}\right)}_{f_{1}\left(X_{1}\right)}) \cdot P\left(X_{1}\right) \cdot P\left(X_{2} \mid X_{1}\right) \cdot(\underbrace{\sum_{X_{3}} P\left(X_{3} \mid X_{2}, X_{4}\right)}_{f_{2}\left(X_{2}, X_{4}\right)}) \cdot P\left(X_{4}\right)\}
$$

And now we can move the summation over $X_{4}$.


## Ordering the computations effectively (summary)

- Brute-force approach:

$$
\sum_{X_{1}, X_{3}, X_{4}, X_{5}}\left\{P\left(X_{1}\right) \cdot P\left(X_{2} \mid X_{1}\right) \cdot P\left(X_{3} \mid X_{2}, X_{4}\right) \cdot P\left(X_{4}\right) \cdot P\left(X_{5} \mid X_{1}\right)\right\}
$$

This means to build a table with 5 variables and 32 entries. Then, we need:

- 160 multiplications (in most implementations)
- 52 multiplications (selecting the tables in the appropriate way).
- 30 additions for the marginalization of $X_{1}, X_{3}, X_{4}$ and $X_{5}$ (16, 8, 4 and 2 ).
- Taking advantage from the factorisation and the distributive law:

$$
=\sum_{X_{1}}\left\{\left(\sum_{X_{5}} P\left(X_{5} \mid X_{1}\right)\right) \cdot P\left(X_{1}\right) \cdot P\left(X_{2} \mid X_{1}\right) \cdot\left[\sum_{X_{4}}\left(\sum_{X_{3}} P\left(X_{3} \mid X_{2}, X_{4}\right)\right) \cdot P\left(X_{4}\right)\right]\right\}
$$

This means to deal with a table of size 8 and three of size 4 . Then, we need:

- 14 multiplications.
- 10 additions for the marginalization.


## Complexity of exact inference in BNs

- If the DAG no cycles in the underlying undirected graph (poly-trees), inference is easy because we can move the additions in such a way that we never create a table larger than those included in the BN representation.
- In the general case (the underlying undirected graph has cycles) inference is NP-Complete (Cooper, 1990)

■ The complexity of the previous method is exponential in the width (number of variables minus one) of the largest factor set involved in the pocess.

■ The key to efficient inference with this method lies in finding a good summation order (or elimination order or deletion sequence or ...)

## Entering evidence

- Up to this moment we have supposed the lack of evidence. But, what happens if we have some observations, i.e, $\mathbf{e}=\left(E_{1}=e_{1}, \ldots, E_{n}=e_{n}\right)$ ?.
- The answer is quite simple, before running our algorithm, for each $E_{i}$ we identify the potentials or prob. fucntions in which it is included, then:

$$
f(x)= \begin{cases}f(x) & \text { if } \mathrm{x} \text { is consistent with } \mathbf{e} \\ 0 & \text { otherwise }\end{cases}
$$

- Sometimes we can use evidence absorption, which implies the removal of the observed variable from the potential.
- Example: $\mathbf{e}=(B=b)$

$$
\left(\begin{array}{lllll} 
& b, c & b, \bar{c} & \bar{b}, c & \bar{b}, \bar{c} \\
a & 0.5 & 0.2 & 0.0 & 0.0 \\
\bar{a} & 0.0 & 0.3 & 0.0 & 0.0
\end{array}\right) \longleftarrow\left(\begin{array}{lllll} 
& b, c & b, \bar{c} & \bar{b}, c & \bar{b}, \bar{c} \\
a & 0.5 & 0.2 & 0.8 & 0.32 \\
\bar{a} & 0.0 & 0.3 & 0.0 & 0.12
\end{array}\right) \longrightarrow\left(\begin{array}{lll} 
& c & \bar{c} \\
a & 0.50 & 0.20 \\
\bar{a} & 0.00 & 0.30
\end{array}\right)
$$

## Variable Elimination Algorithm

- Input: A BN over $\mathcal{U}=\left\{X_{1}, \ldots, X_{n}\right\}$, the evidence $\mathbf{e}$ and ONE target variable $X_{i}$.
- Output: $P\left(X_{i} \mid \mathbf{e}\right)$.

1. Let $\mathcal{L}$ be a list containing all the probability functions $\left\{f_{1}, f_{2}, \ldots, f_{n}\right\}$.
2. Enter the evidence $\mathbf{e}$.
3. Select an elimination order $\sigma$ containing all the variables but the target one $\left(X_{i}\right)$.
4. For $k=1$ to $n-1$ do
(a) $X_{k} \leftarrow \sigma(k)$.
(b) Let $F$ be the set of prob. functions in $\mathcal{L}$ that contains variable $X_{k}$.
(c) $\mathcal{L}=\mathcal{L}-F$.
(d) $f^{\prime}=\sum_{X_{k}}\left(\prod_{f \in F} f\right)$
(e) $\mathcal{L}=\mathcal{L} \cup f^{\prime}$.
5. Combine in a single function $f$ all the functions in $\mathcal{L}$. Normalize $f$ to obtain $P\left(X_{i}\right)$.

This algorithm has to be repeated for each target variable.

## Examples

Let us consider the following BN (ASIA or chest-clinic) for the examples:


## Examples (cont.)

Example 1. Get the probability of having Dysnoea (D), using the following elimination order $\sigma_{1}=T, S, E, A, L, B, X$.
$1 \mathcal{L}=\{f_{A}(A), \underbrace{f_{T}(T, A)}, f_{S}(S), f_{L}(L, S), f_{B}(B, S), \underbrace{f_{E}(E, T, L)}, f_{X}(X, E), f_{D}(D, E, B)\}$. Delete T.

$$
g_{1}(A, E, L)=\sum_{T}\left(f_{T}(A, T) \times f_{E}(E, T, L)\right)
$$

size $=16$
$2 \mathcal{L}=\{f_{A}(A), \underbrace{f_{S}(S), f_{L}(L, S), f_{B}(B, S)}, f_{X}(X, E), f_{D}(D, E, B), g_{1}(A, E, L)\}$. Delete $\mathbf{S}$.

$$
g_{2}(L, B)=\sum_{S}\left(f_{S}(S) \times f_{L}(L, S) \times f_{B}(B, S)\right)
$$

size $=8$
$3 \mathcal{L}=\{f_{A}(A), \underbrace{f_{X}(X, E), f_{D}(D, E, B), g_{1}(A, E, L)}, g_{2}(L, B)\}$. Del. E

$$
g_{3}(X, D, B, A, L)=\sum_{E}\left(f_{X}(X, E) \times f_{D}(D, E, B) \times g_{1}(A, E, L)\right)
$$

size $=64$

## Examples (cont.)

$$
\begin{aligned}
& 4 \mathcal{L}=\{\underbrace{f_{A}(A)}, g_{2}(L, B), \underbrace{g_{3}(X, D, B, A, L)}\} \text {. Delete A } \\
& \text { size }=32 \\
& g_{4}(X, D, B, L)=\sum_{A}\left(f_{A}(A) \times g_{3}(X, D, B, A, L)\right) \\
& 5 \mathcal{L}=\{\underbrace{g_{2}(L, B), g_{4}(X, D, B, L)}\} . \text { Delete } \mathbf{L} \text {. } \\
& \text { size }=16 \\
& g_{5}(X, D, B)=\sum_{L} g_{2}(L, B) \times g_{4}(X, D, B, L) \\
& 6 \mathcal{L}=\{\underbrace{g_{5}(X, D, B)}\} \text {. Delete B. } \\
& \text { size }=8 \\
& g_{6}(X, D)=\sum_{B} g_{5}(X, D, B)
\end{aligned}
$$

$7 \mathcal{L}=\{\underbrace{g_{6}(X, D)}\}$. Delete X.

$$
\begin{array}{r}
\text { size }=8 \\
g_{7}(D)=\sum_{X} g_{6}(X, D)
\end{array}
$$

8 return normalize $\left(g_{7}(D)\right)$

## Examples (cont.)

Ejemplo 2. Get the probability of having Dysnoea (D), by using the following elimination order $\sigma_{1}=A, X, T, S, L, E, B$.

$$
\begin{gathered}
f_{A}(A), f_{T}(T, A), f_{S}(S), f_{L}(L, S), f_{B}(B, S), f_{E}(E, T, L), f_{X}(X, E), f_{D}(D, E, B) \\
\text { Delete A Use: } f_{A}(A), f_{T}(A, T) \\
f_{S}(S), f_{L}(L, S), f_{B}(B, S), f_{E}(E, T, L), f_{X}(X, E), f_{D}(D, E, B), g_{1}(T) \\
\text { Delete X Use: } f_{X}(X, E) \\
\begin{array}{cl}
\text { New: } g_{2}(E) & 4 \\
f_{S}(S), f_{L}(L, S), f_{B}(B, S), f_{E}(E, T, L), f_{D}(D, E, B), g_{1}(T), g_{2}(E) \\
\text { Delete T Use: } f_{E}(E, T, L), g_{1}(T) & \text { New: } g_{3}(E, L) \\
f_{S}(S), f_{L}(L, S), f_{B}(B, S), f_{D}(D, E, B), g_{2}(E), g_{3}(E, L)
\end{array}
\end{gathered}
$$

## Examples (cont.)

$$
f_{S}(S), f_{L}(L, S), f_{B}(B, S), f_{D}(D, E, B), g_{2}(E), g_{3}(E, L)
$$

Delete $S \quad$ Use: $f_{S}(S), f_{L}(L, S), f_{B}(B, S) \quad$ New: $g_{4}(L, B) \quad 8$

$$
f_{D}(D, E, B), g_{2}(E), g_{3}(E, L), g_{4}(L, B)
$$

Delete L Use: $g_{3}(E, L), g_{4}(L, B) \quad$ New: $g_{5}(E, B) \quad 8$

$$
f_{D}(D, E, B), g_{2}(E), g_{5}(E, B)
$$

Delete E Use: $f_{D}(D, E, B), g_{2}(E), g_{5}(E, B) \quad$ New: $g_{6}(D, B) \quad 8$

$$
g_{5}(D, B)
$$

Delete B Use: $g_{6}(D, B) \quad$ New: $g_{7}(D) \quad 4$

## Query-based inference

- In a concrete scenary the network's variables can be divided into: interest (I) variables, observed variables or evidence ( $\mathbb{E}=\mathrm{e}$ ) and the remaining ones ( $\mathbf{R}$ ).
- The question now is: do we need to consider all the variables in R?
- Answer: usually no
- Then, prior to solving the query, the network can be pruned to include only the variables relevant for the query.

To prune the network (i.e. to discard some variables in $\mathbf{R}$ ) we will use as tools the concepts of barren nodes and $d$-separation

- D-separation: We can prune all variables $\mathbf{K}$ such that $I(\mathbf{I}|\mathbf{E}| \mathbf{K})$. There exists efficient algorithms for this task (i.e. BayesBall (Schacther 1998)

