## CS 3710 Advanced Topics in AI

Lecture 3

## Probabilistic graphical models

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## Modeling uncertainty with probabilities

- Representing large multivariate distributions directly and exhaustively is hopeless:
- The number of parameters is exponential in the number of random variables
- Inference can be exponential in the number of variables
- Breakthrough (late 80 s , beginning of 90 s )
- Bayesian belief networks
- Give solutions to the space, acquisition bottlenecks
- Partial solutions for time complexities


## Graphical models

Aim: alleviate the representational and computational bottlenecks
Idea: Take advantage of the structure, more specifically, independences and conditional independences that hold among random variables

Two classes of models:

- Bayesian belief networks
- Modeling asymmetric (causal) effects and dependencies
- Markov random fields
- Modeling symmetric effects and dependencies among random variables
- Used often to model spatial dependences (image analysis)

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## Bayesian belief networks (BBNs)

Bayesian belief networks.

- Represent the full joint distribution over the variables more compactly using a smaller number of parameters.
- Take advantage of conditional and marginal independences among random variables
- $A$ and $B$ are independent

$$
P(A, B)=P(A) P(B)
$$

- A and B are conditionally independent given $\mathbf{C}$

$$
\begin{aligned}
& P(A, B \mid C)=P(A \mid C) P(B \mid C) \\
& P(A \mid C, B)=P(A \mid C)
\end{aligned}
$$

## Bayesian belief networks (general)

Two components: $B=\left(S, \Theta_{S}\right)$

- Directed acyclic graph
- Nodes correspond to random variables
- (Missing) links encode independences

- Parameters
- Local conditional probability distributions
for every variable-parent configuration $\mathbf{P}\left(X_{i} \mid p a\left(X_{i}\right)\right)$

Where:
$p a\left(X_{i}\right)$ - stand for parents of $X_{i}$

| $\mathbf{P}(\mathrm{A} \mid \mathrm{B}, \mathrm{E})$ |  |  |
| :---: | :---: | :---: |
| B | E | $\mathbf{T}$ |
| $\mathbf{T}$ | $\mathbf{F}$ |  |
| T | T | 0.95 |
| T | 0.05 |  |
| F | 0.94 | 0.06 |
| F | T | 0.29 |
|  | F | 0.71 |
| 0.001 | 0.999 |  |

## Bayesian belief network.



## Full joint distribution in BBNs

Full joint distribution is defined in terms of local conditional distributions (obtained via the chain rule):

$$
\mathbf{P}\left(X_{1}, X_{2}, . ., X_{n}\right)=\prod_{i=1, . . n} \mathbf{P}\left(X_{i} \mid p a\left(X_{i}\right)\right)
$$

## Example:

Assume the following assignment of values to random variables

$$
B=T, E=T, A=T, J=T, M=F
$$



Then its probability is:

$$
\begin{aligned}
& P(B=T, E=T, A=T, J=T, M=F)= \\
& \quad P(B=T) P(E=T) P(A=T \mid B=T, E=T) P(J=T \mid A=T) P(M=F \mid A=T)
\end{aligned}
$$

## Bayesian belief networks (BBNs)

## Bayesian belief networks

- Represent the full joint distribution over the variables more compactly using the product of local conditionals.
- But how did we get to local parameterizations?

Answer:

- Graphical structure encodes conditional and marginal independences among random variables
- $\mathbf{A}$ and $B$ are independent $P(A, B)=P(A) P(B)$
- A and B are conditionally independent given $\mathbf{C}$

$$
\begin{gathered}
P(A \mid C, B)=P(A \mid C) \\
P(A, B \mid C)=P(A \mid C) P(B \mid C)
\end{gathered}
$$

- The graph structure implies the decomposition !!!


## Independences in BBNs

3 basic independence structures:
1.


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## Independences in BBN

- BBN distribution models many conditional independence relations among distant variables and sets of variables
- These are defined in terms of the graphical criterion called dseparation
- D-separation and independence
- Let X,Y and Z be three sets of nodes
- If $X$ and $Y$ are d-separated by $Z$, then $X$ and $Y$ are conditionally independent given Z
- D-separation :
- A is d-separated from B given C if every undirected path between them is blocked with $\mathbf{C}$
- Path blocking
- 3 cases that expand on three basic independence structures


## Independences in BBNs



- Earthquake and Burglary are independent given MaryCalls $\quad$ F
- Burglary and MaryCalls are independent (not knowing Alarm) F
- Burglary and RadioReport are independent given Earthquake T
- Burglary and RadioReport are independent given MaryCalls F


## Bayesian belief networks (BBNs)

## Bayesian belief networks

- Represents the full joint distribution over the variables more compactly using the product of local conditionals.
- So how did we get to local parameterizations?

$$
\mathbf{P}\left(X_{1}, X_{2}, . ., X_{n}\right)=\prod_{i=1, . . n} \mathbf{P}\left(X_{i} \mid p a\left(X_{i}\right)\right)
$$

- The decomposition is implied by the set of independences encoded in the belief network.


## Full joint distribution in BBNs

Rewrite the full joint probability using the product rule:


$$
\begin{aligned}
& P(B=T, E=T, A=T, J=T, M=F)= \\
& =P(J=T \mid B=T, E=T, A=T, M=F) P(B=T, E=T, A=T, M=F) \\
& =\underline{P(J=T \mid A=T}) \underline{P(B=T, E=T, A=T, M=F)} \\
& P(M=F \mid B=T, E=T, A=T) P(B=T, E=T, A=T) \\
& \underline{P(M=F \mid A=T)} P(B=T, E=T, A=T) \\
& \underline{P(A=T \mid B=T, E=T)} \underline{P(B=T, E=T)} \\
& P(B=T) P(E=T) \\
& =P(J=T \mid A=T) P(M=F \mid A=T) P(A=T \mid B=T, E=T) P(B=T) P(E=T)
\end{aligned}
$$

## Parameter complexity problem

- In the BBN the full joint distribution is defined as:

$$
\mathbf{P}\left(X_{1}, X_{2}, . ., X_{n}\right)=\prod_{i=1, . . n} \mathbf{P}\left(X_{i} \mid p a\left(X_{i}\right)\right)
$$

- What did we save?

Alarm example: 5 binary (True, False) variables \# of parameters of the full joint:

$$
2^{5}=32
$$

One parameter is for free:

$$
2^{5}-1=31
$$



## Parameter complexity problem

- In the BBN the full joint distribution is defined as:

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\mathbf{P}\left(X_{1}, X_{2}, . ., X_{n}\right)=\prod_{i=1, \ldots n} \mathbf{P}\left(X_{i} \mid p a\left(X_{i}\right)\right)
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$$

One parameter is for free:

$$
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$$

\# of parameters of the BBN: ?


## Bayesian belief network.

- In the BBN the full joint distribution is expressed using a set of local conditional distributions



## Parameter complexity problem

- In the BBN the full joint distribution is defined as:

$$
\mathbf{P}\left(X_{1}, X_{2}, \ldots, X_{n}\right)=\prod_{i=1, \ldots n} \mathbf{P}\left(X_{i} \mid p a\left(X_{i}\right)\right)
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- What did we save?

Alarm example: 5 binary (True, False) variables \# of parameters of the full joint:

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$$

One parameter is for free:

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2^{5}-1=31
$$

\# of parameters of the BBN:

$$
2^{3}+2\left(2^{2}\right)+2(2)=20
$$



One parameter in every conditional is for free:

## Parameter complexity problem

- In the BBN the full joint distribution is defined as:

$$
\mathbf{P}\left(X_{1}, X_{2}, . ., X_{n}\right)=\prod_{i=1, . . n} \mathbf{P}\left(X_{i} \mid p a\left(X_{i}\right)\right)
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- What did we save?

Alarm example: 5 binary (True, False) variables \# of parameters of the full joint:

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One parameter is for free:

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\# of parameters of the BBN:

$$
2^{3}+2\left(2^{2}\right)+2(2)=20
$$



One parameter in every conditional is for free:

$$
2^{2}+2(2)+2(1)=10
$$

## Model acquisition problem

## The structure of the BBN

- typically reflects causal relations (BBNs are also sometime referred to as causal networks)
- Causal structure is intuitive in many applications domain and it is relatively easy to define to the domain expert


## Probability parameters of BBN

- are conditional distributions relating random variables and their parents
- Complexity is much smaller than the full joint
- It is much easier to obtain such probabilities from the expert or learn them automatically from data


## BBNs built in practice

- In various areas:
- Intelligent user interfaces (Microsoft)
- Troubleshooting, diagnosis of a technical device
- Medical diagnosis:
- Pathfinder (Intellipath)
- CPSC
- Munin
- QMR-DT
- Collaborative filtering
- Military applications
- Business and finance
- Insurance, credit applications


## Diagnosis of car engine

- Diagnose the engine start problem



## Car insurance example

- Predict claim costs (medical, liability) based on application data



## (ICU) Alarm network



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## CPCS

- Computer-based Patient Case Simulation system (CPCS-PM) developed by Parker and Miller (University of Pittsburgh)
- 422 nodes and 867 arcs



## QMR-DT

- Medical diagnosis in internal medicine

Bipartite network of disease/findings relations

QMR-DT derived from Internist-1/ QMR KB


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## Inference in Bayesian networks

- BBN models compactly the full joint distribution by taking advantage of existing independences between variables
- Simplifies the acquisition of a probabilistic model
- But we are interested in solving various inference tasks:
- Diagnostic task. (from effect to cause)
$\mathbf{P}$ (Burglary | JohnCalls $=T$ )
- Prediction task. (from cause to effect)

$$
\mathbf{P}(\text { JohnCalls } \mid \text { Burglary }=T)
$$

- Other probabilistic queries (queries on joint distributions). P (Alarm)
- Main issue: Can we take advantage of independences to construct special algorithms and speeding up the inference?


## Inference in Bayesian network

- Bad news:
- Exact inference problem in BBNs is NP-hard (Cooper)
- Approximate inference is NP-hard (Dagum, Luby)
- But very often we can achieve significant improvements
- Assume our Alarm network

- Assume we want to compute: $\quad P(J=T)$


## Inference in Bayesian networks

Computing: $\quad P(J=T)$

## Approach 1. Blind approach.

- Sum out all un-instantiated variables from the full joint,
- express the joint distribution as a product of conditionals
$P(J=T)=$
$=\sum_{b \in T, F} \sum_{e \in T, F} \sum_{a \in T, F} \sum_{m \in T, F} P(B=b, E=e, A=a, J=T, M=m)$
$=\sum_{b \in T, F} \sum_{e \in T, F} \sum_{a \in T, F} \sum_{m \in T, F} P(J=T \mid A=a) P(M=m \mid A=a) P(A=a \mid B=b, E=e) P(B=b) P(E=e)$


## Computational cost:

Number of additions: ?
Number of products: ?

## Inference in Bayesian networks

Computing: $\quad P(J=T)$
Approach 1. Blind approach.

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$=\sum_{b \in T, F} \sum_{e \in T, F} \sum_{a \in T, F} \sum_{m \in T, F} P(B=b, E=e, A=a, J=T, M=m)$
$=\sum_{b \in T, F \in T, F} \sum_{i \in T, F} \sum_{m \in T, F} P(J=T \mid A=a) P(M=m \mid A=a) P(A=a \mid B=b, E=e) P(B=b) P(E=e)$
Computational cost:
Number of additions: 15
Number of products: ?


## Inference in Bayesian networks

Computing: $\quad P(J=T)$

## Approach 1. Blind approach.

- Sum out all un-instantiated variables from the full joint,
- express the joint distribution as a product of conditionals
$P(J=T)=$
$=\sum_{b \in T, F} \sum_{e \in T, F} \sum_{a \in T, F} \sum_{m \in T, F} P(B=b, E=e, A=a, J=T, M=m)$
$=\sum_{b \in T, F \in \in T, F} \sum_{a \in T, F} \sum_{m \in T, F} P(J=T \mid A=a) P(M=m \mid A=a) P(A=a \mid B=b, E=e) P(B=b) P(E=e)$


## Computational cost:

Number of additions: 15
Number of products: $16 * 4=64$

## Inference in Bayesian networks

## Approach 2. Interleave sums and products

- Combines sums and product in a smart way (multiplications by constants can be taken out of the sum)
$P(J=T)=$
$=\sum_{b \in T, F e \in T, F} \sum_{a \in T, F} \sum_{m \in T, F} P(J=T \mid A=a) P(M=m \mid A=a) P(A=a \mid B=b, E=e) P(B=b) P(E=e)$
$=\sum_{b \in \in, F, F \in T F, F m \in T, F} \sum P(J=T \mid A=a) P(M=m \mid A=a) P(B=b)\left[\sum_{e \in T, F} P(A=a \mid B=b, E=e) P(E=e)\right]$
$=\sum_{a \in T, F} P(J=T \mid A=a)\left[\sum_{m \in T, F} P(M=m \mid A=a)\right]\left[\sum_{b \in T, F} P(B=b)\left[\sum_{e \in T, F} P(A=a \mid B=b, E=e) P(E=e)\right]\right.$


## Computational cost:

Number of additions: $1+2 *[1+1+2 * 1]=$ ?
Number of products: $2 *[2+2 *(1+2 * 1)]=$ ?

## Inference in Bayesian networks

## Approach 2. Interleave sums and products

- Combines sums and product in a smart way (multiplications by constants can be taken out of the sum)
$P(J=T)=$
$=\sum_{b \in T, F \in T, F} \sum_{a \in T, F} \sum_{m \in T, F} P(J=T \mid A=a) P(M=m \mid A=a) P(A=a \mid B=b, E=e) P(B=b) P(E=e)$
$=\sum_{b \in T, F a \in T F, F \in T, F} \sum_{n} P(J=T \mid A=a) P(M=m \mid A=a) P(B=b)\left[\sum_{e \in T, F} P(A=a \mid B=b, E=e) P(E=e)\right]$
$=\sum_{a \in T, F} P(J=T \mid A=a)\left[\sum_{m \in T, F} P(M=m \mid A=a)\right]\left[\sum_{b \in T, F} P(B=b)\left[\sum_{c e T, F} P(A=a \mid B=b, E=e) P(E=e)\right]\right.$


## Computational cost:

Number of additions: $1+2 *[1+1+2 * 1]=\mathbf{9}$
Number of products: $2 *[2+2 *(1+2 * 1)]=$ ?

## Inference in Bayesian networks

## Approach 2. Interleave sums and products

- Combines sums and product in a smart way (multiplications by constants can be taken out of the sum)
$P(J=T)=$
$=\sum_{b \in T, F e \in T, F} \sum_{a \in T, F} \sum_{m \in T, F} P(J=T \mid A=a) P(M=m \mid A=a) P(A=a \mid B=b, E=e) P(B=b) P(E=e)$
$=\sum_{b \in T, F \in \in \in T F} \sum_{m \in T, F} P(J=T \mid A=a) P(M=m \mid A=a) P(B=b)\left[\sum_{e \in T, F} P(A=a \mid B=b, E=e) P(E=e)\right]$
$=\sum_{a \in T, F} P(J=T \mid A=a)\left[\sum_{m \in T, F} P(M=m \mid A=a)\right]\left[\sum_{b \in T, F} P(B=b)\left[\sum_{e \in T, F} P(A=a \mid B=b, E=e) P(E=e)\right]\right.$


## Computational cost:

Number of additions: $1+2 *[1+1+2 * 1]=\mathbf{9}$
Number of products: $2 *[2+2 *(1+2 * 1)]=16$

## Inference in Bayesian networks

- The smart interleaving of sums and products can help us to speed up the computation of joint probability queries
- What if we want to compute: $P(B=T, J=T)$
$P(B=T, J=T)=$
$\left.\quad=\sum_{a \in T, F} P(J=T \mid A=a)\left[\sum_{m \in T, F} P(M=m \mid A=a)\right] P(B=T)\left[\sum_{e \in T, F} P(A=a \mid B=T, E=e) P(E=e)\right]\right]$
$P(J=T)=$
$=\sum_{a \in T, F} P(J=T \mid A=a)\left[\sum_{m \in T, F} P(M=m \mid A=a)\left[\sum_{b e T, F} P(B=b)\left[\sum_{c e T, F} P(A=a \mid B=b, E=e) P(E=e)\right]\right]\right.$
- A lot of shared computation
- Smart cashing of results can save the time for more queries


## Inference in Bayesian networks

- The smart interleaving of sums and products can help us to speed up the computation of joint probability queries
- What if we want to compute: $P(B=T, J=T)$

$$
\begin{aligned}
& P(B=T, J=T)= \\
& \quad=\sum_{a \in T, F} P(J=T \mid A=a)\left[\sum_{m \in T, F} P(M=m \mid A=a)\right] P(B=T)\left[\sum_{e \in T, F} P(A=a \mid B=T, E=e) P(E=e)\right] \\
& P(J=T)= \\
& =\sum_{a \in T, F} P(J=T \mid A=a)\left[\sum_{k \in T, F} P(M=m \mid A=a)\right]\left[\sum_{b \in T, f} P(B=b)\left[\sum_{e \in T, F} P(A=a \mid B=b, E=e) P(E=e)\right]\right]
\end{aligned}
$$

- A lot of shared computation
- Smart cashing of results can save the time if more queries


## Inference in Bayesian networks

- When cashing of results becomes handy?
- What if we want to compute a diagnostic query:

$$
P(B=T \mid J=T)=\frac{P(B=T, J=T)}{P(J=T)}
$$

- Exactly probabilities we have just compared !!
- There are other queries when cashing and ordering of sums and products can be shared and saves computation

$$
\mathbf{P}(B \mid J=T)=\frac{\mathbf{P}(B, J=T)}{P(J=T)}=\alpha \mathbf{P}(B, J=T)
$$

- General technique: Variable elimination


## Inference in Bayesian networks

- General idea of variable elimination

$$
\begin{aligned}
& P(\text { True })=1= \\
& =\sum_{a \in T, F}[\underbrace{\sum_{j \in T, F} P(J=j \mid A=a)}_{f_{J}(a)}][\underbrace{\sum_{m \in T, F} P(M=m \mid A=a)}_{f_{M}(a)}][\underbrace{\sum_{b} P(B=b)}_{b \in T, F}[\underbrace{\sum_{e \in T, F} P(A=a \mid B=b, E=e) P(E=e)}_{f_{E}(a, b)}] \\
& \text { Variable order: } \\
& f_{B}(a) \\
& \text { B } \\
& \text { Results cashed in } \\
& \text { the tree structure } \\
& \text { Complexity: } \\
& \text { treewidth of the graph }
\end{aligned}
$$

## Inference in Bayesian network

- Exact inference algorithms:
- Variable elimination
- Symbolic inference (D'Ambrosio)
- Recursive decomposition (Cooper)
- Message passing algorithm (Pearl)
- Clustering and joint tree approach (Lauritzen, Spiegelhalter)
- Arc reversal (Olmsted, Schachter)
- Approximate inference algorithms:


## - Monte Carlo methods:

- Forward sampling, Likelihood sampling
- Variational methods


## Markov random fields

- Probabilistic models with symmetric dependences.
- Typically models of spatially varying quantities

$$
P(x) \propto \prod_{c \in c l(x)} f_{c}\left(x_{c}\right)
$$

$f_{c}\left(x_{c}\right)$ - A potential function (defined over factors)
$P(x)=\frac{1}{Z} \exp \left(-\sum_{c \in c l(x)} \phi_{c}\left(x_{c}\right)\right)$

- Gibbs (Boltzman) distribution
$Z=\sum_{x \in\{x\}} \exp \left(-\sum_{c \in c l(x)} \phi_{c}\left(x_{c}\right)\right) \quad$ - A partition function


## Markov random fields

- Interactions induced by the factorized form are captured by an undirected network (also called independence graph)
- $\mathrm{G}=(\mathrm{S}, \mathrm{E})$
- $\mathrm{S}=1,2, . . \mathrm{N}$ correspond to random variables
- $(i, j) \in E \Leftrightarrow \exists c:\{i, j\} \subset c$ or $\mathrm{x}_{\mathrm{i}}$ and $\mathrm{x}_{\mathrm{j}}$ appear within the same factor c


## - Consequence:

- factors c correspond to cliques of the graph


## Markov random fields

- regular lattice (Ising model)

- Arbitrary graph



## Markov random fields

- regular lattice (Ising model)

- Arbitrary graph



## Markov random fields

- Pairwise Markov property
- Two nodes in the network that are not directly connected can be made independent given all other nodes


$$
\begin{aligned}
P\left(x_{A}, x_{B} \mid x_{r}\right)=\frac{P\left(x_{A}, x_{B}, x_{r}\right)}{P\left(x_{r}\right)} & \propto \exp \left(-\sum_{c: c \cap A \neq\}} \phi_{c}\left(x_{c}\right)-\sum_{c: c \cap A=c} \phi_{c}\left(x_{c}\right)\right) \\
& \propto \exp \left(-\sum_{c: \subset \cap A \neq\}} \phi_{c}\left(x_{c}\right)\right)=P\left(x_{A} \mid x_{r}\right)
\end{aligned}
$$

## Markov random fields

- Pairwise Markov property
- Two nodes in the network that are not directly connected can be made independent given all other nodes
- Local Markov property
- A set of nodes (variables) can be made independent from the rest of nodes variables given its immediate neighbors
- Global Markov property
- A vertex set $A$ is independent of the vertex set $B$ ( $A$ and $B$ are disjoint) given set C if all chains in between elements in $A$ and $B$ intersect $C$

