# Lecture 7 <br> Inference in Bayesian Networks 

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## Course Overview

$\checkmark$ Introduction
$\checkmark$ Artificial Intelligence
$\checkmark$ Intelligent Agents
$\checkmark$ Search
$\checkmark$ Uninformed Search
$\checkmark$ Heuristic Search

- Uncertain knowledge and Reasoning
$\checkmark$ Probability and Bayesian approach
- Bayesian Networks
- Hidden Markov Chains
- Kalman Filters
- Learning
- Supervised

Learning Bayesian Networks, Neural Networks

- Unsupervised

EM Algorithm

- Reinforcement Learning
- Games and Adversarial Search
- Minimax search and

Alpha-beta pruning

- Multiagent search
- Knowledge representation and Reasoning
- Propositional logic
- First order logic
- Inference
- Plannning


## Bayesian networks, Resume

Encode local conditional independences

$$
\operatorname{Pr}\left(X_{i} \mid X_{-i}\right)=\operatorname{Pr}\left(X_{i} \mid \operatorname{Parents}\left(X_{i}\right)\right)
$$

Thus the global semantics simplifies to (joint probability factorization):

$$
\begin{aligned}
\operatorname{Pr}\left(X_{1}, \ldots, X_{n}\right) & =\prod_{i=1}^{n} \operatorname{Pr}\left(X_{i} \mid X_{1}, \ldots, X_{i-1}\right) \quad \text { (chain rule) } \\
& =\prod_{i=1}^{n} \operatorname{Pr}\left(X_{i} \mid \operatorname{Parents}\left(X_{i}\right)\right) \quad \text { (by construction) }
\end{aligned}
$$

## Outline

## Inference in BN

1. Inference in BN

## Inference tasks

- Simple queries: compute posterior marginal $\operatorname{Pr}\left(X_{i} \mid \mathbf{E}=\mathbf{e}\right)$

$$
\text { e.g., P(NoGas | Gauge = empty, Lights =on, Starts = false })
$$

- Conjunctive queries:

$$
\operatorname{Pr}\left(X_{i}, X_{j} \mid \mathbf{E}=\mathbf{e}\right)=\operatorname{Pr}\left(X_{i} \mid \mathbf{E}=\mathbf{e}\right) \operatorname{Pr}\left(X_{j} \mid X_{i}, \mathbf{E}=\mathbf{e}\right)
$$

- Optimal decisions: decision networks include utility information; probabilistic inference required for $P$ (outcome | action, evidence)
- Value of information: which evidence to seek next?
- Sensitivity analysis: which probability values are most critical?
- Explanation: why do I need a new starter motor?


## Inference by enumeration

Sum out variables from the joint without actually constructing its explicit representation

Simple query on the burglary network:

$$
\begin{aligned}
\operatorname{Pr}(B \mid j, m) & =\operatorname{Pr}(B, j, m) / P(j, m) \\
& =\alpha \operatorname{Pr}(B, j, m) \\
& =\alpha \sum_{e} \sum_{a} \operatorname{Pr}(B, e, a, j, m)
\end{aligned}
$$



Rewrite full joint entries using product of CPT entries:

$$
\begin{aligned}
\operatorname{Pr}(B \mid j, m) & =\alpha \sum_{e} \sum_{a} \operatorname{Pr}(B) P(e) \operatorname{Pr}(a \mid B, e) P(j \mid a) P(m \mid a) \\
& =\alpha \operatorname{Pr}(B) \sum_{e} P(e) \sum_{a} \operatorname{Pr}(a \mid B, e) P(j \mid a) P(m \mid a)
\end{aligned}
$$

Recursive depth-first enumeration: $O(n)$ space, $O\left(d^{n}\right)$ time

## Enumeration algorithm

function Enumeration- $\operatorname{Ask}(X, \mathrm{e}, b n)$ returns a distribution over $X$ inputs: $X$, the query variable
e, observed values for variables E
$b n$, a Bayesian network with variables $\{X\} \cup E \cup Y$
$\mathrm{Q}(X) \leftarrow$ a distribution over $X$, initially empty for each value $x_{i}$ of $X$ do $\mathrm{Q}\left(x_{i}\right) \leftarrow$ Enumerate-All(bn.Vars, $\left.\mathrm{e} \cup\left\{X=x_{i}\right\}\right)$ return Normalize( $\mathrm{Q}(X)$ )
function Enumerate-All(vars, e) returns a real number
if Empty? (vars) then return 1.0
$Y \leftarrow$ First(vars)
if $Y$ has value $y$ in $e$
then return $P(y \mid \operatorname{parent}(Y)) \times$ Enumerate-All(Rest(vars), e) else return $\sum_{y} P(y \mid \operatorname{parent}(Y)) \times$ Enumerate-All(Rest(vars), $\left.\mathrm{e} \cup\{Y=y\}\right)$

## Evaluation tree



Enumeration is inefficient: repeated computation e.g., computes $P(j \mid a) P(m \mid a)$ for each value of $e$

## Inference by variable elimination

Variable elimination: carry out summations right-to-left, storing intermediate results (factors) to avoid recomputation $\operatorname{Pr}(B \mid j, m)$

$$
\begin{aligned}
& =\alpha \underbrace{\operatorname{Pr}(B)}_{B} \sum_{e} \underbrace{P(e)}_{E} \sum_{a} \underbrace{\operatorname{Pr}(a \mid B, e)}_{A} \underbrace{P(j \mid a)}_{J} \underbrace{P(m \mid a)}_{M} \\
& =\alpha \operatorname{Pr}(B) \sum_{e^{e}} P(e) \sum_{a} \operatorname{Pr}(a \mid B, e) P(j \mid a) f_{M}(a) \\
& =\alpha \operatorname{Pr}(B) \sum_{e} P(e) \sum_{a} \operatorname{Pr}(a \mid B, e) f_{J}(a) f_{M}(a) \\
& =\alpha \operatorname{Pr}(B) \sum_{e} P(e) \sum_{a} f_{A}(a, b, e) f_{J}(a) f_{M}(a) \\
& =\alpha \operatorname{Pr}(B) \sum_{e} P(e) f_{\bar{A} J M}(b, e)(\text { sum out } A) \\
& =\alpha \operatorname{Pr}(B) f_{\bar{E} \bar{A} J M}(b)(\text { sum out } E) \\
& =\alpha f_{B}(b) \times f_{\bar{E} \bar{A} J M}(b)
\end{aligned}
$$

## Variable elimination: Basic operations

Summing out a variable from a product of factors:

1. move any constant factors outside the summation:

$$
\begin{aligned}
& \sum_{f_{1} \times \cdots \times f_{i} \times f_{\bar{X}}} f_{1} \times \cdots \times f_{k}=f_{1} \times \cdots \times f_{i} \sum_{x} f_{i+1} \times \cdots \times f_{k}= \\
& \text { assuming } f_{1}, \ldots, f_{i} \text { do not depend on } x
\end{aligned}
$$

2. add up submatrices in pointwise product of remaining factors:

Eg: pointwise product of $f_{1}$ and $f_{2}$ :

$$
\begin{aligned}
& \quad f_{1}\left(x_{1}, \ldots, x_{j}, y_{1}, \ldots, y_{k}\right) \times f_{2}\left(y_{1}, \ldots, y_{k}, z_{1}, \ldots, z_{l}\right) \\
& \quad=f\left(x_{1}, \ldots, x_{j}, y_{1}, \ldots, y_{k}, z_{1}, \ldots, z_{l}\right) \\
& \text { E.g., } f_{1}(a, b) \times f_{2}(b, c)=f(a, b, c)
\end{aligned}
$$

## Irrelevant variables

Consider the query $P($ JohnCalls $\mid$ Burglary $=$ true $)$

$$
\begin{aligned}
& P(J \mid b)=\alpha P(b) \sum_{e} P(e) \sum_{a} P(a \mid b, e) P(J \mid a) \sum_{m} P(m \mid \\
& \text { m over } m \text { is identically } 1 ; M \text { is irrelevant to the } \\
& \text { ry }
\end{aligned}
$$

Theorem
$Y$ is irrelevant unless $Y \in \operatorname{Ancestors}(\{X\} \cup \mathrm{E})$
Here, $X=$ JohnCalls, $\mathbf{E}=\{$ Burglary $\}$, and Ancestors $(\{X\} \cup E)=\{$ Alarm, Earthquake $\}$ so MaryCalls is irrelevant

## Irrelevant variables contd.

Defn: moral graph of DAG Bayes net: marry all parents and drop arrows Defn: $\overline{\mathbf{A}}$ is $\underline{m}$-separated from $B$ by $C$ iff separated by $\mathbf{C}$ in the moral graph

Theorem
$Y$ is irrelevant if m-separated from $X$ by $E$

For $P($ JohnCalls $\mid$ Alarm = true $)$, both Burglary and Earthquake are irrelevant


## Complexity of exact inference

Singly connected networks (or polytrees):

- any two nodes are connected by at most one (undirected) path
- time and space cost (with variable elimination) are $O\left(d^{k} n\right)$
- hence time and space cost are linear in $n$ and $k$ bounded by a constant

Multiply connected networks:

- can reduce 3SAT to exact inference $\Longrightarrow$ NP-hard
- equivalent to counting 3SAT models $\Longrightarrow$ \#P-complete

Proof of this in one of the exercises for Thursday.

## Inference by stochastic simulation

Basic idea:

- Draw $N$ samples from a sampling distribution $S$
- Compute an approximate posterior probability $\hat{P}$
- Show this converges to the true probability


Outline:

- Sampling from an empty network
- Rejection sampling: reject samples disagreeing with evidence
- Likelihood weighting: use evidence to weight samples
- Markov chain Monte Carlo (MCMC): sample from a stochastic process whose stationary distribution is the true posterior


## Sampling from an empty network

function Prior-Sample( $b n$ ) returns an event sampled from $b n$ inputs: $b n$, a belief network specifying joint distribution $\operatorname{Pr}\left(X_{1}, \ldots, X_{n}\right)$
$\mathbf{x} \leftarrow$ an event with $n$ elements
for $i=1$ to $n$ do
$x_{i} \leftarrow$ a random sample from $\operatorname{Pr}\left(X_{i} \mid \operatorname{parents}\left(X_{i}\right)\right)$
given the values of $\operatorname{Parents}\left(X_{i}\right)$ in $\mathbf{x}$
return x

Ancestor sampling

## Example



## Sampling from an empty network contdr. ${ }^{\text {lnference in BN }}$

Probability that PriorSample generates a particular event

$$
S_{P S}\left(x_{1} \ldots x_{n}\right)=P\left(x_{1} \ldots x_{n}\right)
$$

i.e., the true prior probability
E.g., $S_{P S}(t, f, t, t)=0.5 \times 0.9 \times 0.8 \times 0.9=0.324=P(t, f, t, t)$

Proof: Let $N_{P S}\left(x_{1} \ldots x_{n}\right)$ be the number of samples generated for event $x_{1}, \ldots, x_{n}$. Then we have

$$
\begin{aligned}
\lim _{N \rightarrow \infty} \hat{P}\left(x_{1}, \ldots, x_{n}\right) & =\lim _{N \rightarrow \infty} N_{P S}\left(x_{1}, \ldots, x_{n}\right) / N \\
& =S_{P S}\left(x_{1}, \ldots, x_{n}\right) \\
& =\prod_{i=1}^{n} P\left(x_{i} \mid \operatorname{parents}\left(X_{i}\right)\right)=P\left(x_{1} \ldots x_{n}\right)
\end{aligned}
$$

$\rightsquigarrow$ That is, estimates derived from PriorSample are consistent Shorthand: $\hat{P}\left(x_{1}, \ldots, x_{n}\right) \approx P\left(x_{1} \ldots x_{n}\right)$

## Rejection sampling

$\hat{\operatorname{Pr}}(X \mid \mathbf{e})$ estimated from samples agreeing with $\mathbf{e}$
function Rejection-Sampling $(X, \mathbf{e}, b n, N)$ returns an estimate of $P(X \mid \mathbf{e})$
local variables: N , a vector of counts over $X$, initially zero

$$
\begin{aligned}
& \text { for } j=1 \text { to } N \text { do } \\
& \mathrm{x} \leftarrow \text { Prior-Sample }(b n) \\
& \text { if } \mathrm{x} \text { is consistent with } \mathrm{e} \text { then } \\
& \mathrm{N}[x] \leftarrow \mathbf{N}[x]+1 \text { where } \mathrm{x} \text { is the value of } X \text { in } \mathrm{x} \\
& \text { return Normalize }(\mathrm{N}[X])
\end{aligned}
$$

E.g., estimate $\operatorname{Pr}($ Rain $\mid$ Sprinkler $=$ true) using 100 samples

27 samples have Sprinkler $=$ true
Of these, 8 have Rain = true and 19 have Rain $=$ false.
$\hat{\operatorname{Pr}}($ Rain $\mid$ Sprinkler $=$ true $)=\operatorname{Normalize~}(\langle 8,19\rangle)=\langle 0.296,0.704\rangle$
Similar to a basic real-world empirical estimation procedure

## Analysis of rejection sampling

Rejection sampling returns consistent posterior estimates
Proof:

$$
\begin{array}{ccc}
\hat{\operatorname{Pr}}(X \mid \mathbf{e})=\alpha \mathbf{N}_{P S}(X, \mathbf{e}) & \text { (algorithm defn.) } \\
\quad=N_{P S}(X, \mathbf{e}) / N_{P S}(\mathbf{e}) & \text { (normalized by } \left.N_{P S}(\mathbf{e})\right) \\
& \approx \operatorname{Pr}(X, \mathbf{e}) / P(\mathbf{e}) & \text { (property of PriorSample) } \\
& =\operatorname{Pr}(X \mid \mathbf{e}) & \text { (defn. of conditional probability) }
\end{array}
$$

Problem: hopelessly expensive if $P(\mathrm{e})$ is small
$P($ e $)$ drops off exponentially with number of evidence variables!

## Likelihood weighting

Idea: fix evidence variables, sample only nonevidence variables, and weight each sample by the likelihood it accords the evidence
function Likelihood-Weighting $(X, \mathbf{e}, b n, N)$ returns an estimate of $P(X \mid \mathbf{e})$
local variables: W , a vector of weighted counts over $X$, initially zero

$$
\begin{aligned}
& \text { for } j=1 \text { to } N \text { do } \\
& \quad \mathbf{x}, W \leftarrow \text { Weighted-Sample }(b n) \\
& \mathbf{W}[x] \leftarrow \mathbf{W}[x]+W \text { where } x \text { is the value of } X \text { in } \mathrm{x} \\
& \text { return Normalize }(\mathbf{W}[X])
\end{aligned}
$$

function Weighted-Sample(bn, e) returns an event and a weight
$\mathbf{x} \leftarrow$ an event with $n$ elements; $w \leftarrow 1$
for $i=1$ to $n$ do
if $X_{i}$ has a value $x_{i}$ in e
then $w \leftarrow w \times P\left(X_{i}=x_{i} \mid \operatorname{parents}\left(X_{i}\right)\right)$
else $x_{i} \leftarrow$ a random sample from $\operatorname{Pr}\left(X_{i} \mid\right.$ parents $\left.\left(X_{i}\right)\right)$
return $\mathrm{x}, \mathrm{w}$

## Likelihood weighting example



## Likelihood weighting analysis

Likelihood weighting returns consistent estimates
Sampling probability for WeightedSample is

$$
S_{W S}(\mathbf{z}, \mathbf{e})=\prod_{i=1}^{\prime} P\left(z_{i} \mid \operatorname{parents}\left(Z_{i}\right)\right)
$$

(pays attention to evidence in ancestors only) $\rightsquigarrow$ somewhere "in between" prior and posterior distribution

Weight for a given sample $z, e$ is

$$
w(\mathbf{z}, \mathbf{e})=\prod_{i=1}^{m} P\left(e_{i} \mid \operatorname{parents}\left(E_{i}\right)\right)
$$


but performance still degrades with many evidence variables because a few samples have nearly all the total weight
Weighted sampling probability is

$$
S_{w s}(\mathbf{z}, \mathbf{e}) w(\mathbf{z}, \mathbf{e})=\prod_{i=1}^{\prime} P\left(z_{i} \mid \text { parents }\left(Z_{i}\right)\right) \prod_{i-1}^{m} P\left(e_{i} \mid \text { parents }\left(E_{i}\right)\right)=P(\mathbf{z}, \mathbf{e})
$$

## Summary

Approximate inference by LW:

- LW does poorly when there is lots of (late-in-the-order) evidence
- LW generally insensitive to topology
- Convergence can be very slow with probabilities close to 1 or 0
- Can handle arbitrary combinations of discrete and continuous variables


## Approximate inference using MCMC

"State" of network = current assignment to all variables.
Generate next state by sampling one variable given Markov blanket
Sample each variable in turn, keeping evidence fixed

```
function MCMC-Ask(X, e,bn,N) returns an estimate of P(X|e)
    local variables: }\mathbf{N}[X]\mathrm{ , a vector of counts over }X\mathrm{ , initially zero
                        Z, nonevidence variables in bn, hidden + query
                        x, current state of the network, initially copied from e
    initialize x with random values for the variables in Z
    for j=1 to N do
        N}[x]\leftarrow\textrm{N}[x]+1\mathrm{ where }x\mathrm{ is the value of X in x
        for each Z}\mp@subsup{Z}{i}{}\mathrm{ in Z do
        sample the value of Z}\mp@subsup{Z}{i}{}\mathrm{ in x from }\operatorname{Pr}(\mp@subsup{Z}{i}{}|mb(\mp@subsup{Z}{i}{})
            given the values of MB(Z
    return Normalize(N[X])
```

Can also choose a variable to sample at random each time

## The Markov chain

With Sprinkler $=$ true, $W$ etGrass $=$ true, there are four states:


Wander about for a while, average what you see
Probabilistic finite state machine

## MCMC example contd.

Estimate $\operatorname{Pr}($ Rain $\mid$ Sprinkler $=$ true, $W$ etGrass $=$ true $)$
Sample Cloudy or Rain given its Markov blanket, repeat.
Count number of times Rain is true and false in the samples.
E.g., visit 100 states

31 have Rain = true, 69 have Rain $=$ false
$\hat{\operatorname{Pr}}($ Rain $\mid$ Sprinkler $=$ true, WetGrass $=$ true $)=\operatorname{Normalize~}(\langle 31,69\rangle)=\langle 0.31,0.69\rangle$

Theorem
The Markov Chain approaches a stationary distribution:
long-run fraction of time spent in each state is exactly proportional to its posterior probability

## Markov blanket sampling

Markov blanket of Cloudy is
Sprinkler and Rain
Markov blanket of Rain is
Cloudy, Sprinkler, and WetGrass


Main computational problems:

1) Difficult to tell if convergence has been achieved
2) Can be wasteful if Markov blanket is large:
$P\left(X_{i} \mid m b\left(X_{i}\right)\right)$ won't change much (law of large numbers)

## Local semantics and Markov Blanket

Local semantics: each node is conditionally independent of its nondescendants given its parents


Each node is conditionally independent of all others given its Markov blanket: parents + children + children's parents


## MCMC analysis: Outline

- Transition probability $q\left(x \rightarrow x^{\prime}\right)$
- Occupancy probability $\pi_{t}(\mathbf{x})$ at time $t$
- Equilibrium condition on $\pi_{t}$ defines stationary distribution $\pi(\mathbf{x})$

Note: stationary distribution depends on choice of $q\left(x \rightarrow x^{\prime}\right)$

- Pairwise detailed balance on states guarantees equilibrium
- Gibbs sampling transition probability: sample each variable given current values of all others
$\Longrightarrow$ detailed balance with the true posterior
- For Bayesian networks, Gibbs sampling reduces to sampling conditioned on each variable's Markov blanket


## Stationary distribution

- $\pi_{t}(\mathbf{x})=$ probability in state $\mathbf{x}$ at time $t$
$\pi_{t+1}\left(\mathbf{x}^{\prime}\right)=$ probability in state $\mathbf{x}^{\prime}$ at time $t+1$
- $\pi_{t+1}$ in terms of $\pi_{t}$ and $q\left(\mathbf{x} \rightarrow \mathbf{x}^{\prime}\right)$

$$
\pi_{t+1}\left(\mathbf{x}^{\prime}\right)=\sum_{\mathbf{x}} \pi_{t}(\mathbf{x}) q\left(\mathbf{x} \rightarrow \mathbf{x}^{\prime}\right)
$$

- Stationary distribution: $\pi_{t}=\pi_{t+1}=\pi$

$$
\pi\left(\mathbf{x}^{\prime}\right)=\sum_{\mathbf{x}} \pi(\mathbf{x}) q\left(\mathbf{x} \rightarrow \mathbf{x}^{\prime}\right) \quad \text { for all } \mathbf{x}^{\prime}
$$

- If $\pi$ exists, it is unique (specific to $q\left(x \rightarrow x^{\prime}\right)$ )
- In equilibrium, expected "outflow" = expected "inflow"


## Detailed balance

- "Outflow" = "inflow" for each pair of states:

$$
\pi(\mathbf{x}) q\left(\mathbf{x} \rightarrow \mathbf{x}^{\prime}\right)=\pi\left(\mathbf{x}^{\prime}\right) q\left(\mathbf{x}^{\prime} \rightarrow \mathbf{x}\right) \quad \text { for all } \mathbf{x}, \mathbf{x}^{\prime}
$$

- Detailed balance $\Longrightarrow$ stationarity:

$$
\begin{aligned}
\sum_{\mathbf{x}} \pi(\mathbf{x}) q\left(\mathbf{x} \rightarrow \mathbf{x}^{\prime}\right) & =\sum_{\mathbf{x}} \pi\left(\mathbf{x}^{\prime}\right) q\left(\mathbf{x}^{\prime} \rightarrow \mathbf{x}\right) \\
& =\pi\left(\mathbf{x}^{\prime}\right) \sum_{\mathbf{x}} q\left(\mathbf{x}^{\prime} \rightarrow \mathbf{x}\right) \\
& =\pi\left(\mathbf{x}^{\prime}\right)
\end{aligned}
$$

- MCMC algorithms typically constructed by designing a transition probability $q$ that is in detailed balance with desired $\pi$


## Gibbs sampling

- Sample each variable in turn, given all other variables
- Sampling $X_{i}$, let $\bar{X}_{i}$ be all other nonevidence variables
- Current values are $x_{i}$ and $\overline{x_{i}} ; \mathbf{e}$ is fixed
- Transition probability is given by

$$
q\left(\mathbf{x} \rightarrow \mathbf{x}^{\prime}\right)=q\left(x_{i}, \overline{\mathbf{x}_{i}} \rightarrow x_{i}^{\prime}, \overline{\mathbf{x}_{i}}\right)=P\left(x_{i}^{\prime} \mid \overline{\mathbf{x}_{i}}, \mathbf{e}\right)
$$

- This gives detailed balance with true posterior $P(\mathbf{x} \mid \mathbf{e})$ :

$$
\begin{aligned}
\pi(\mathbf{x}) q\left(\mathbf{x} \rightarrow \mathbf{x}^{\prime}\right) & =P(\mathbf{x} \mid \mathbf{e}) P\left(x_{i}^{\prime} \mid \overline{\mathbf{x}_{i}}, \mathbf{e}\right)=P\left(x_{i}, \overline{,} \mid \mathbf{e}\right) P\left(x_{i}^{\prime} \mid \overline{\mathbf{x}_{i}}, \mathbf{e}\right) \\
& =P\left(x_{i} \mid \overline{\mathbf{x}_{i}}, \mathbf{e}\right) P\left(\overline{\mathbf{x}_{i}} \mid \mathbf{e}\right) P\left(x_{i}^{\prime} \mid \overline{\mathbf{x}_{i}}, \mathbf{e}\right) \quad \text { (chain rule) } \\
& =P\left(x_{i} \mid \overline{\mathbf{x}_{i}}, \mathbf{e}\right) P\left(x_{i}^{\prime}, \overline{\mathbf{x}_{i}} \mid \mathbf{e}\right) \quad \text { (chain rule backwards) } \\
& =q\left(\mathbf{x}^{\prime} \rightarrow \mathbf{x}\right) \pi\left(\mathbf{x}^{\prime}\right)=\pi\left(\mathbf{x}^{\prime}\right) q\left(\mathbf{x}^{\prime} \rightarrow \mathbf{x}\right)
\end{aligned}
$$

## Summary

Exact inference by variable elimination:

- polytime on polytrees, NP-hard on general graphs
- space $=$ time, very sensitive to topology

Approximate inference by LW, MCMC:

- PriorSampling and RejectionSampling unusable as evidence grow
- LW does poorly when there is lots of (late-in-the-order) evidence
- LW, MCMC generally insensitive to topology
- Convergence can be very slow with probabilities close to 1 or 0
- Can handle arbitrary combinations of discrete and continuous variables

