DM825
Introduction to Machine Learning

## Lecture 12 <br> Bayesian Networks

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## Outline

## 1. Conditional Independence

2. Inference in BN

Exact inference by enumeration Exact inference by variable elimination Exact inference by message passing Approximate inference by stochastic simulation Approximate inference by Markov chain Monte Carlo

## Factorization

BN encode local conditional independences

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

Joint probability factorization (the global semantics simplifies to):

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

## Important Rules

When working with Bayesian Networks, the following probability theory rules are worth remembering:

- Product rule
- Sum rule (marginalization)
- Bayes rule
- Factorization


## Outline

1. Conditional Independence
```
2. Inference in BN
    Exact inference by enumeration
    Exact inference by variable elimination
    Exact inference by message passing
    Approximate inference by stochastic simulation
    Approximate inference by Markov chain Monte Carlo
```


## Three Examples

$p(a, b, c)=p(a \mid c) p(b \mid c) p(c)$

$$
p(a, b)=\sum_{c} p(a, b, c)=\sum_{c} p(a \mid c) p(b \mid c) p(c)
$$

$$
p(a, b \mid c)=\frac{p(a, b, c)}{p(c)}=\frac{p(a \mid c) p(b \mid c) p(c)}{p(c)}=p(a \mid c) p(b \mid c)
$$



$$
\begin{aligned}
p(a, b, c) & =p(a) p(c \mid a) p(b \mid c) \\
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p(a, b \mid c) & =\frac{p(a, b, c)}{p(c)}=\frac{p(a) p(b) p(c \mid a, b)}{p(c)}
\end{aligned}
$$

## Example

$$
\begin{aligned}
& p(G=1 \mid B=1, F=1)=0.8 \\
& p(G=1 \mid B=1, F=0)=0.2 \\
& p(B=1)=0.9 \\
& p(F=1)=0.9
\end{aligned}
$$


$p(F=0 \mid G=0)=?$
$p(F=0 \mid G=0) \geq p(F=0)$
$p(F=0 \mid G=0, B=0)=?$
$p(F=0 \mid G=0, B=0) \leq p(F=0 \mid G=0)$ (not conditional independent)
$B$ explains away $F$

## d-separation

Definition (d-separation)
Two distinct variables $A$ and $B$ in a causal network are $d$-separated (" $d$ " for "directed graph") if for all paths between $A$ and $B$, there is an intermediate variable $C$ (distinct from $A$ and $B$ ) such that either

1. the connection is tail-to-tail or head-to-tail and $C$ is instantiated or
2. the connection is head-to-head, and neither $C$ nor any of $C$ 's descendants have received evidence.
If $A$ and $B$ are not d-separated, we call them d -connected.

If (1) then $A$ indep. of $B$ given $C$
If (2) then $A$ indep. of $B$

Conditional Independence


## Markov Blanket

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

$$
\begin{aligned}
p\left(\mathbf{x}_{i} \mid \mathbf{x}_{j \neq i}\right) & =\frac{p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{D}\right)}{\sum_{\mathbf{x}_{i}} p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{D}\right)} \\
& =\frac{\prod_{k} p\left(\mathbf{x}_{k} \mid \mathrm{pa}_{k}\right)}{\sum_{\mathbf{x}_{i}} \prod_{k}\left(\mathbf{x}_{k} \mid \mathrm{pa}_{k}\right)}
\end{aligned}
$$



## Algebra of Potentials

- General algebra of multiplication and marginalization on tables.
- For each outcome a variable has a corresponding state. States are mutually exclusive and exhaustive. The set of states associated with a variable $A$ is denoted by $\operatorname{sp}(A)=\left(a_{1}, a_{2}, \ldots, a_{n}\right)$.
- Potential $\phi: s p(\mathcal{X}) \rightarrow \mathbb{R}$
- $\operatorname{dom}(\phi(A, B \mid C))=\{A, B, C\}$ domain
- multiplication: $\phi_{1} \phi_{2}: \operatorname{dom}\left(\phi_{1} \phi_{2}\right)=\operatorname{dom}\left(\phi_{1}\right) \cup \operatorname{dom}\left(\phi_{2}\right)$
- marginalization: $\sum_{A} \phi$ has domain $\operatorname{dom}(\phi) \backslash\{A\}$
- unit potential property: $\sum_{A} P(A \mid \mathcal{V})=1$
- projection for marginalization. Eg: if $A$ and $B$ are marginalized out of $\phi(A, B, C)$, we say $\phi$ is projected down to $C$


## Moralization



Converting a directed graph into an undirected graph: On the undirected:

$$
p(\mathbf{x})=\frac{1}{Z} \prod_{C} \psi_{C}\left(\mathbf{x}_{c}\right)
$$

On the directed:

$$
p(\mathbf{x})=p\left(x_{1}\right) p\left(x_{2}\right) p\left(x_{3}\right) p\left(x_{4} \mid x_{1}, x_{2}, x_{3}\right)
$$

we introduce and edge for every arc and we marry parents

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Exact inference by enumeration Exact inference by variable elimination Exact inference by message passing Approximate inference by stochastic simulation Approximate inference by Markov chain Monte Carlo

## Inference tasks

$\vec{e}$ assignment of values to some variables $\mathbb{E}$ (instantiation, evidence)

- Probability of Evidence $\operatorname{Pr}(\vec{e})$

Example: probability that an individual will come out positive on both tests $\operatorname{Pr}(T 1=+\mathrm{ve}, T 2=+\mathrm{ve})$ overall reliability of the system $\operatorname{Pr}(S=$ avail $)$ related: node marginals query: probability $\operatorname{Pr}(x \mid e)$ for each $X$ and for each of $x \in X$.

- Most Probable Explanation (MPE) $\left.\arg _{\max }^{\vec{q} \in \mathbf{Q}} \operatorname{Pr}^{\operatorname{Pr}} \mid \vec{e}\right), \mathbf{Q}=\overline{\mathbf{E}}$ Example: find the most likely group, dissected by sex and condition, that will yield negative results for both tests $\left(\vec{e}=\left\{T_{1}=-\mathrm{ve} ; T 2=-\mathrm{ve}\right\}\right.$ and $Q=\{S, C\}$ )
- Maximum a Posteriori Hypothesis (MAP) $\arg \max _{\vec{q} \in \mathbf{Q}} \operatorname{Pr}(\vec{q} \mid \vec{e}), \mathbf{Q} \subseteq \overline{\mathbf{E}}$ Example: find most likely configuration of the two fans given that the system is unavailable ( $\vec{e}=\{S=$ unavail $\}, Q=\{F 1, F 2\}$ ).


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## Inference by enumeration

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

Simple query on the burglary network:

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



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Rewrite full joint entries using product of CPT entries:

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

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 $\{X\} \cup \mathbf{E} \cup \mathbf{Y}$
$\mathrm{Q}(X) \leftarrow$ a distribution over $X$, initially empty
for each value $x_{i}$ of $X$ do
$\mathrm{Q}\left(x_{i}\right) \leftarrow$ Enumerate-All $\left(\right.$ 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), $\mathbf{e} \cup\{Y=$ $y\}$ )

## Evaluation tree



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

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## Inference by variable elimination

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

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

## Variable elimination: Basic operations

Summing out a variable from a product of factors:

1. move any constant factors outside the summation:
2. add up submatrices in pointwise product of remaining factors:

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

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\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 $)$

Sum over $m$ is identically $1 ; M$ is irrelevant to the query

## Irrelevant variables contd.

Defn: moral graph of DAG Bayes net: marry all parents and drop arrows Defn: $\overline{\mathrm{A}}$ is m-separated from B by C iff separated by 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 $O\left(d^{k} n\right), k$ number of parents
- 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


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If we want the posteriror of each variable then even if poly tree $O(n) O(n)$ Join tree reduce the complexity to $O(n)$
Idea: join individual nodes such that the resulting network is a polytree

## Chains



We want to infer maringal of $x_{j}$ with no evidence

## Chains



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$$
\begin{align*}
& p\left(x_{n}\right)=\frac{1}{Z} \\
& \underbrace{\left[\sum_{x_{n-1}} \psi_{n-1, n}\left(x_{n-1}, x_{n}\right) \cdots\left[\sum_{x_{2}} \psi_{2,3}\left(x_{2}, x_{3}\right)\left[\sum_{x_{1}} \psi_{1,2}\left(x_{1}, x_{2}\right)\right]\right] \cdots\right]}_{\mu_{\alpha}\left(x_{n}\right)} \\
& \underbrace{\left[\sum_{x_{n+1}} \psi_{n, n+1}\left(x_{n}, x_{n+1}\right) \cdots\left[\sum_{x_{N}} \psi_{N-1, N}\left(x_{N-1}, x_{N}\right)\right] \cdots\right]}_{\mu_{\beta}\left(x_{n}\right)} . \tag{8.52}
\end{align*}
$$

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## Inference by stochastic simulation

Basic idea:

- Draw $N$ samples from a sampling distribution $S$


## 0.5 ooin

- Compute an approximate posterior probability $\hat{P}$
- Show this converges to the true probability $P$

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(bn) returns an event sampled from bn
    inputs: bn, a belief network specifying joint distribution
Pr}(\mp@subsup{X}{1}{},\ldots,\mp@subsup{X}{n}{}
    x}\leftarrow\mathrm{ an event with n elements
    for }i=1\mathrm{ to }n\mathrm{ do
    xi}\leftarrow\mathrm{ a random sample from }\operatorname{Pr}(\mp@subsup{X}{i}{}|\operatorname{parents}(\mp@subsup{X}{i}{})
    given the values of pa( }\mp@subsup{X}{i}{})\mathrm{ in }\textrm{x
    return x
```

Ancestor sampling

## Example



## Example



## Example



## Example



## Example



## Example



## Example



## Sampling from an empty network contd.

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

## Sampling from an empty network contd.

Probability that PriorSample generates a particular event

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S_{P S}\left(x_{1} \ldots x_{n}\right)=P\left(x_{1} \ldots x_{n}\right)
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i.e., the true prior probability
E.g., $S_{P S}(t, f, t, t)=0.5 \times 0.9 \times 0.8 \times 0.9=0.324 \rightarrow P(t, f, t, t)$

## Sampling from an empty network contd.

Probability that PriorSample generates a particular event

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

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

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

## Sampling from an empty network contd.

Probability that PriorSample generates a particular event

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

$\rightsquigarrow$ 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 $\mathbf{e}$

## Rejection sampling

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

$$
\text { for } j=1 \text { to } N \text { do }
$$

$\mathrm{x} \leftarrow$ Prior-Sample(bn)
if x is consistent with e then
$\mathrm{N}[x] \leftarrow \mathrm{N}[x]+1$ where $x$ is the value of $X$ in x
return Normalize( $\mathrm{N}[X]$ )

## Rejection sampling

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

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

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 $)=$ 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:
Pr}(X|\mathbf{e})=\alpha\mp@subsup{\mathbf{N}}{PS}{(}(X,\mathbf{e})\quad\mathrm{ (algorithm defn.)
    = N
    \approx\operatorname{Pr}(X,\mathbf{e})/P(\mathbf{e})\quad\mathrm{ (property of PriorSample)}
    = Pr(X|e) (defn. of conditional probability)
```


## Analysis of rejection sampling

Rejection sampling returns consistent posterior estimates

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

Problem: hopelessly expensive if $P(\mathbf{e})$ 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

## Likelihood weighting

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

```
for j=1 to N do
    x},w\leftarrow\mathrm{ Weighted-Sample(bn)
    W}[x]\leftarrow\mathbf{W}[x]+w\mathrm{ where x is the value of X in }\mathbf{x
    return Normalize(W[X])
```

function Weighted-Sample(bn, e) returns an event and a weight
$\mathrm{x} \leftarrow$ 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 example



## Likelihood weighting example



## Likelihood weighting example



## Likelihood weighting example



## Likelihood weighting example



## Likelihood weighting example



## Likelihood weighting analysis

Likelihood weighting returns consistent estimates
Sampling probability for WeightedSample is

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

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


Weight for a given sample $\mathrm{z}, \mathrm{e}$ is

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

## Likelihood weighting analysis

Likelihood weighting returns consistent estimates
Sampling probability for WeightedSample is

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

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


Weight for a given sample $\mathrm{z}, \mathrm{e}$ is

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

## Likelihood weighting analysis

Likelihood weighting returns consistent estimates
Sampling probability for WeightedSample is

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but performance still degrades with many evidence variables because a few samples have nearly all the total weight
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## 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


## Outline

## 1. Conditional Independence

2. Inference in BN

Exact inference by enumeration
Exact inference by variable elimination
Exact inference by message passing
Approximate inference by stochastic simulation
Approximate inference by Markov chain Monte Carlo

## 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 \(P(X \mid \mathbf{e})\)
    local variables: \(\mathbf{N}[X]\), a vector of counts over \(X\), initially zero
    Z , nonevidence variables in \(b n\), 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
        \(\mathbf{N}[x] \leftarrow \mathbf{N}[x]+1\) where \(\mathbf{x}\) is the value of \(\boldsymbol{X}\) in \(\mathbf{x}\)
        for each \(Z_{i}\) in Z do
            sample the value of \(Z_{i}\) in x from \(\operatorname{Pr}\left(Z_{i} \mid m b\left(Z_{i}\right)\right)\)
            given the values of \(M B\left(Z_{i}\right)\) in x
    return Normalize( \(\mathbf{N}[X]\) )
```

Can also choose a variable to sample at random each time

## The Markov chain

With Sprinkler $=$ true, WetGrass $=$ true, there are four states:


Wander about for a while, average what you see

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With Sprinkler $=$ true, WetGrass $=$ 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, WetGrass $=$ true $)$

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E.g., visit 100 states

31 have Rain = true, 69 have Rain $=$ false
$\hat{\operatorname{Pr}}($ Rain $\mid$ Sprinkler $=$ true, WetGrass $=$ true $)=\operatorname{Normalize~}(\langle 31,69\rangle)=\langle 0.31,0$.

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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


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Probability given the Markov blanket is calculated as follows:

$$
P\left(x_{i}^{\prime} \mid m b\left(X_{i}\right)\right)=P\left(x_{i}^{\prime} \mid \operatorname{parents}\left(X_{i}\right)\right) \prod_{Z_{j} \in C h i l d r e n\left(X_{i}\right)} P\left(z_{j} \mid \operatorname{parents}\left(Z_{j}\right)\right)
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Easily implemented in message-passing parallel systems

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$$

Easily implemented in message-passing parallel systems 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 $q\left(\mathrm{x} \rightarrow \mathrm{x}^{\prime}\right)$


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- 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 $t$
$\pi_{t+1}\left(\mathrm{x}^{\prime}\right)=$ probability in state $\mathrm{x}^{\prime}$ at time $t+1$


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- If $\pi$ exists, it is unique (specific to $q\left(\mathrm{x} \rightarrow \mathbf{x}^{\prime}\right)$ )
- 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}
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- Detailed balance $\Longrightarrow$ stationarity:

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

- 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


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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)
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$$

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

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

## 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

