Lecture 11
Probabilistic Graphical Models
Inference

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Outline

1. Inference in BN

2. Inference by Randomized Algorithms

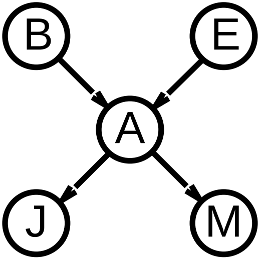
Inference tasks

- Simple queries: compute posterior marginal $\mathbf{P}(X_i|\mathbf{E}=\mathbf{e})$
  e.g., $P(NoGas|Gauge=empty, Lights=on, Starts=false)$
- Conjunctive queries: $\mathbf{P}(X_i, X_j|\mathbf{E}=\mathbf{e}) = \mathbf{P}(X_i|\mathbf{E}=\mathbf{e})\mathbf{P}(X_j|X_i, \mathbf{E}=\mathbf{e})$
- 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:



$$\begin{aligned}\mathbf{P}(B|j,m) &= \mathbf{P}(B,j,m)/P(j,m)\\ &= \alpha\mathbf{P}(B,j,m)\\ &= \alpha\ \textstyle\sum_e\ \sum_a\ \mathbf{P}(B,e,a,j,m)\end{aligned}$$

Rewrite full joint entries using product of CPT entries:

$$\begin{aligned}\mathbf{P}(B|j,m) &= \alpha\ \textstyle\sum_e\ \sum_a\ \mathbf{P}(B)P(e)\mathbf{P}(a|B,e)P(j|a)P(m|a)\\ &= \alpha\mathbf{P}(B)\ \textstyle\sum_e\ P(e)\ \sum_a\ \mathbf{P}(a|B,e)P(j|a)P(m|a)\end{aligned}$$

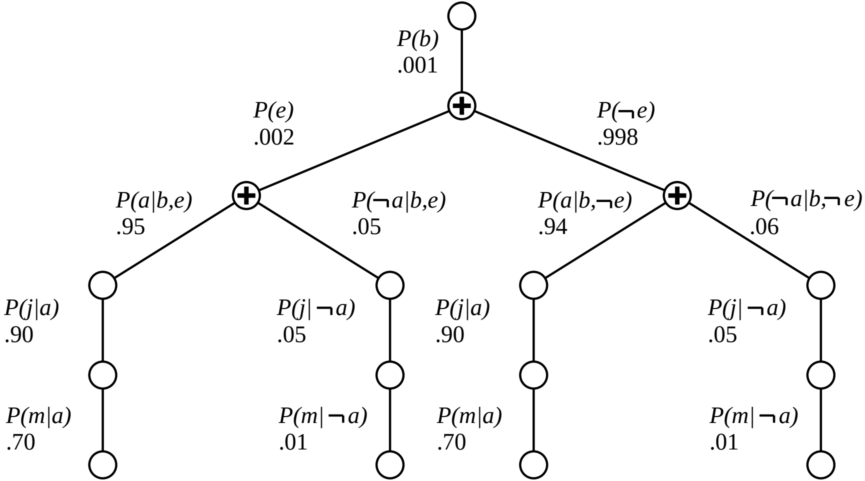
Recursive depth-first enumeration: $O(n)$ space, $O(d^n)$ time

Enumeration algorithm

```
function Enumeration-Ask(X, e, bn) returns a distribution over X
   inputs: X,  the query variable
           e, observed values for variables E
           bn, a Bayesian network with variables {X} ∪ E ∪ Y

   Q(X) ← a distribution over X, initially empty
   for each value x_i of X do
       extend e with value x_i for X
       Q(x_i) ← Enumerate-All(Vars[bn], e)
   return Normalize(Q(X))
-----------------------------------------------------------------------
function Enumerate-All(vars, e) returns a real number
   if Empty?(vars) then return 1.0
   Y ← First(vars)
   if Y has value y in e
       then return P(y | parent(Y)) × Enumerate-All(Rest(vars), e)
      else return Σ_y P(y | parent(Y)) × Enumerate-All(Rest(vars), e_y)
            where e_y is e extended with Y = y
```

Evaluation tree



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

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 $O(d^k n)$
- hence time and space cost are linear in n and k bounded by a constant

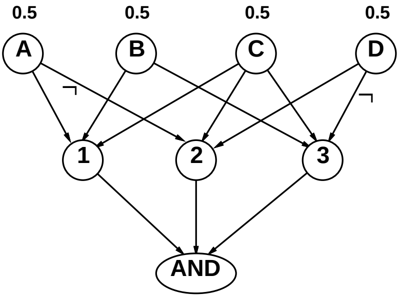
Multiply connected networks:

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

1. A v B v C

2. C v D v ¬A

3. B v C v ¬D



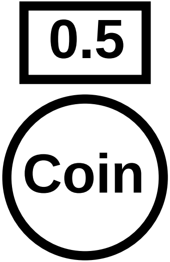
Outline

1. Inference in BN
2. Inference by Randomized Algorithms

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 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

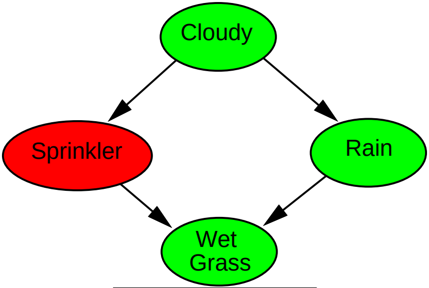
Sampling from an empty network

```
function Prior-Sample(bn) returns an event sampled from bn
      inputs: bn, a belief network specifying joint distribution P(X_1, ..., X_n)

   x ← an event with n elements
   for i = 1 to n do
        x_i ← a random sample from P(X_i | parents(X_i))
              given the values of Parents(X_i) in x
   return x
```

Example

P(C)
.50



C	P(S|C)
T	.10
F	.50

C	P(R|C)
T	.80
F	.20

S	R	P(W|S,R)
T	T	.99
T	F	.90
F	T	.90
F	F	.01

Sampling from an empty network contd.

Probability that PriorSample generates a particular event

$$S_{PS}(x_1 \ldots x_n) = P(x_1 \ldots x_n)$$

i.e., the true prior probability

E.g., $S_{PS}(t, f, t, t) = 0.5 \times 0.9 \times 0.8 \times 0.9 = 0.324 = P(t, f, t, t)$

Proof: Let $N_{PS}(x_1 \ldots x_n)$ be the number of samples generated for event $x_1, \ldots, x_n$. Then we have

$$\begin{aligned} \lim_{N \to \infty} \hat{P}(x_1, \ldots, x_n) &= \lim_{N \to \infty} N_{PS}(x_1, \ldots, x_n)/N \\ &= S_{PS}(x_1, \ldots, x_n) \\ &= \prod_{i=1}^{n} P(x_i | parents(X_i)) = P(x_1 \ldots x_n) \end{aligned}$$

$\rightsquigarrow$ That is, estimates derived from PriorSample are consistent
Shorthand: $\hat{P}(x_1, \ldots, x_n) \approx P(x_1 \ldots x_n)$

Rejection sampling

$\hat{\mathbf{P}}(X|\mathbf{e})$ estimated from samples agreeing with $\mathbf{e}$

function Rejection-Sampling($X, \mathbf{e}, bn, N$) **returns** an estimate of $P(X|\mathbf{e})$
  local variables: $\mathbf{N}$, a vector of counts over X, initially zero

  for $j = 1$ to N **do**
    $\mathbf{x} \leftarrow$ Prior-Sample(bn)
    if $\mathbf{x}$ is consistent with $\mathbf{e}$ **then**
      $\mathbf{N}[x] \leftarrow \mathbf{N}[x]+1$ where x is the value of X in $\mathbf{x}$
  return Normalize($\mathbf{N}[X]$)

E.g., estimate $\mathbf{P}(Rain|Sprinkler = true)$ using 100 samples
  27 samples have $Sprinkler = true$
    Of these, 8 have $Rain = true$ and 19 have $Rain = false$.

$\hat{\mathbf{P}}(Rain|Sprinkler = true) = \text{Normalize}(\langle 8, 19\rangle) = \langle 0.296, 0.704\rangle$
Similar to a basic real-world empirical estimation procedure

Analysis of rejection sampling

Rejection sampling returns consistent posterior estimates

Proof:

$\hat{\mathbf{P}}(X|\mathbf{e}) = \alpha \mathbf{N}_{PS}(X, \mathbf{e})$ (algorithm defn.)

$= \mathbf{N}_{PS}(X, \mathbf{e})/N_{PS}(\mathbf{e})$ (normalized by $N_{PS}(\mathbf{e})$)

$\approx \mathbf{P}(X, \mathbf{e})/P(\mathbf{e})$ (property of PriorSample)

$= \mathbf{P}(X|\mathbf{e})$ (defn. of conditional probability)

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

$P(\mathbf{e})$ 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($X, \mathbf{e}, bn, N$) **returns** an estimate of $P(X|\mathbf{e})$
  local variables: $\mathbf{W}$, a vector of weighted counts over X, initially zero

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

---

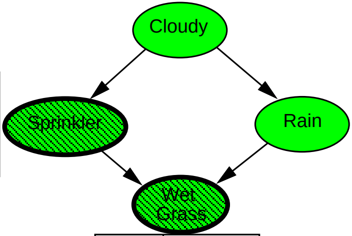
function Weighted-Sample($bn, \mathbf{e}$) **returns** an event and a weight

  $\mathbf{x} \leftarrow$ an event with n elements; $w \leftarrow 1$
  for $i = 1$ **to** n **do**
    if X_i has a value x_i in $\mathbf{e}$
      then $w \leftarrow w \times P(X_i = x_i \mid parents(X_i))$
      else $x_i \leftarrow$ a random sample from $\mathbf{P}(X_i \mid parents(X_i))$
  return $\mathbf{x}$, w

Likelihood weighting example

$P(Rain|Sprinkler = true, WetGrass = true)$

P(C)
.50



C	P(S|C)
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S	R	P(W|S,R)
T	T	.99
T	F	.90
F	T	.90
F	F	.01

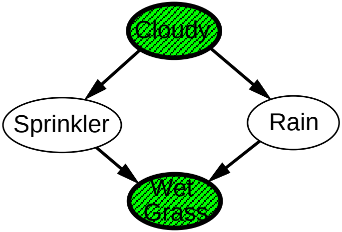
Likelihood weighting analysis

Likelihood weighting returns consistent estimates

Sampling probability for WeightedSample is

$$S_{WS}(\mathbf{z},\mathbf{e}) = \prod_{i=1}^{l} P(z_i|parents(Z_i))$$

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



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

$$w(\mathbf{z},\mathbf{e}) = \prod_{i=1}^{m} P(e_i|parents(E_i))$$

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

Weighted sampling probability is

$$S_{WS}(\mathbf{z},\mathbf{e})w(\mathbf{z},\mathbf{e}) = \prod_{i=1}^{l} P(z_i|parents(Z_i)) \prod_{i=1}^{m} P(e_i|parents(E_i)) = P(\mathbf{z},\mathbf{e})$$

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

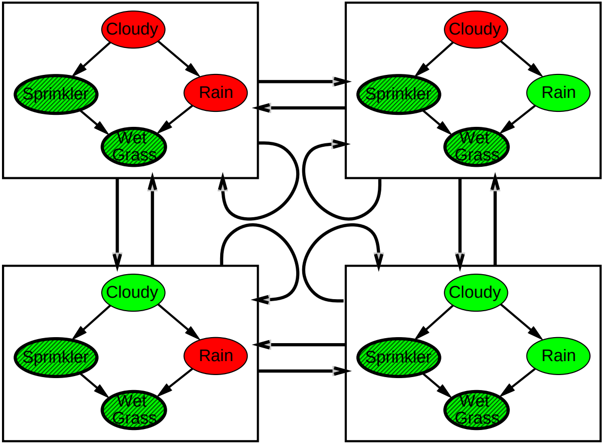
function MCMC-Ask(X, **e**, bn, N) **returns** an estimate of $P(X|\mathbf{e})$
  local variables: $\mathbf{N}[X]$, a vector of counts over X, initially zero
    $\mathbf{Z}$, nonevidence variables in bn, hidden + query
    $\mathbf{x}$, current state of the network, initially copied from $\mathbf{e}$

  initialize $\mathbf{x}$ with random values for the variables in $\mathbf{Z}$
  for $j = 1$ to N **do**
    $\mathbf{N}[x] \leftarrow \mathbf{N}[x] + 1$ where x is the value of X in $\mathbf{x}$
    for each Z_i in $\mathbf{Z}$ **do**
      sample the value of Z_i in $\mathbf{x}$ from $\mathbf{P}(Z_i|mb(Z_i))$
        given the values of $MB(Z_i)$ in $\mathbf{x}$
  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

Probabilistic finite state machine

MCMC example contd.

Estimate $\mathbf{P}(Rain|Sprinkler = true, WetGrass = true)$

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 $Rain = false$

$\hat{\mathbf{P}}(Rain|Sprinkler = true, WetGrass = true) = \text{Normalize}(\langle 31, 69\rangle) = \langle 0.31, 0.69\rangle$

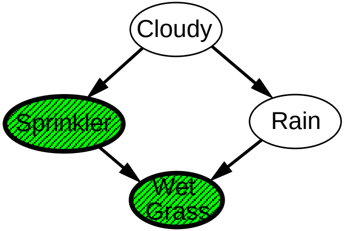
Theorem

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*

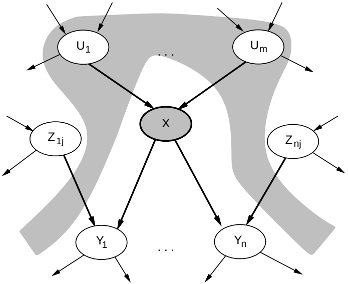
Markov blanket of *Rain* is
Cloudy, *Sprinkler*, and *WetGrass*



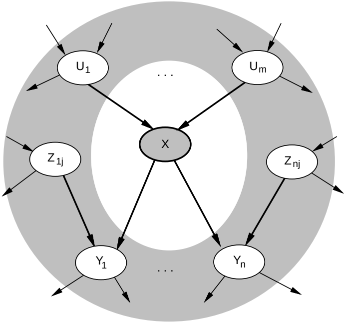
Main computational problems:
1) Difficult to tell if convergence has been achieved
2) Can be wasteful if Markov blanket is large:
$P(X_i|mb(X_i))$ won't change much (law of large numbers)

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 $q(\mathbf{x} \to \mathbf{x}')$
- Occupancy probability $\pi_t(\mathbf{x})$ at time t
- Equilibrium condition on π_t defines stationary distribution $\pi(\mathbf{x})$
  Note: stationary distribution depends on choice of $q(\mathbf{x} \to \mathbf{x}')$
- 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
  $\pi_{t+1}(\mathbf{x}')$ = probability in state $\mathbf{x}'$ at time $t+1$

- π_{t+1} in terms of π_t and $q(\mathbf{x} \to \mathbf{x}')$

$$\pi_{t+1}(\mathbf{x}') = \sum_{\mathbf{x}} \pi_t(\mathbf{x}) q(\mathbf{x} \to \mathbf{x}')$$

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

$$\pi(\mathbf{x}') = \sum_{\mathbf{x}} \pi(\mathbf{x}) q(\mathbf{x} \to \mathbf{x}') \qquad \text{for all } \mathbf{x}'$$

- If π exists, it is unique (specific to $q(\mathbf{x} \to \mathbf{x}')$)

- In equilibrium, expected "outflow" = expected "inflow"

Detailed balance

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

$$\pi(\mathbf{x})q(\mathbf{x} \to \mathbf{x}') = \pi(\mathbf{x}')q(\mathbf{x}' \to \mathbf{x}) \qquad \text{for all } \mathbf{x},\ \mathbf{x}'$$

- Detailed balance $\implies$ stationarity:

$$\begin{aligned} \sum_{\mathbf{x}} \pi(\mathbf{x})q(\mathbf{x} \to \mathbf{x}') &= \sum_{\mathbf{x}} \pi(\mathbf{x}')q(\mathbf{x}' \to \mathbf{x}) \\ &= \pi(\mathbf{x}') \sum_{\mathbf{x}} q(\mathbf{x}' \to \mathbf{x}) \\ &= \pi(\mathbf{x}') \end{aligned}$$

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

Gibbs sampling

- Sample each variable in turn, given **all other variables**
- Sampling X_i, let $\bar{\mathbf{X}}_i$ be all other nonevidence variables
- Current values are x_i and $\bar{\mathbf{x}}_i$; $\mathbf{e}$ is fixed
- Transition probability is given by

$$q(\mathbf{x} \rightarrow \mathbf{x}') = q(x_i, \bar{\mathbf{x}}_i \rightarrow x_i', \bar{\mathbf{x}}_i) = P(x_i' | \bar{\mathbf{x}}_i, \mathbf{e})$$

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

$$\begin{aligned}
\pi(\mathbf{x}) q(\mathbf{x} \rightarrow \mathbf{x}') &= P(\mathbf{x}|\mathbf{e}) P(x_i'|\bar{\mathbf{x}}_i, \mathbf{e}) = P(x_i, \bar{\mathbf{x}}_i|\mathbf{e}) P(x_i'|\bar{\mathbf{x}}_i, \mathbf{e}) \\
&= P(x_i|\bar{\mathbf{x}}_i, \mathbf{e}) P(\bar{\mathbf{x}}_i|\mathbf{e}) P(x_i'|\bar{\mathbf{x}}_i, \mathbf{e}) \quad \text{(chain rule)} \\
&= P(x_i|\bar{\mathbf{x}}_i, \mathbf{e}) P(x_i', \bar{\mathbf{x}}_i|\mathbf{e}) \quad \text{(chain rule backwards)} \\
&= q(\mathbf{x}' \rightarrow \mathbf{x}) \pi(\mathbf{x}') = \pi(\mathbf{x}') q(\mathbf{x}' \rightarrow \mathbf{x})
\end{aligned}$$

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