

COMS W4701: Artificial Intelligence

Lecture 11: Inference and Sampling

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Today

- Exact inference in Bayes nets
- Variable elimination
- Direct sampling methods: Prior, rejection, importance
- MCMC methods: Gibbs sampling

Inference in Bayes Nets

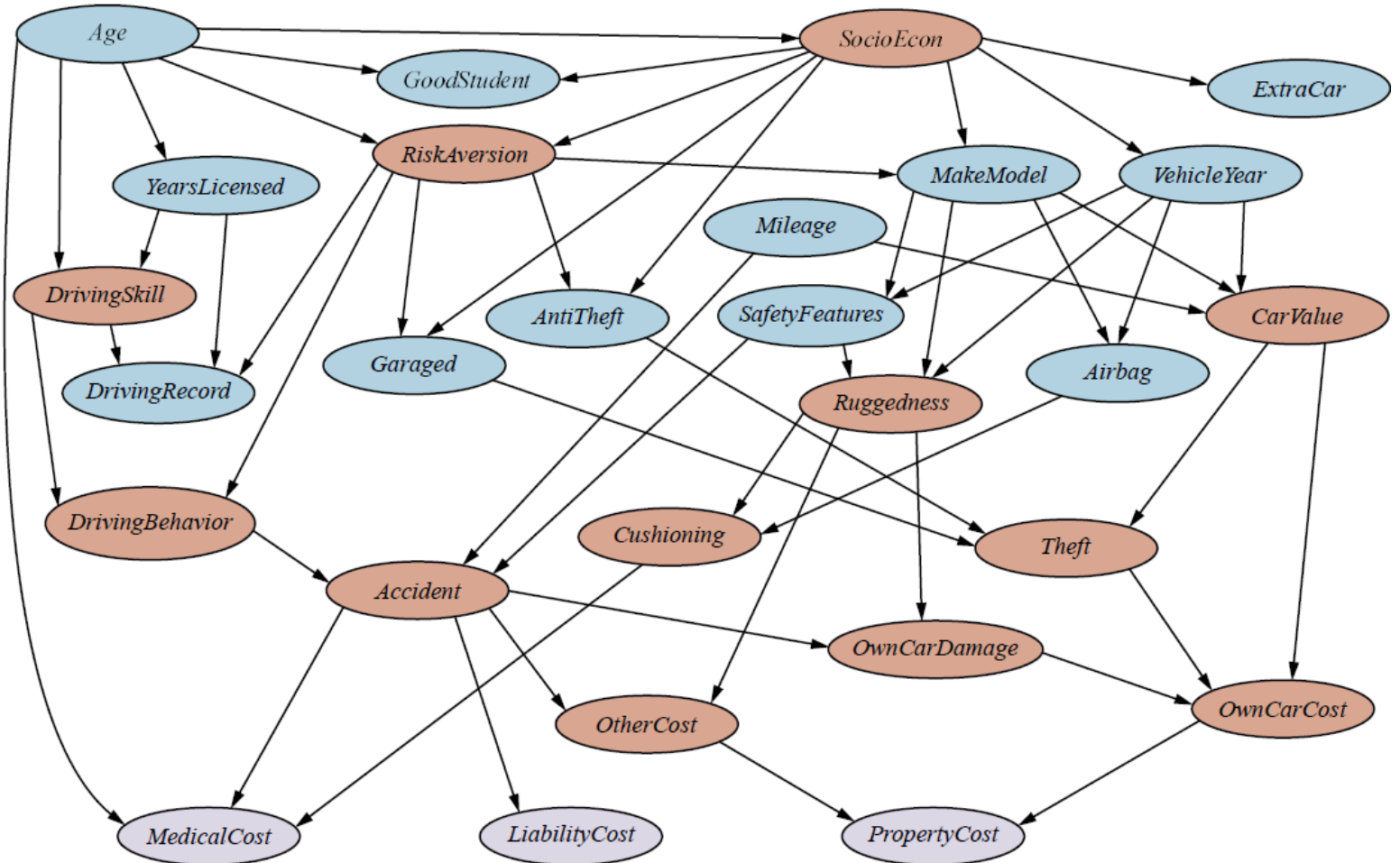
- General task: Find the posterior distribution of a set of **query** variables X given a set of observed **evidence** e
- There may also be **hidden** variables Y interacting with X and E
- General strategy: Construct joint distributions via chain rule and remove hidden variables via marginalization

$$P(X \mid e) = \alpha P(X, e) = \alpha \sum_y P(X, y, e)$$

- Can be computationally heavy; conditional independences can help

Example: Car Insurance

- Queries: Costs of insurance (purple)
- Evidence: Entries requested by insurance company (blue)
- Hidden variables: Not observed, but may play role in determining insurance costs (red)



Example: Alarm Network

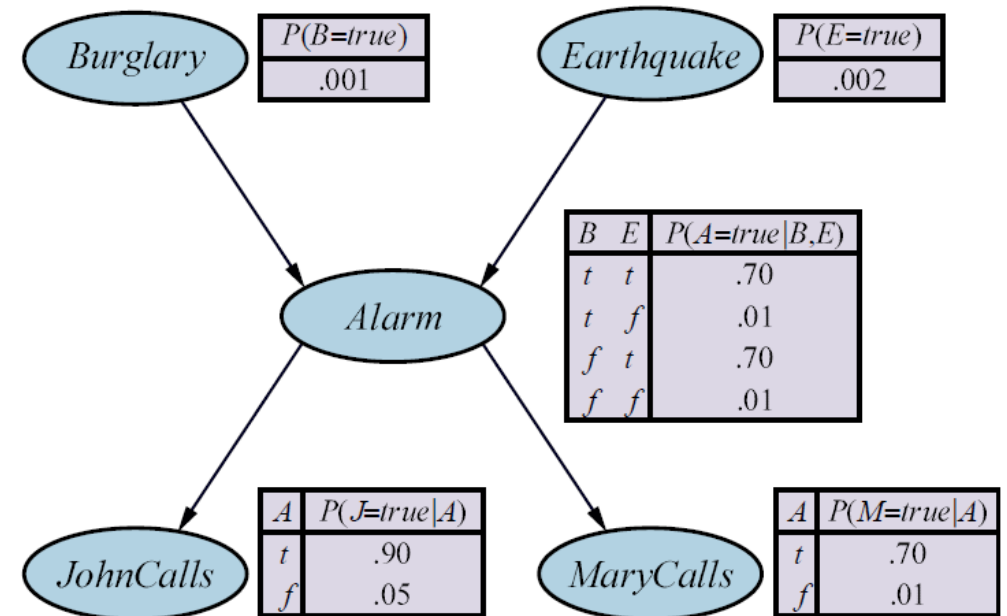
- Let's query individual probabilities first, instead of entire distributions
- Query** variables **X**; **evidence** variables **e**; **hidden** variables **Y**

$$P(+b, -e, +a) = P(+b)P(-e)P(+a | +b, -e) \\ = (.001)(.998)(.01) = 9.98 \times 10^{-6}$$

$$P(+j | -a, +e) = P(+j | -a) = 0.05$$

$$P(+j, +m | -a) = P(+j | -a)P(+m | -a) \\ = (0.05)(0.01) = 0.0005$$

$$P(+a) = \sum_{b,e} P(b, e, +a) = \sum_{b,e} P(b)P(e)P(+a | b, e) \\ = (.001)(.002)(.7) + (.001)(.998)(.01) + (.999)(.002)(.7) + (.999)(.998)(.01) = .01138$$



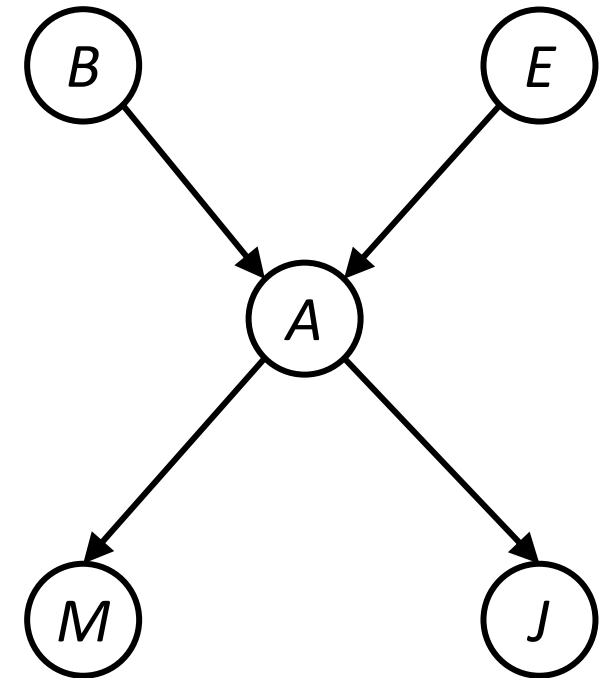
Example: Alarm Network

$$\sum_e P(b)P(e)P(a \mid b, e)$$

$$\sum_{b,e,a} P(b)P(e)P(a \mid b, e)P(m \mid a)P(j \mid a)$$

$$\frac{P(b)P(e)P(a \mid b, e)}{\sum_{b,e} P(b)P(e)P(a \mid b, e)}$$

$$\frac{\sum_{b,e} P(b)P(e)P(a \mid b, e) P(m \mid a)}{\sum_{b,e,m} P(b)P(e)P(a \mid b, e)P(m \mid a)}$$



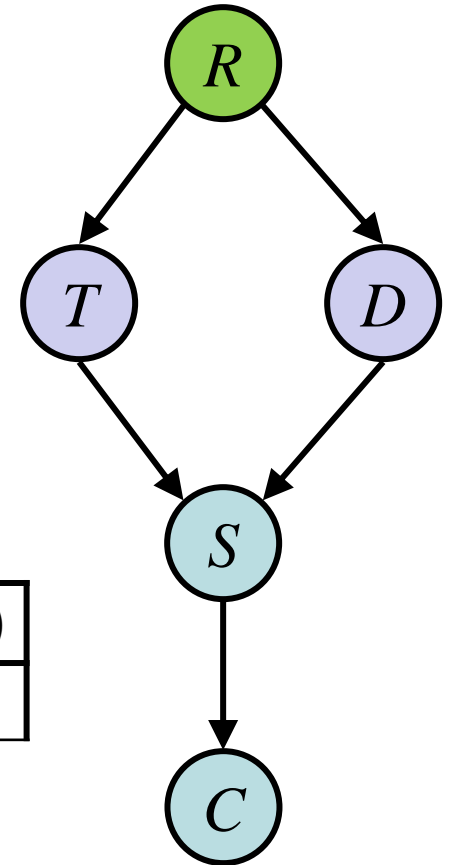
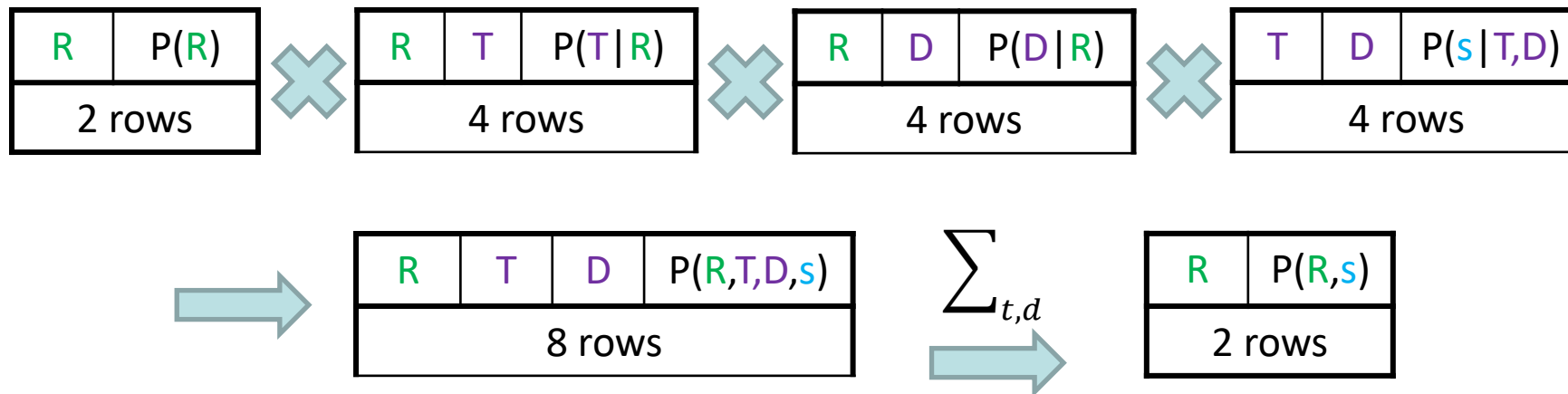
Querying Distributions

- The chain rule can be used to form an entire joint distribution all at once by *pointwise multiplying* matching rows

$$P(R|s, c) = P(R|s) \propto P(R, s) = \sum_{t,d} P(R, t, d, s)$$

Conditional independence

$$= \sum_{t,d} P(R)P(t|R)P(d|R)P(s|t, d)$$



Example 1

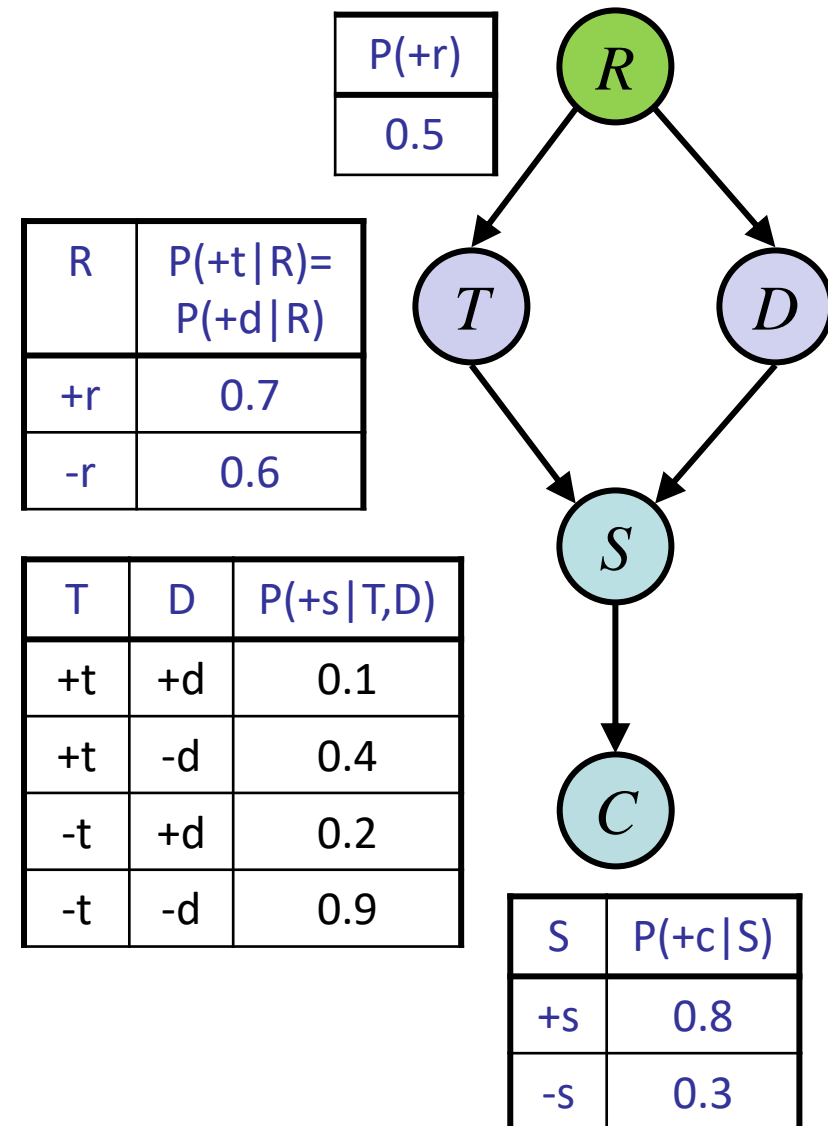
$$P(R|+s, +c) \propto \sum_{t,d} P(R)P(t|R)P(d|R)P(+s|t,d)$$

$$= \frac{P(R, +t, +d|+s, +c)}{P(R, -t, +d|+s, +c)} \frac{P(R, +t, -d|+s, +c)}{P(R, -t, -d|+s, +c)} \\ + \frac{P(R, +t, +d|+s, +c)}{P(R, -t, +d|+s, +c)} \frac{P(R, +t, -d|+s, +c)}{P(R, -t, -d|+s, +c)} \\ + \frac{P(R, +t, +d|+s, +c)}{P(R, -t, +d|+s, +c)} \frac{P(R, +t, -d|+s, +c)}{P(R, -t, -d|+s, +c)} \frac{P(R, +t, -d|+s, +c)}{P(R, -t, -d|+s, +c)} \\ + \frac{P(R, +t, +d|+s, +c)}{P(R, -t, +d|+s, +c)} \frac{P(R, +t, -d|+s, +c)}{P(R, -t, -d|+s, +c)} \frac{P(R, +t, -d|+s, +c)}{P(R, -t, -d|+s, +c)} \frac{P(R, +t, -d|+s, +c)}{P(R, -t, -d|+s, +c)}$$

$$= \frac{0.128}{0.162} \propto \frac{0.441}{0.559} = P(R | +s, +c)$$

$$P(R, +s, +c)$$

Prior to summing, we are building a distribution over R, T, D (3 variables)



Example 2

$$P(R \mid +c, +d) \propto \sum_{t,s} P(R)P(t \mid R)P(+d \mid R)P(s \mid t, +d)P(+c \mid s)$$

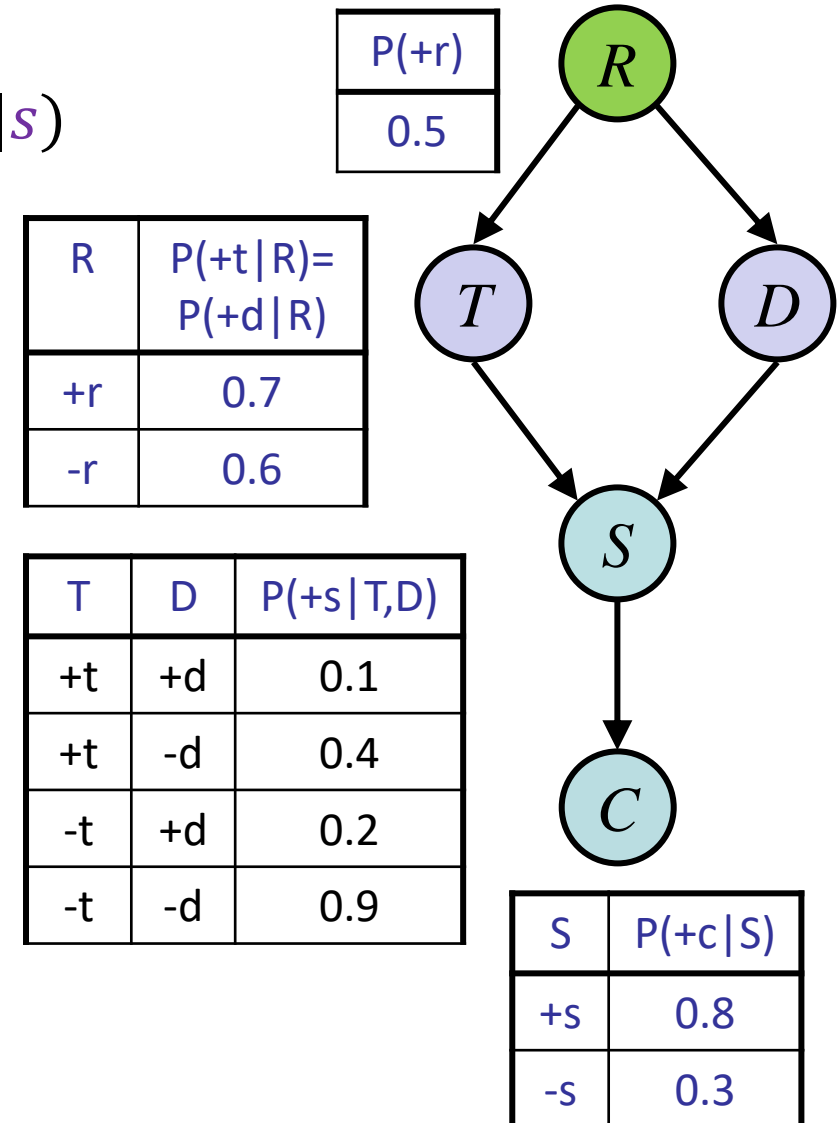
$$= \begin{matrix} P(R, +t, +s \mid +d, +c) \\ \left(\frac{0.5}{0.5}\right) * \left(\frac{0.7}{0.6}\right) * \left(\frac{0.7}{0.6}\right) * 0.1 * 0.8 \end{matrix} + \begin{matrix} P(R, +t, -s \mid +d, +c) \\ \left(\frac{0.5}{0.5}\right) * \left(\frac{0.7}{0.6}\right) * \left(\frac{0.7}{0.6}\right) * 0.9 * 0.3 \end{matrix}$$

$$+ \begin{matrix} P(R, -t, +s \mid +d, +c) \\ \left(\frac{0.5}{0.5}\right) * \left(\frac{0.3}{0.4}\right) * \left(\frac{0.7}{0.6}\right) * 0.2 * 0.8 \end{matrix} + \begin{matrix} P(R, -t, -s \mid +d, +c) \\ \left(\frac{0.5}{0.5}\right) * \left(\frac{0.3}{0.4}\right) * \left(\frac{0.7}{0.6}\right) * 0.8 * 0.3 \end{matrix}$$

$$= \begin{pmatrix} 0.1278 \\ 0.1111 \end{pmatrix} \propto \begin{pmatrix} 0.535 \\ 0.465 \end{pmatrix} = P(R \mid +c, +d)$$

$$P(R, +c, +d)$$

Prior to summing, we are building a distribution over R, T, S (3 variables)



Complexity of Inference

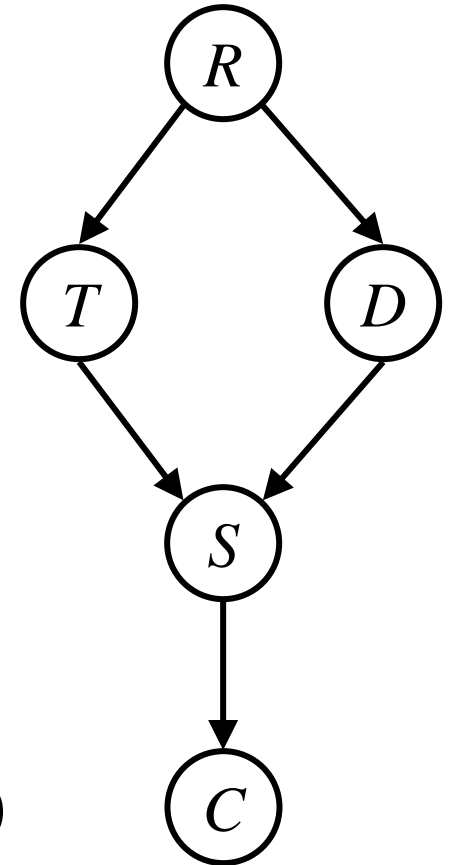
- Inference process involves building up a joint distribution encompassing all relevant variables, followed by marginalization down to the original query
- Worst case: Joint distribution over the entire Bayes net!
- Inference is NP-hard in general
- We can try to make process more efficient by marginalizing early and often
- Alternate between building up and summing out

Variable Elimination

- Idea: Alternate between building up and marginalizing

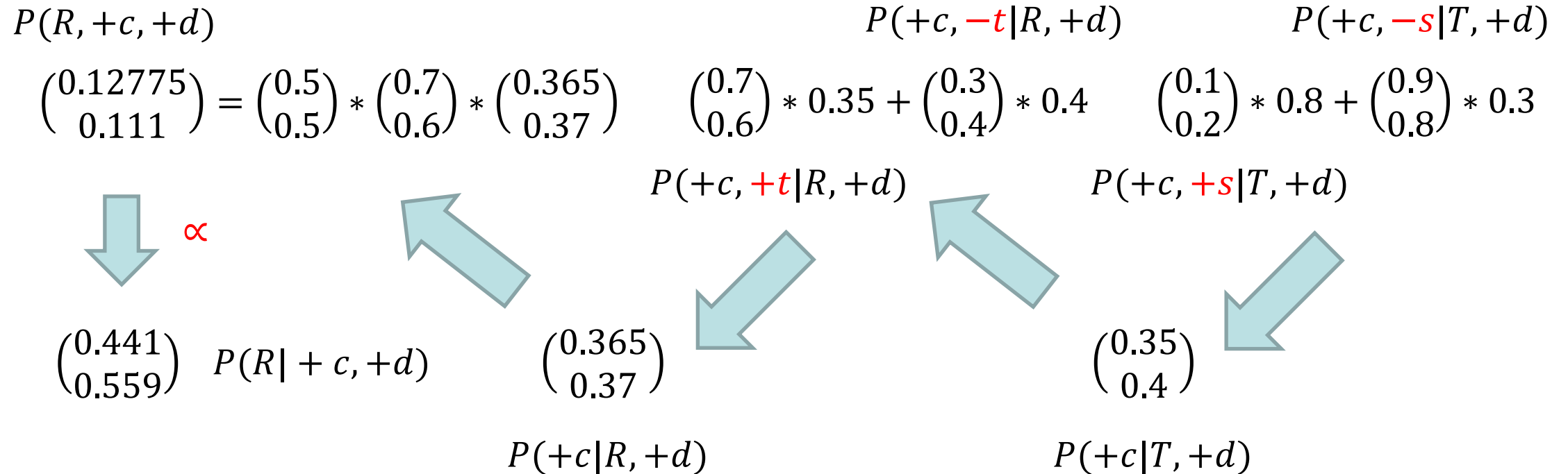
$$\begin{aligned} P(S|r) &\propto P(r, S) = \sum_{t,d} P(r)P(t|r)P(d|r)P(S|t, d) \\ &= P(r) \sum_t P(t|r) \sum_d P(d|r)P(S|t, d) \end{aligned}$$

$$\begin{aligned} P(S|c) &\propto P(S, c) = \sum_{r,t,d} P(r)P(t|r)P(d|r)P(S|t, d)P(c|S) \\ &= P(c|S) \sum_r P(r) \sum_t P(t|r) \sum_d P(d|r)P(S|t, d) \end{aligned}$$



Example: Variable Elimination

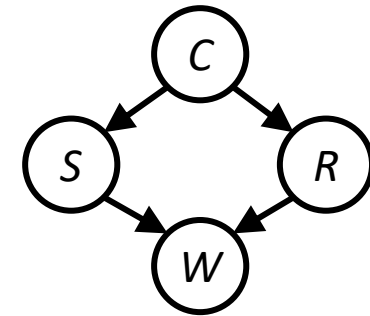
$$P(R|+c, +d) \propto P(R)P(+d|R) \sum_t P(t|R) \sum_s P(s|t, +d)P(+c|s)$$



Largest distribution at any point is over 2 variables

Approximate Inference: Sampling

- Exact inference becomes impossible when we have hundreds of variables
- **Monte Carlo:** Sampling from *known* probability distribution to estimate *unknown* distribution
- The more samples we get, the better the accuracy
- We can sample the variables in topological order according to each conditional probability table



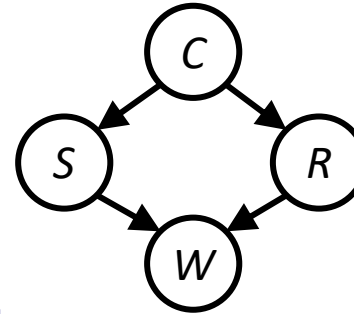
Ordering: C, S, R, W

1. Sample C using $P(C)$
2. Sample S using $P(S|c)$
3. Sample R using $P(R|c)$
4. Sample W using $P(W|s, r)$

Ordering C, R, S, W also works

Prior Sampling

- Inferences can be computed by counting samples corresponding to the query
- Prior sampling is **consistent**
- Probability that an event is generated equal to the true probability



Suppose we get 5 samples:

- (+c, -s, +r, +w)
- (+c, +s, +r, +w)
- (-c, +s, +r, -w)
- (+c, -s, +r, +w)
- (-c, -s, -r, +w)

$$\prod_{i=1}^n P(X_i | \text{parents}(X_i))$$

- Proportion of an event in samples approaches true probability in large-sample limit

$\hat{P}(R)$

| | |
|----|-----|
| +r | 0.8 |
| -r | 0.2 |

$\hat{P}(C, W)$

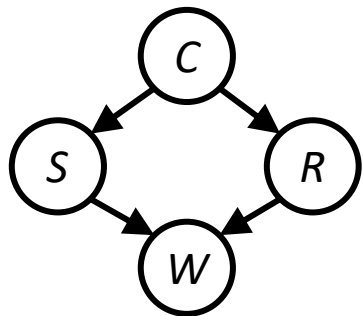
| | | |
|----|----|-----|
| +c | +w | 0.6 |
| | -w | 0 |
| -c | +w | 0.2 |
| | -w | 0.2 |

$\hat{P}(S|W)$

| | | |
|----|----|------|
| +w | +s | 0.25 |
| | -s | 0.75 |
| -w | +s | 1 |
| | -s | 0 |

Rejection Sampling

- Counting samples can be done online instead of all at the end
- If query contains evidence, many samples may be irrelevant
- E.g., want $P(A|+b)$, all samples with $-b$ are useless to us!
- Idea: Discard irrelevant samples as they come and only count *consistent* ones



1. $(+c, -s, +r, +w)$
2. $(+c, +s, +r, +w)$
3. $(-c, +s, +r, -w)$
4. $(+c, -s, +r, +w)$
5. $(-c, -s, -r, +w)$

$$P(C|+s)$$

| | |
|----|-----|
| +c | 0.5 |
| -c | 0.5 |

Reject 1, 4, 5

$$P(R|-c)$$

| | |
|----|-----|
| +r | 0.5 |
| -r | 0.5 |

Reject 1, 2, 4

$$P(S|+r, +w)$$

| | |
|----|-----|
| +s | 0.3 |
| -s | 0.7 |

Reject 3, 5

Rejection Sampling

```
initialize  $C = 0$ , vector of counts for values of query variable  $X$   
for  $i = 1:N$  (number of samples requested)  
    sample  $s$  via prior sampling from the Bayes net  
    if  $s$  is consistent with evidence  $e$ :  
         $C[j] \leftarrow C[j] + 1$  where  $X = j$  in  $s$   
return  $\text{normalize}(C)$ 
```

- Problem: Lots of potentially wasted work due to rejected samples!
- Fraction of accepted samples = probability of evidence
- With more evidence variables, fraction of consistent samples drops *exponentially*
- Need to wait a long time for rare evidence to occur

Likelihood Weighting

```
initialize  $W = 0$ , vector of counts for values of query variable  $X$ 
for  $i = 1:N$ 
    sample  $s$  while fixing evidence variables  $e$ 
     $w \leftarrow \prod_{e_i} P(e_i | \text{parents}(E_i))$  in  $s$ 
     $W[j] \leftarrow W[j] + w$  where  $X = j$  in  $s$ 
return normalize( $C$ )
```

- Idea: **Fix** evidence variables to the values that we want
- Compensate by **weighting** each sample using probability of evidence given parents
- Weights are *cumulative products* for each evidence variable

Example: Likelihood Weighting

- We want $P(C, R \mid +s, +w)$

- Fix $+s$ and $+w$; sample all other variables

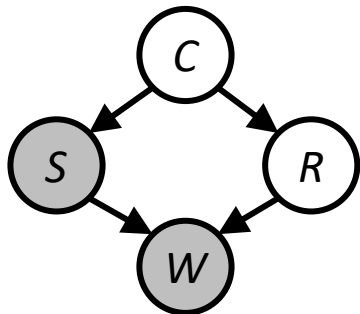
- Each sample has a weight given by

$$P(+s \mid \text{parents}(S))P(+w \mid \text{parents}(W)) \\ = P(+s \mid c)P(+w \mid +s, r)$$

| C | $P(+s \mid C)$ |
|----|----------------|
| +c | 0.1 |
| -c | 0.5 |

| R | $P(+w \mid +s, R)$ |
|----|--------------------|
| +r | 0.99 |
| -r | 0.90 |

- When counting, **sum up the weights of each sample**, and then normalize



- $(+c, +s, +r, +w)$ $0.1 \times .99 = .099$
- $(+c, +s, -r, +w)$ $0.1 \times .99 = .099$
- $(+c, +s, -r, +w)$ $0.1 \times 0.9 = 0.09$
- $(-c, +s, -r, +w)$ $0.5 \times 0.9 = 0.45$

$$\hat{P}(C, R, +s, +w) \quad \hat{P}(C, R \mid +s, +w)$$

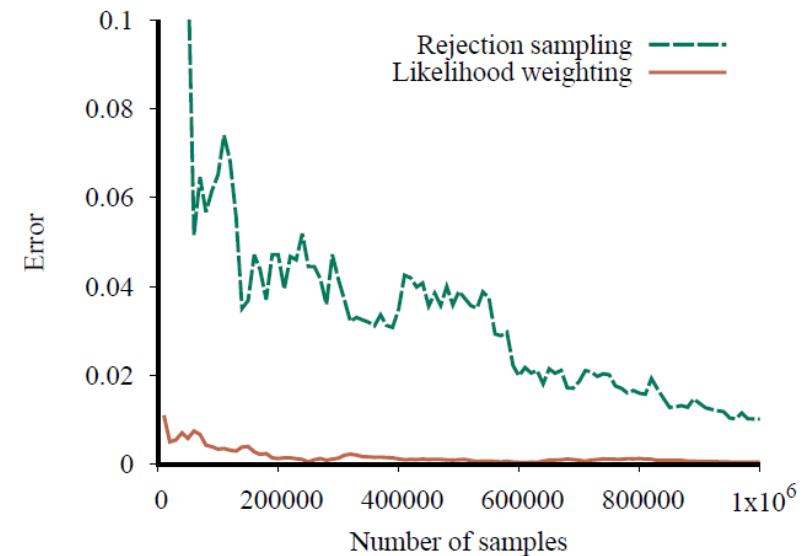
| | | |
|----|----|-------|
| +c | +r | 0.198 |
| | -r | 0.09 |
| -c | +r | 0 |
| | -r | 0.45 |

\propto

| | | |
|----|----|-------|
| +c | +r | 0.268 |
| | -r | 0.122 |
| -c | +r | 0 |
| | -r | 0.610 |

Importance Sampling*

- Likelihood weighting is an example of **importance sampling**: Use *sampling distribution* g and a correction factor to simulate sampling from *target distribution* f
- f is too hard to sample from, so use g instead
- For a sample x , correction factor is the *weight* $f(x)/g(x)$
- This works no matter what g we use!
- Much more efficient than rejection sampling
- Can get good accuracies with fewer samples



Likelihood Weighting Consistency*

- When performing inference in a Bayes net, the target distribution is $f(\mathbf{z}) = P(\mathbf{z}|\mathbf{e})$, where \mathbf{Z} are nonevidence variables
- Sampling distribution is $Q(\mathbf{z}) = \prod_i P(z_i|\text{parents}(Z_i))$ (how we generate samples)

- Sample weight is as follows:

$$w(\mathbf{z}) = \frac{f(\mathbf{z})}{g(\mathbf{z})} = \frac{P(\mathbf{z}|\mathbf{e})}{Q(\mathbf{z})} \propto \frac{P(\mathbf{z}, \mathbf{e})}{Q(\mathbf{z})} = \frac{\prod_i P(z_i|\text{parents}(Z_i)) \prod_j P(e_j|\text{parents}(E_j))}{\prod_i P(z_i|\text{parents}(Z_i))}$$

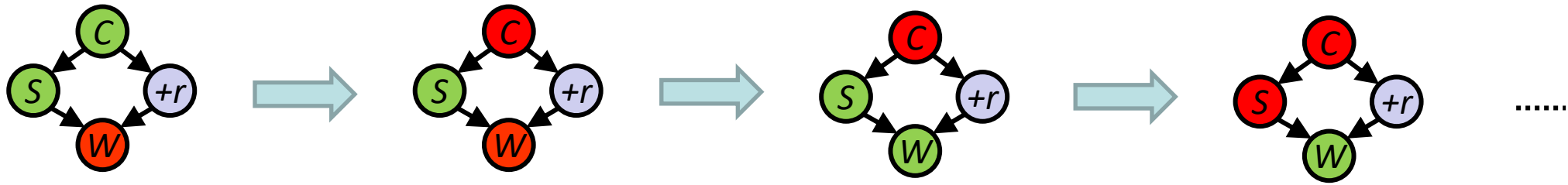
- Likelihood weights each sample by $\prod_j P(e_j|\text{parents}(E_j))$ and normalizes the counts at the end, so our estimates are consistent!

Sampling as Local Search

- Drawback of likelihood weighting: With lots of evidence, weights become small and tallies are dominated by a few samples with larger weights
- Another problem: Evidence variables “downstream” from their parents cannot influence the generation of their values
- How can we “condition” on both ancestors as well as descendants?
- Idea: Instead of generating each new sample from scratch, make small change to current one (just like local search!)

Gibbs Sampling

- **Gibbs sampling:** Fix evidence e and randomly sample non-evidence variables \mathbf{Z} . Then repeatedly choose and sample a variable Z_i conditioned on the *current* sample.
- Example: Evidence $+r$. Start (randomly) with $(+c, -w, +r)$ and sample S .



Sample from
 $P(S \mid +c, +r, -w)$
and obtain $+s$

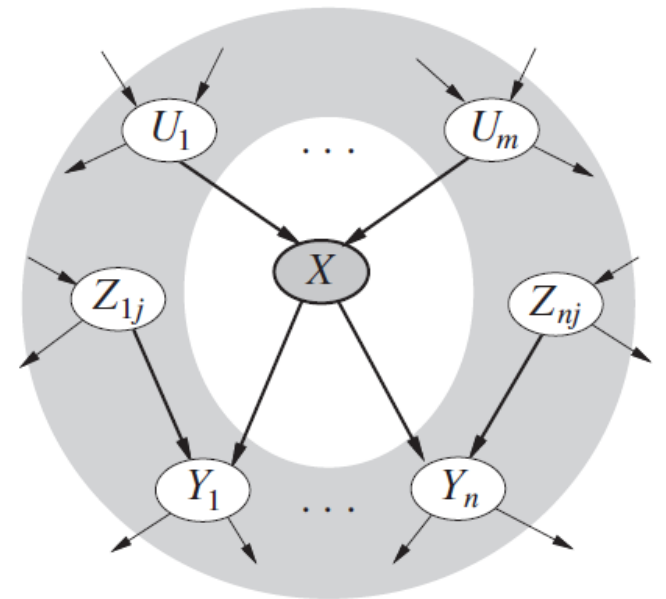
Sample from
 $P(C \mid +s, +r, -w)$
and obtain $-c$

Sample from
 $P(W \mid -c, +s, +r)$
and obtain $+w$

Sample from
 $P(S \mid -c, +r, +w)$
and obtain $-s$

Markov Blanket

- Problem: How do we sample from $P(X_i \mid \text{all other nodes in the BN})$?
- We actually only have to worry about a smaller subset of nodes
- A RV is conditionally independent of all other nodes given its **Markov blanket**: parents, children, children's parents
- Parents(X) *block* causal chains and common causes
- Children(X) *enable* common effects, but...
- Parents(Y_i) again block causal chains and common causes

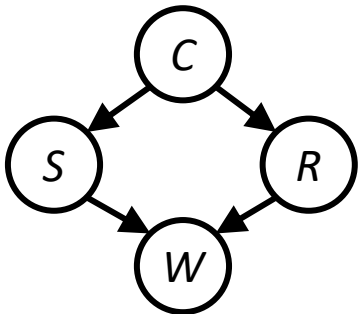


Gibbs Sampling

- To sample from $P(X_i | mb(X_i))$, find the joint distribution and normalize
- All variables in $mb(X_i)$ are fixed, so easy to compute analytically
- Size is $O(|X_i|)$

$$P(x'_i | mb(X_i)) = \alpha P(x'_i | parents(X_i)) \times \prod_{Y_j \in Children(X_i)} P(y_j | parents(Y_j))$$

- Examples:



$$P(C | s, r, w) = P(C | s, r) \propto P(C)P(s|C)P(r|C)$$

$$P(S | c, r, w) \propto P(c)P(S|c)P(r|c)P(w|S, r) \propto P(S|c)P(w|S, r)$$

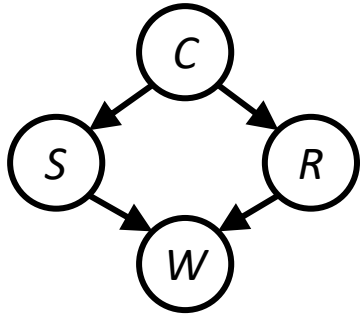
$$P(R | c, s, w) \propto P(c)P(s|c)P(R|c)P(w|s, R) \propto P(R|c)P(w|s, R)$$

$$P(W | c, s, r) = P(W | s, r)$$

Example: Gibbs Sampling

| C | P(+s C) |
|----|---------|
| +c | 0.1 |
| -c | 0.5 |

| C | P(C) |
|----|------|
| +c | 0.5 |



| C | P(+r C) |
|----|---------|
| +c | 0.8 |
| -c | 0.2 |

| S | R | P(+w S,R) |
|----|----|-----------|
| +s | +r | 0.99 |
| +s | -r | 0.90 |
| -s | +r | 0.90 |
| -s | -r | 0 |

$$P(S \mid +c, +r, -w) \propto P(S|+c)P(-w|S, +r)$$

| S | P(S,+c+r,-w) |
|----|--------------|
| +s | 0.001 |
| -s | 0.09 |

=

| S | P(S +c) |
|----|---------|
| +s | 0.1 |
| -s | 0.9 |

×

| S | P(-w S,+r) |
|----|------------|
| +s | 0.01 |
| -s | 0.1 |

$$P(C \mid +s, +r, -w) \propto P(C)P(+s|C)P(+r|C)$$

| C | P(C,+s,+r) |
|----|------------|
| +c | 0.04 |
| -c | 0.05 |

=

| C | P(C) |
|----|------|
| +c | 0.5 |
| -c | 0.5 |

×

| C | P(+s C) |
|----|---------|
| +c | 0.1 |
| -c | 0.5 |

×

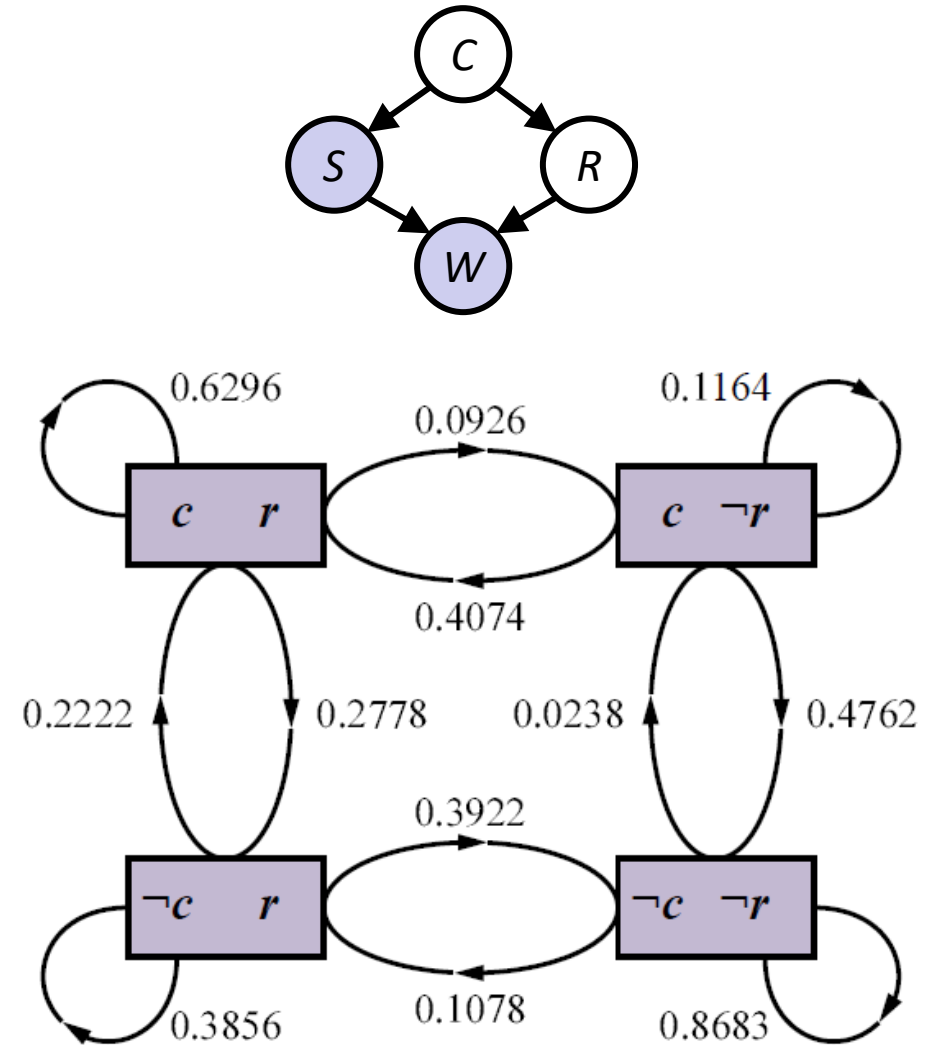
| C | P(+r C) |
|----|---------|
| +c | 0.8 |
| -c | 0.2 |

$$P(W \mid -c, +s, +r) = P(W \mid +s, +r)$$

| W | P(W +s,+r) |
|----|------------|
| +w | 0.99 |
| -w | 0.01 |

Markov Chain Monte Carlo

- Gibbs sampling is a **Markov chain Monte Carlo (MCMC)** method
- Traverses a Markov chain in the space of RVs
- Transition probabilities are the *likelihoods* of obtaining a sample given its predecessor
- The posterior distribution of the BN, conditioned on the evidence, is the *stationary distribution* of this Markov chain
- This is exactly what we want!



Gibbs Sampling Performance

- Each sampling step only depends on a node's immediate neighbors
- Good news: Independent of network size
- Generally performs better than likelihood weighting when evidence is “downstream”
- Information from evidence propagates outward in all directions
- However, convergence (**mixing rate**) is sensitive to the relationships among the RVs
- If certain states are hard to reach (low transition probabilities), then convergence can take a long time—same issues as in local search!

Metropolis-Hastings Sampling*

- Idea: As in local search algorithms like simulated annealing, sample locally *most* of the time, but occasionally allow for *jumps* to other part of the state space
- This can be specified by a **proposal distribution** $q(x' | x)$
- Ex: With small probability ε , generate sample x' using likelihood weighting (jump); otherwise, generate x' via Gibbs sampling
- But not all samples are good candidates, especially when jumping around
- Should only accept samples from the proposal according to their likelihood
- Otherwise, reject it (and stay put)

Acceptance Probability*

- Although we can use any arbitrary proposal $q(x'|x)$, let's restrict ourselves to *symmetric* distributions only: $q(x'|x) = q(x|x')$
- Equally likely to go from x' to x as it is to go from x to x' , e.g. uniform distributions
- Suppose current sample is x ; we sample x' according to proposal q and compute the **acceptance probability**:

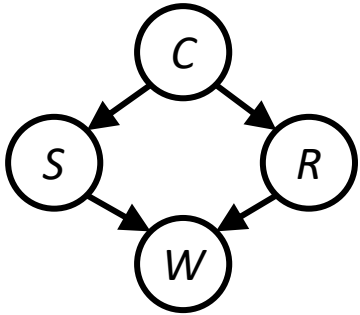
$$a(x'|x) = \min\left(1, \frac{P(x', e)}{P(x, e)}\right)$$

- If x' is more likely than x , accept it
- If x' is less likely than x , accept it with probability given by their likelihood ratios
- If x' is rejected, then new sample is x again (stay put)

Example: MH Sampling*

| C | P(+s C) |
|----|---------|
| +c | 0.1 |
| -c | 0.5 |

| C | P(C) |
|----|------|
| +c | 0.5 |



| C | P(+r C) |
|----|---------|
| +c | 0.8 |
| -c | 0.2 |

| S | R | P(+w S,R) |
|----|----|-----------|
| +s | +r | 0.99 |
| +s | -r | 0.90 |
| -s | +r | 0.90 |
| -s | -r | 0 |

- Current sample: $x = (+c, +s, +r, -w)$
- Proposed sample: $x' = (+c, -s, +r, -w)$
- Acceptance ratio: $\frac{P(x')}{P(x)} = \frac{(0.5)(0.9)(0.8)(0.1)}{(0.5)(0.1)(0.8)(0.01)} = 90$
- x' is much more likely than x , so accept
- Current sample: $x = (+c, -s, +r, -w)$
- Proposed sample: $x' = (-c, +s, +r, -w)$
- Acceptance ratio: $\frac{P(x')}{P(x)} = \frac{(0.5)(0.5)(0.2)(0.01)}{(0.5)(0.9)(0.8)(0.1)} = 0.035$
- x' is very unlikely to occur; most likely reject

MH Properties*

- The form of the acceptance probability ensures that the underlying Markov chain has a stationary distribution (just like in Gibbs)
- Convergence is guaranteed for any choice of (symmetric) proposal distribution
- Gibbs is just special case of MH in which proposals are always accepted
- Computation of acceptance probability can be optimized
- Since samples usually only change locally, most of the terms can be reused
- Ex: $P(x')$ becomes $P(x)$ in the next acceptance probability

More Sampling Applications*

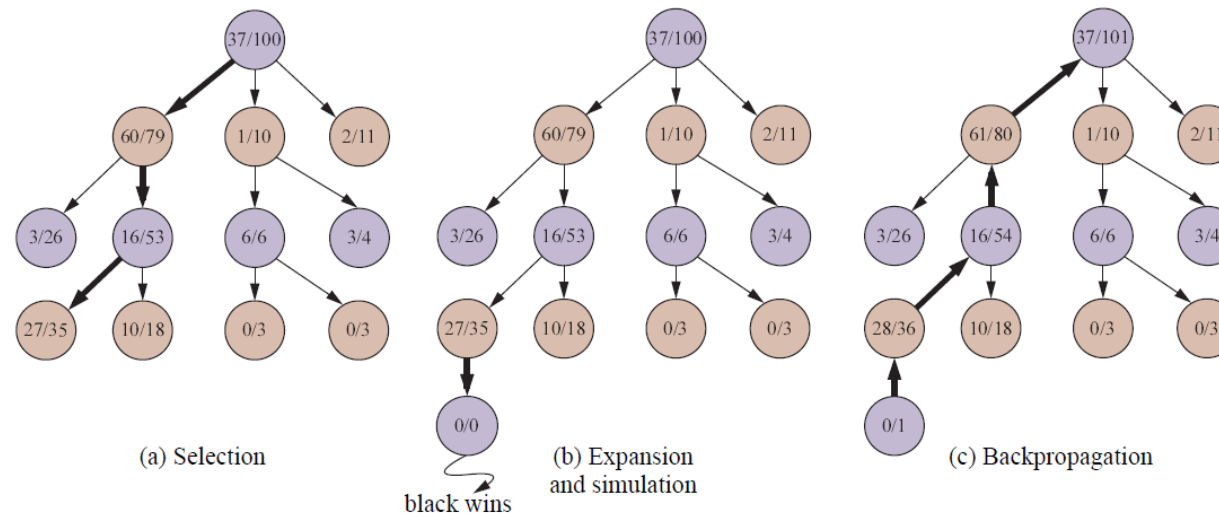
- Where else have we seen Monte Carlo methods before?
- Monte Carlo tree search for games
- Reinforcement learning
- Many problems in which solving for exact solutions is too hard!

Sampling in Games*

- Recall some of the challenges of performing search in game trees
- Huge branching factors, e.g. in games like Go
- Difficult to define good eval functions; most info at the end of the game
- **Monte Carlo tree search:** Instead of using an eval function, a state value is estimated through many simulated playouts from the state to the end of the game
- A *playout policy* may be learned from experience or follow some weak heuristics
- A *selection policy* chooses which states to simulate and play
- As in RL, need to balance exploitation and exploration, e.g. using UCB

Monte Carlo Tree Search*

- Given a current game tree, perform the following steps:
 1. Follow selection policy down to a leaf of the tree
 2. Expand the leaf and simulate a playout to the end of the game
 3. Record and backpropagate the result to all nodes in the simulated path



- After a number of iterations, choose the move with the most playouts

Sampling in Reinforcement Learning*

- We have already discussed using Monte Carlo methods in RL for both prediction (estimate values for a fixed policy) and control (find an optimal policy)
- Control example: Generate many episodes in the MDP following a ϵ -greedy policy
- If we do not decrease ϵ to 0, we may not actually learn a purely greedy optimal policy!
- We have a different behavior (ϵ -greedy) and target (greedy) policy
- How to address this discrepancy?
- Use importance sampling: Weight each sample by the relative likelihoods according to the target and behavior policies

Sampling in HMMs*

- We know how to perform exact state estimation for a general HMM
- This may be computationally intractable for large problems, e.g. robot localization
- **Particle filtering:** Instead of keeping track of exact distributions of belief states, keep track of a number of particles (samples) that estimate the belief state
- Each particle evolves according to transition and sensor models

| | | |
|------|------|------|
| 0.01 | 0.17 | 0.45 |
| 0.08 | 0.03 | 0.21 |
| 0.02 | 0.01 | 0.02 |



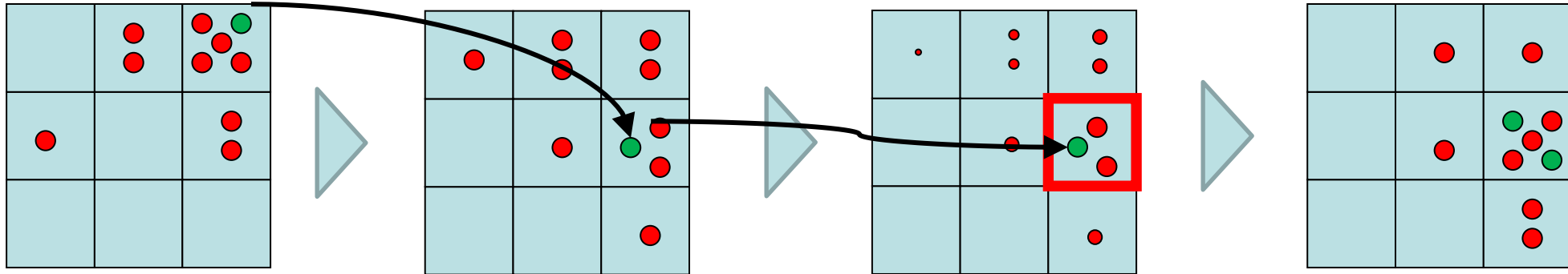
| | | |
|---|--------|------------------|
| | ● ● | ● ● ● ● |
| ● | | ● ● |
| | | |

Particle Filter*

sample $p(x_t | x_{t-1}^j)$

weight $w_t^j = p(z_t | x_t^j)$

Resample
(renormalize):



Particles:

(3,3)
(2,3)
(3,3)
(3,2)
(3,3)
(3,2)
(1,2)
(3,3)
(3,3)
(2,3)

Particles:

(3,2)
(2,3)
(3,2)
(3,1)
(3,3)
(3,2)
(1,3)
(2,3)
(3,2)
(2,2)

Particles:

(3,2) $w=.9$
(2,3) $w=.2$
(3,2) $w=.9$
(3,1) $w=.4$
(3,3) $w=.4$
(3,2) $w=.9$
(1,3) $w=.1$
(2,3) $w=.2$
(3,2) $w=.9$
(2,2) $w=.4$

(New) Particles:

(3,2)
(2,2)
(3,2)
(2,3)
(3,3)
(3,2)
(1,3)
(2,3)
(3,2)
(3,2)

Summary

- Performing inference in Bayes nets involves querying distributions given evidence
- Computationally heavy in large networks with many hidden variables
- Monte Carlo sampling allows us to *estimate* probability distributions
- Direct sampling methods draw samples independently
- Reject inconsistent samples or enforce consistency through likelihood weighting
- MCMC methods (e.g., Gibbs) treat sampling as local search
- Transitions follow a Markov chain; stationary distribution gives us posterior