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- Suppose we have a *biased* coin that comes up heads with some unknown probability p; how can we use it to produce random bits with probabilities of exactly 0.5 for 0 and 1?
- Answer (von Neumann):
  - Flip coin twice, repeat until the outcomes are different
  - HT = 0, TH = 1, each has probability p(1-p)

## CS 188: Artificial Intelligence

#### Bayes Nets: Approximate Inference



Instructors: Stuart Russell and Dawn Song

University of California, Berkeley

# Sampling

- Basic idea
  - Draw N samples from a sampling distribution S
  - Compute an approximate posterior probability
  - Show this converges to the true probability P

- Why sample?
  - Often very fast to get a decent approximate answer
  - The algorithms are very simple and general (easy to apply to fancy models)
  - They require very little memory (O(n))
  - They can be applied to large models, whereas exact algorithms blow up



# Example

- Suppose you have two agent programs A and B for Monopoly
- What is the probability that A wins?
  - Method 1:
    - Let s be a sequence of dice rolls and Chance and Community Chest cards
    - Given s, the outcome V(s) is determined (1 for a win, 0 for a loss)
    - Probability that **A** wins is  $\sum_{s} P(s) V(s)$
    - Problem: infinitely many sequences s !
  - Method 2:
    - Sample N sequences from P(s), play N games (maybe 100)
    - Probability that **A** wins is roughly  $1/N \sum_i V(s_i)$  i.e., fraction of wins in the sample

# Sampling basics: discrete (*categorical*) distribution

- To simulate a biased d-sided coin P(x): Example
  - Step 1: Get sample *u* from uniform distribution over [0, 1)
    - E.g. random() in python
  - Step 2: Convert this sample *u* into an outcome for the given distribution by associating each outcome *x<sub>i</sub>* with a *P(x<sub>i</sub>)*-sized sub-interval of [0,1)

 $0.0 \le u < 0.6, \rightarrow C=red$  $0.6 \le u < 0.7, \rightarrow C=green$  $0.7 \le u < 1.0, \rightarrow C=blue$ 

- If random() returns u = 0.83, then the sample is C = blue
- E.g, after sampling 8 times:



#### Sampling in Bayes nets

- Prior sampling
- Rejection sampling
- Likelihood weighting
- Gibbs sampling

## **Prior sampling**



## **Prior sampling**



# **Prior sampling**

- For *i*=1, 2, ..., *n* (in topological order)
  - Sample X<sub>i</sub> from P(X<sub>i</sub> | parents(X<sub>i</sub>))
- Return (x<sub>1</sub>, x<sub>2</sub>, ..., x<sub>n</sub>)



# **Prior Sampling**

This process generates samples with probability:

 $S_{PS}(x_1,...,x_n) = \prod_i P(x_i \mid parents(X_i)) = P(x_1,...,x_n)$ ...i.e. the BN's joint probability

- Let the number of samples of an event be  $N_{PS}(x_1,...,x_n)$
- Estimate from N samples is  $Q_N(x_1,...,x_n) = N_{PS}(x_1,...,x_n)/N$
- Then  $\lim_{N\to\infty} Q_N(x_1,...,x_n) = \lim_{N\to\infty} N_{PS}(x_1,...,x_n)/N$ =  $S_{PS}(x_1,...,x_n)$ =  $P(x_1,...,x_n)$
- I.e., the sampling procedure is *consistent*

## Example

- We'll get a bunch of samples from the BN:
  - c, ¬s, r, w
  - c, s, r, w
  - ¬−C, S, r, ¬W
  - c, ¬s, r, w
  - ¬−C, ¬¬S, ¬¬r, W
- If we want to know P(W)
  - We have counts <w:4, ¬w:1>
  - Normalize to get *P(W)* = <w:0.8, ¬w:0.2>
  - This will get closer to the true distribution with more samples



#### **Rejection sampling**



# **Rejection sampling**

- A simple application of prior sampling for estimating conditional probabilities
  - Let's say we want  $P(C | r, w) = \alpha P(C, r, w)$
  - For these counts, samples with ¬r or ¬w are not relevant
  - So count the C outcomes for samples with r, w and reject all other samples
- This is called *rejection sampling* 
  - It is also consistent for conditional probabilities (i.e., correct in the limit)





## **Rejection sampling**

- Input: evidence e<sub>1</sub>,...,e<sub>k</sub>
- For i=1, 2, ..., n
  - Sample X<sub>i</sub> from P(X<sub>i</sub> | parents(X<sub>i</sub>))
  - If x<sub>i</sub> not consistent with evidence
    - Reject: Return, and no sample is generated in this cycle
- Return (x<sub>1</sub>, x<sub>2</sub>, ..., x<sub>n</sub>)



#### Car Insurance: *P*(*PropertyCost* | *e*)



#### Likelihood weighting



# Likelihood weighting

- Problem with rejection sampling:
  - If evidence is unlikely, rejects lots of samples
  - Evidence not exploited as you sample
  - Consider P(Shape | Color=blue)

- Idea: fix evidence variables, sample the rest
  - Problem: sample distribution not consistent!
  - Solution: *weight* each sample by probability of evidence variables given parents



#### Likelihood Weighting



# Likelihood weighting

- Input: evidence  $e_1, \dots, e_k$
- *w* = 1.0
- for i=1, 2, ..., n
  - if *X<sub>i</sub>* is an evidence variable
    - x<sub>i</sub> = observed value<sub>i</sub> for X<sub>i</sub>
    - Set  $w = w * P(x_i | parents(X_i))$
  - else
    - Sample x<sub>i</sub> from P(X<sub>i</sub> | parents(X<sub>i</sub>))
- return (x<sub>1</sub>, x<sub>2</sub>, ..., x<sub>n</sub>), w



## Likelihood weighting is consistent

• Sampling distribution if **Z** sampled and **e** fixed evidence  $S_{WS}(\mathbf{z}, \mathbf{e}) = \prod_{j} P(z_j \mid parents(Z_j))$ 

Now, samples have weights

 $w(\mathbf{z}, \mathbf{e}) = \prod_{k} P(e_k \mid parents(E_k))$ 



- Together, weighted sampling distribution is consistent  $S_{WS}(\mathbf{z}, \mathbf{e}) \cdot w(\mathbf{z}, \mathbf{e}) = \prod_{j} P(z_j \mid parents(Z_j)) \prod_{k} P(e_k \mid parents(E_k))$  $= P(\mathbf{z}, \mathbf{e})$
- Likelihood weighting is an example of *importance sampling*
  - Would like to estimate some quantity based on samples from P
  - P is hard to sample from, so use Q instead
  - Weight each sample x by P(x)/Q(x)

#### Car Insurance: *P*(*PropertyCost* | *e*)



# Likelihood weighting

- Likelihood weighting is good
  - All samples are used
  - The values of *downstream* variables are influenced by *upstream* evidence



- Likelihood weighting still has weaknesses
  - The values of *upstream* variables are unaffected by *downstream* evidence
    - E.g., suppose evidence is a video of a traffic accident
  - With evidence in k leaf nodes, weights will be O(2<sup>-k</sup>)
  - With high probability, one lucky sample will have much larger weight than the others, dominating the result
- We would like each variable to "see" all the evidence!

## Quiz

- Suppose I perform a random walk on a graph, following the arcs out of a node *uniformly at random*. In the infinite limit, what fraction of time do I spend at each node?
  - Consider these two examples:



#### Markov Chain Monte Carlo

- MCMC (Markov chain Monte Carlo) is a family of randomized algorithms for approximating some quantity of interest over a very large state space
  - Markov chain = a sequence of randomly chosen states ("random walk"), where each state is chosen conditioned on the previous state
  - Monte Carlo = a very expensive city in Monaco with a famous casino



#### Markov Chain Monte Carlo

- MCMC (Markov chain Monte Carlo) is a family of randomized algorithms for approximating some quantity of interest over a very large state space
  - Markov chain = a sequence of randomly chosen states ("random walk"), where each state is chosen conditioned on the previous state
  - Monte Carlo = a very expensive city in Monaco with a famous casino
  - Monte Carlo = an algorithm (usually based on sampling) that has some probability of producing an incorrect answer
- MCMC = wander around for a bit, average what you see

# Gibbs sampling

#### A particular kind of MCMC

- States are complete assignments to all variables
  - (Cf local search: closely related to simulated annealing!)
- Evidence variables remain fixed, other variables change
- To generate the next state, pick a variable and sample a value for it conditioned on all the other variables:  $X'_i \sim P(X_i \mid x_1, ..., x_{i-1}, x_{i+1}, ..., x_n)$ 
  - Will tend to move towards states of higher probability, but can go down too
  - In a Bayes net,  $P(X_i | x_1, ..., x_{i-1}, x_{i+1}, ..., x_n) = P(X_i | markov_blanket(X_i))$

#### Theorem: Gibbs sampling is consistent\*

Provided all Gibbs distributions are bounded away from 0 and 1 and variable selection is fair

## Advantages of MCMC



Samples soon begin to reflect all the evidence in the network

Eventually they are being drawn from the true posterior!

#### Car Insurance: *P*(*PropertyCost* | *e*)



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# Gibbs sampling algorithm

- Repeat many times
  - Sample a non-evidence variable X<sub>i</sub> from
  - $P(X_i | x_1, ..., x_{i-1}, x_{i+1}, ..., x_n) = P(X_i | markov_blanket(X_i))$ 
    - =  $\alpha P(X_i \mid parents(X_i)) \prod_j P(y_j \mid parents(Y_j))$



# Gibbs Sampling Example: P(S | r)

- Step 1: Fix evidence
  - *R* = true



- Step 2: Initialize other variables
  - Randomly



- Step 3: Repeat
  - Choose a non-evidence variable X
  - Resample X from P(X | markov\_blanket(X))



Sample  $S \sim P(S \mid c, r, \neg w)$ 

Sample  $C \sim P(C \mid s, r)$ 

Sample  $W \sim P(W \mid s, r)$ 

#### Markov chain given s, w



# Gibbs sampling and MCMC in practice

- The most commonly used method for large Bayes nets
  - See, e.g., BUGS, JAGS, STAN, infer.net, BLOG, etc.
- Can be <u>compiled</u> to run very fast
  - Eliminate all data structure references, just multiply and sample
  - ~100 million samples per second on a laptop
- Can run asynchronously in parallel (one processor per variable)
- Many cognitive scientists suggest the brain runs on MCMC

## Consistency of Gibbs (see AIMA 13.4.2 for details)

- Suppose we run it for a long time and predict the probability of reaching any given state at time  $t: \pi_t(x_1, ..., x_n)$  or  $\pi_t(\underline{x})$
- Each Gibbs sampling step (pick a variable, resample its value) applied to a state <u>x</u> has a probability k(<u>x' | x</u>) of reaching a next state <u>x'</u>
- So  $\pi_{t+1}(\underline{\mathbf{x'}}) = \sum_{\mathbf{x}} k(\underline{\mathbf{x'}} | \underline{\mathbf{x}}) \pi_t(\underline{\mathbf{x}})$  or, in matrix/vector form  $\pi_{t+1} = \mathbf{K}\pi_t$
- When the process is in equilibrium  $\pi_{t+1} = \pi_t = \pi$  so  $K\pi = \pi$
- This has a unique\* solution  $\pi = P(x_1, ..., x_n | e_1, ..., e_k)$ 
  - \* Markov chain must be *ergodic*, i.e., completely connected and aperiodic
  - Satisfied if all probabilities are bounded away from 0 and 1
- So for large enough t the next sample will be drawn from the true posterior
  - "Large enough" depends on CPTs in the Bayes net; takes *longer* if nearly deterministic

# **Bayes Net Sampling Summary**

- Prior Sampling P :
  - Generate complete samples from P(x1,...,xn)



- Likelihood Weighting P(Q | e):
  - Weight samples by how well they predict *e*



- Rejection Sampling P(Q | e):
  - Reject samples that don't match *e*



- Gibbs sampling P(Q | e) :
  - Wander around in *e* space
  - Average what you see