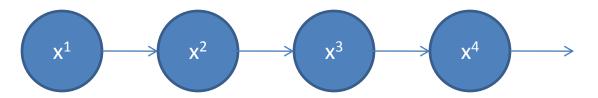
Sampling Techniques for Probabilistic and Deterministic Graphical models

ICS 276, Fall 2014
Bozhena Bidyuk
Rina Dechter

Overview

- 1. Probabilistic Reasoning/Graphical models
- 2. Importance Sampling
- 3. Markov Chain Monte Carlo: Gibbs Sampling
- 4. Sampling in presence of Determinism
- 5. Rao-Blackwellisation
- 6. AND/OR importance sampling

Markov Chain



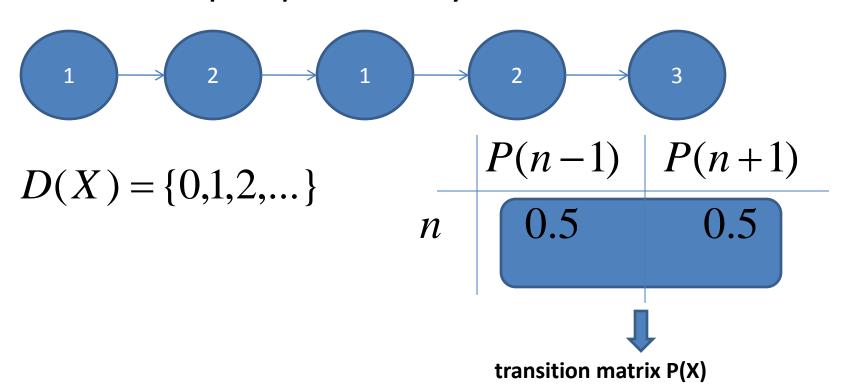
 A Markov chain is a discrete random process with the property that the next state depends only on the current state (Markov Property):

$$P(x^{t} | x^{1}, x^{2}, ..., x^{t-1}) = P(x^{t} | x^{t-1})$$

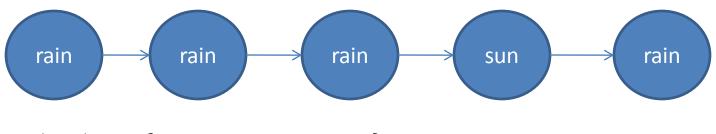
• If $P(X^t|x^{t-1})$ does not depend on t (time homogeneous) and state space is finite, then it is often expressed as a transition function (aka transition matrix) $\sum P(X = x) = 1$

Example: Drunkard's Walk

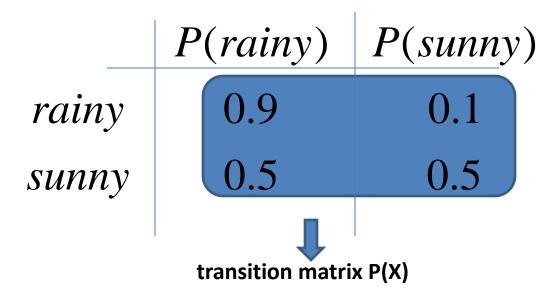
 a random walk on the number line where, at each step, the position may change by +1 or
 –1 with equal probability



Example: Weather Model



$$D(X) = \{rainy, sunny\}$$

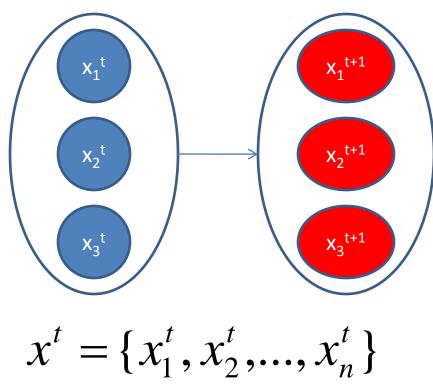


Multi-Variable System

$$X = \{X_{1}, X_{2}, X_{3}\}, D(X_{i}) = discrete, finite$$

state is an assignment of values to all the

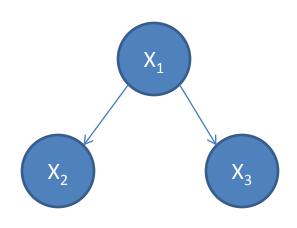
variables



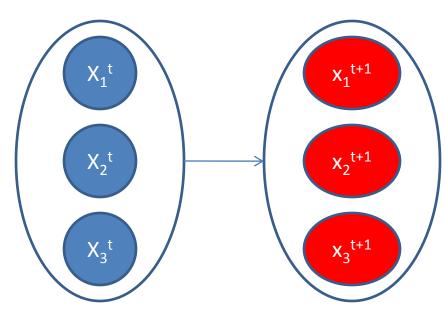
Bayesian Network System

 Bayesian Network is a representation of the joint probability distribution over 2 or more

variables



$$X = \{X_1, X_2, X_3\}$$



$$x^{t} = \{x_1^{t}, x_2^{t}, x_3^{t}\}$$

Stationary Distribution Existence

• If the Markov chain is time-homogeneous, then the vector $\pi(X)$ is a *stationary* distribution (aka *invariant* or *equilibrium* distribution, aka "fixed point"), if its entries sum up to 1 and satisfy:

 $\pi(x_i) = \sum_{x_i \in D(X)} \pi(x_j) P(x_i \mid x_j)$

- Finite state space Markov chain has a unique stationary distribution if and only if:
 - The chain is irreducible
 - All of its states are positive recurrent

Irreducible

- A state χ is *irreducible* if under the transition rule one has nonzero probability of moving from χ to any other state and then coming back in a finite number of steps
- If one state is irreducible, then all the states must be irreducible

(Liu, Ch. 12, pp. 249, Def. 12.1.1)

Recurrent

- A state χ is *recurrent* if the chain returns to χ with probability 1
- Let M(x) be the expected number of steps to return to state x
- State χ is *positive recurrent* if $M(\chi)$ is finite The recurrent states in a finite state chain are positive recurrent.

Stationary Distribution Convergence

Consider infinite Markov chain:

$$P^{(n)} = P(x^n \mid x^0) = P^0 P^n$$

 If the chain is both *irreducible* and *aperiodic*, then:

$$\pi = \lim_{n \to \infty} P^{(n)}$$

• Initial state is not important in the limit "The most useful feature of a "good" Markov chain is its fast forgetfulness of its past..."

(Liu, Ch. 12.1)

Aperiodic

- Define d(i) = g.c.d.{n > 0 | it is possible to go from i to i in n steps}. Here, g.c.d. means the greatest common divisor of the integers in the set. If d(i)=1 for ∀i, then chain is aperiodic
- Positive recurrent, aperiodic states are ergodic

Markov Chain Monte Carlo

- How do we estimate P(X), e.g., P(X|e)?
- Generate samples that form Markov Chain with stationary distribution $\pi = P(X|e)$
- Estimate π from samples (observed states): visited states $x^0,...,x^n$ can be viewed as "samples" from distribution π

$$\overline{\pi}(x) = \frac{1}{T} \sum_{t=1}^{T} \delta(x, x^{t})$$

$$\pi = \lim_{T \to \infty} \overline{\pi}(x)$$

MCMC Summary

- Convergence is guaranteed in the limit
- Initial state is not important, but... typically, we throw away first K samples - "burn-in"
- Samples are dependent, not i.i.d.
- Convergence (mixing rate) may be slow
- The stronger correlation between states, the slower convergence!

Gibbs Sampling (Geman&Geman,1984)

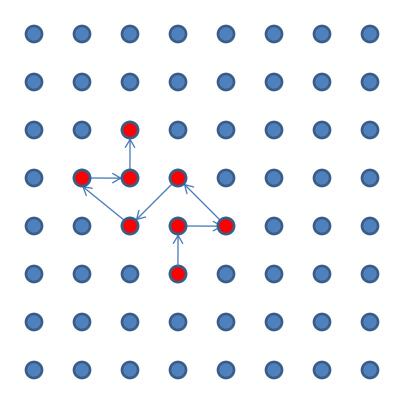
- Gibbs sampler is an algorithm to generate a sequence of samples from the joint probability distribution of two or more random variables
- Sample new variable value one variable at a time from the variable's conditional distribution:

$$P(X_i) = P(X_i \mid x_1^t, ..., x_{i-1}^t, x_{i+1}^t, ..., x_n^t) = P(X_i \mid x^t \setminus x_i)$$

• Samples form a Markov chain with stationary distribution P(X|e)

Gibbs Sampling: Illustration

The process of Gibbs sampling can be understood as a *random walk* in the space of all instantiations of X=x (remember drunkard's walk):



In one step we can reach instantiations that differ from current one by value assignment to at most one variable (assume randomized choice of variables X_i).

Ordered Gibbs Sampler

Generate sample x^{t+1} from x^t :

Process
All
Variables
In Some
Order

$$X_{1} = x_{1}^{t+1} \leftarrow P(X_{1} \mid x_{2}^{t}, x_{3}^{t}, ..., x_{N}^{t}, e)$$

$$X_{2} = x_{2}^{t+1} \leftarrow P(X_{2} \mid x_{1}^{t+1}, x_{3}^{t}, ..., x_{N}^{t}, e)$$

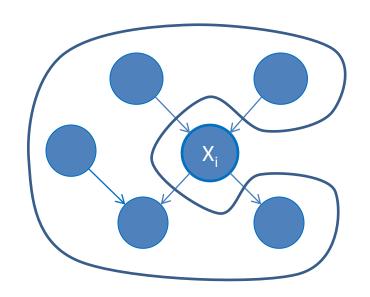
$$...$$

$$X_{N} = x_{N}^{t+1} \leftarrow P(X_{N} \mid x_{1}^{t+1}, x_{2}^{t+1}, ..., x_{N-1}^{t+1}, e)$$

In short, for i=1 to N:

$$X_i = x_i^{t+1} \leftarrow \text{sampled from } P(X_i \mid x^t \setminus x_i, e)$$

Transition Probabilities in BN



Given *Markov blanket* (parents, children, and their parents), X_i is independent of all other nodes

Markov blanket:

$$markov(X_i) = pa_i \bigcup ch_i \bigcup (\bigcup_{X_i \in ch_i} pa_j)$$

$$P(X_i | x^t \setminus x_i) = P(X_i | markov_i^t)$$
:

$$P(x_i \mid x^t \setminus x_i) \propto P(x_i \mid pa_i) \prod_{X_j \in ch_i} P(x_j \mid pa_j)$$

Computation is linear in the size of Markov blanket!

Ordered Gibbs Sampling Algorithm (Pearl, 1988)

Input: *X, E=e*

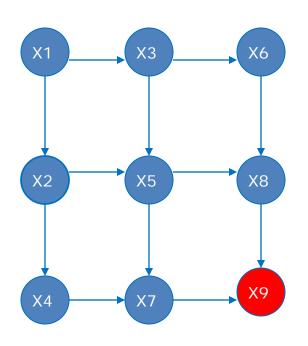
Output: T samples {x^t}

Fix evidence E=e, initialize x^0 at random

- 1. For t = 1 to T (compute samples)
- For i = 1 to N (loop through variables)
- 3. $x_i^{t+1} \leftarrow P(X_i \mid markov_i^t)$
- 4. End For
- 5. End For

Gibbs Sampling Example - BN

$$X = \{X_1, X_2, ..., X_9\}, E = \{X_9\}$$



$$X_1 = X_1^0$$

$$X_6 = X_6^0$$

$$\mathbf{X}_2 = \mathbf{x}_2^0$$

$$X_7 = X_7^0$$

$$\mathbf{X}_3 = \mathbf{x}_3^0$$

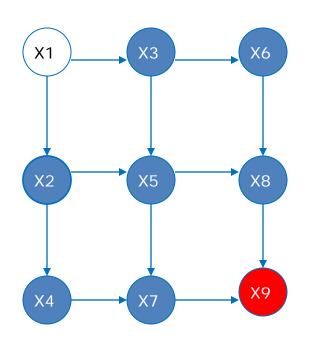
$$X_8 = X_8^0$$

$$X_4 = X_4^0$$

$$\mathbf{X}_5 = \mathbf{x}_5^0$$

Gibbs Sampling Example - BN

$$X = \{X_1, X_2, ..., X_9\}, E = \{X_9\}$$



$$x_1^1 \leftarrow P(X_1 \mid x_2^0, ..., x_8^0, x_9)$$

$$x_2^1 \leftarrow P(X_2 \mid x_1^1, ..., x_8^0, x_9)$$

. . .

Answering Queries $P(x_i | e) = ?$

• **Method 1**: count # of samples where $X_i = x_i$ (histogram estimator):

$$\overline{P}(X_i = x_i) = \frac{1}{T} \sum_{t=1}^{T} \delta(x_i, x^t)$$
 Dirac delta f-n

• **Method 2**: average probability (*mixture estimator*):

$$\overline{P}(X_i = x_i) = \frac{1}{T} \sum_{t=1}^{T} P(X_i = x_i | markov_i^t)$$

 Mixture estimator converges faster (consider estimates for the unobserved values of X_i; prove via Rao-Blackwell theorem)

Rao-Blackwell Theorem

Rao-Blackwell Theorem: Let random variable set X be composed of two groups of variables, R and L. Then, for the joint distribution $\pi(R,L)$ and function g, the following result applies

$$Var[E\{g(R) | L\} \le Var[g(R)]$$

for a function of interest g, e.g., the mean or covariance (Casella&Robert, 1996, Liu et. al. 1995).

- theorem makes a weak promise, but works well in practice!
- improvement depends the choice of R and L

Importance vs. Gibbs

Gibbs:
$$x^t \leftarrow \hat{P}(X \mid e)$$

$$\hat{P}(X \mid e) \xrightarrow{T \to \infty} P(X \mid e)$$

$$\hat{g}(X) = \frac{1}{T} \sum_{t=1}^{T} g(x^t)$$

Importance: $X^t \leftarrow Q(X \mid e)$

$$\overline{g} = \frac{1}{T} \sum_{t=1}^{T} \frac{g(x^t)P(x^t)}{Q(x^t)}$$

 W_{t}

Gibbs Sampling: Convergence

- Sample from $P(X|e) \rightarrow P(X|e)$
- Converges iff chain is irreducible and ergodic
- Intuition must be able to explore all states:
 - if X_i and X_j are strongly correlated, X_i =0↔ X_j =0, then, we cannot explore states with X_i =1 and X_j =1
- All conditions are satisfied when all probabilities are positive
- Convergence rate can be characterized by the second eigen-value of transition matrix

Gibbs: Speeding Convergence

Reduce dependence between samples (autocorrelation)

- Skip samples
- Randomize Variable Sampling Order
- Employ blocking (grouping)
- Multiple chains

Reduce variance (cover in the next section)

Blocking Gibbs Sampler

- Sample several variables together, as a block
- **Example:** Given three variables X, Y, Z, with domains of size 2, group Y and Z together to form a variable $W=\{Y,Z\}$ with domain size 4. Then, given sample (x^t, y^t, z^t) , compute next sample:

$$x^{t+1} \leftarrow P(X \mid y^t, z^t) = P(w^t)$$
$$(y^{t+1}, z^{t+1}) = w^{t+1} \leftarrow P(Y, Z \mid x^{t+1})$$

- + Can improve convergence greatly when two variables are strongly correlated!
- Domain of the block variable grows exponentially with the #variables in a block!

Gibbs: Multiple Chains

- Generate M chains of size K
- Each chain produces independent estimate P_m :

$$\overline{P}_m(x_i \mid e) = \frac{1}{K} \sum_{t=1}^K P(x_i \mid x^t \setminus x_i)$$

• Estimate $P(x_i|e)$ as average of $P_m(x_i|e)$:

$$\hat{P}(\bullet) = \frac{1}{M} \sum_{i=1}^{M} P_m(\bullet)$$

Treat P_m as independent random variables.

Gibbs Sampling Summary

Markov Chain Monte Carlo method

(Gelfand and Smith, 1990, Smith and Roberts, 1993, Tierney, 1994)

- Samples are dependent, form Markov Chain
- Sample from $\overline{P}(X \mid e)$ which converges to $\overline{P}(X \mid e)$
- Guaranteed to converge when all P > 0
- Methods to improve convergence:
 - Blocking
 - Rao-Blackwellised

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Sampling: Performance

- Gibbs sampling
 - Reduce dependence between samples
- Importance sampling
 - Reduce variance
- Achieve both by sampling a subset of variables and integrating out the rest (reduce dimensionality), aka Rao-Blackwellisation
- Exploit graph structure to manage the extra cost

Smaller Subset State-Space

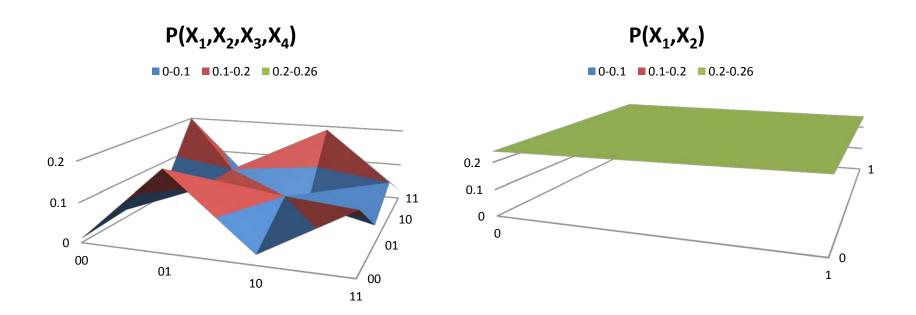
Smaller state-space is easier to cover

$$X = \{X_1, X_2, X_3, X_4\}$$
 $X = \{X_1, X_2\}$

$$D(X) = 64$$

$$D(X) = 16$$

Smoother Distribution



Speeding Up Convergence

Mean Squared Error of the estimator:

$$MSE_{Q}[\overline{P}] = BIAS^{2} + Var_{Q}[\overline{P}]$$

In case of unbiased estimator, BIAS=0

$$MSE_{Q}[\hat{P}] = Var_{Q}[\hat{P}] = \left(E_{Q}[\hat{P}]^{2} - E_{Q}[P]^{2}\right)$$

Reduce variance ⇒ speed up convergence!

Rao-Blackwellisation

$$X = R \bigcup L$$

$$\hat{g}(x) = \frac{1}{T} \{h(x^{1}) + \dots + h(x^{T})\}$$

$$\tilde{g}(x) = \frac{1}{T} \{E[h(x) | l^{1}] + \dots + E[h(x) | l^{T}]\}$$

$$Var\{g(x)\} = Var\{E[g(x) | l]\} + E\{var[g(x) | l]\}$$

$$Var\{\hat{g}(x)\} \ge Var\{E[g(x) | l]\}$$

$$Var\{\hat{g}(x)\} = \frac{Var\{h(x)\}}{T} \ge \frac{Var\{E[h(x) | l]\}}{T} = Var\{\tilde{g}(x)\}$$
Liu, Ch.2.3

Rao-Blackwellisation

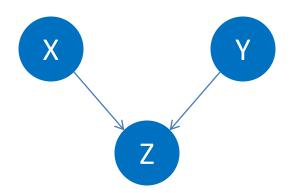
"Carry out analytical computation as much as possible" - Liu

- X=R∪L
- Importance Sampling:

$$Var_{\mathcal{Q}}\left\{\frac{P(R,L)}{Q(R,L)}\right\} \ge Var_{\mathcal{Q}}\left\{\frac{P(R)}{Q(R)}\right\}$$
 Liu, Ch.2.5.5

- Gibbs Sampling:
 - autocovariances are lower (less correlation between samples)
 - if X_i and X_j are strongly correlated, $X_i=0 \leftrightarrow X_j=0$, only include one fo them into a sampling set

Blocking Gibbs Sampler vs. Collapsed



Faster Convergence • Standard Gibbs:

$$P(x | y, z), P(y | x, z), P(z | x, y)$$
 (1)

Blocking:

$$P(x \mid y, z), P(y, z \mid x) \tag{2}$$

• Collapsed:

$$P(x \mid y), P(y \mid x) \tag{3}$$

Collapsed Gibbs Sampling

Generating Samples

Generate sample ct+1 from ct:

$$C_1 = c_1^{t+1} \leftarrow P(c_1 \mid c_2^t, c_3^t, ..., c_K^t, e)$$

$$C_2 = c_2^{t+1} \leftarrow P(c_2 \mid c_1^{t+1}, c_3^t, ..., c_K^t, e)$$

• • •

$$C_K = c_K^{t+1} \leftarrow P(c_K \mid c_1^{t+1}, c_2^{t+1}, ..., c_{K-1}^{t+1}, e)$$

In short, for i=1 to K:

$$C_i = c_i^{t+1} \leftarrow$$
sampled from $P(c_i | c^t \setminus c_i, e)$

Collapsed Gibbs Sampler

- Input: $C \subset X$, E=e
- Output: T samples $\{c^t\}$

Fix evidence E=e, initialize c^0 at random

- 1. For t = 1 to T (compute samples)
- 2. For i = 1 to N (loop through variables)
- 3. $c_i^{t+1} \leftarrow P(C_i \mid c^t \setminus c_i)$
- 4. End For
- 5. End For

Calculation Time

- Computing $P(c_i | c^t \setminus c_i, e)$ is more expensive (requires inference)
- Trading #samples for smaller variance:
 - generate more samples with higher covariance
 - generate fewer samples with lower covariance
- Must control the time spent computing sampling probabilities in order to be timeeffective!

Exploiting Graph Properties

Recall... computation time is exponential in the adjusted induced width of a graph

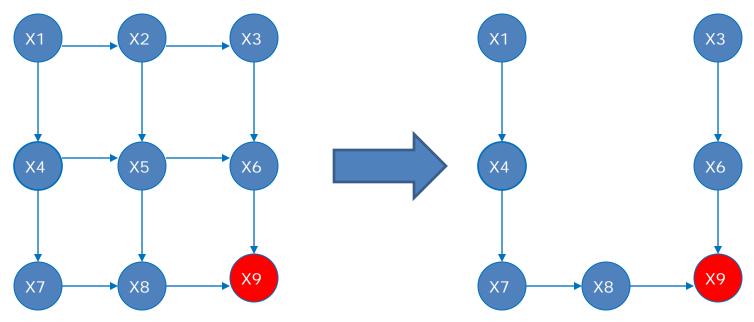
- w-cutset is a subset of variable s.t. when they are observed, induced width of the graph is w
- when sampled variables form a w-cutset, inference is exp(w) (e.g., using Bucket Tree Elimination)
- cycle-cutset is a special case of w-cutset

Sampling w-cutset \Rightarrow w-cutset sampling!

What If C=Cycle-Cutset?

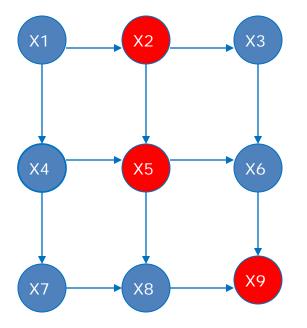
$$c^0 = \{x_2^0, x_5^0\}, E = \{X_9\}$$

 $P(x_2,x_5,x_9)$ – can compute using Bucket Elimination



 $P(x_2,x_5,x_9)$ – computation complexity is O(N)

Computing Transition Probabilities



Compute joint probabilities:

$$BE: P(x_2 = 0, x_3, x_9)$$

$$BE: P(x_2 = 1, x_3, x_9)$$

Normalize:

$$\alpha = P(x_2 = 0, x_3, x_9) + P(x_2 = 1, x_3, x_9)$$

$$P(x_2 = 0 \mid x_3) = \alpha P(x_2 = 0, x_3, x_9)$$

$$P(x_2 = 1 \mid x_3) = \alpha P(x_2 = 1, x_3, x_9)$$

Cutset Sampling-Answering Queries

• Query: $\forall c_i \in C$, $P(c_i \mid e) = ?$ same as Gibbs:

$$\hat{P}(c_i / e) = \frac{1}{T} \sum_{t=1}^{T} P(c_i \mid c^t \setminus c_i, e)$$
computed while generating sample t using bucket tree elimination

• Query: $\forall x_i \in X \setminus C$, $P(x_i \mid e) = ?$

$$\overline{P}(x_i/e) = \frac{1}{T} \sum_{t=1}^{T} P(x_i \mid c^t, e)$$
compute after generating sample t using bucket tree elimination

Cutset Sampling vs. Cutset Conditioning

Cutset Conditioning

$$P(x_i/e) = \sum_{c \in D(C)} P(x_i \mid c, e) \times P(c \mid e)$$

Cutset Sampling

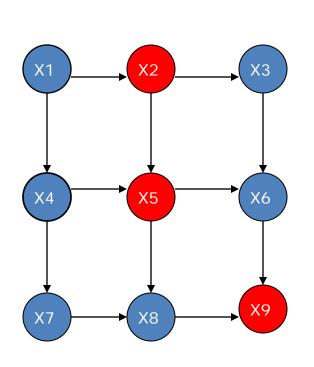
$$\overline{P}(x_i/e) = \frac{1}{T} \sum_{t=1}^{T} P(x_i \mid c^t, e)$$

$$= \sum_{c \in D(C)} P(x_i \mid c, e) \times \frac{count(c)}{T}$$

$$= \sum_{c \in D(C)} P(x_i \mid c, e) \times \overline{P}(c \mid e)$$

Cutset Sampling Example

Estimating $P(x_2|e)$ for sampling node X_2 :



$$x_2^1 \leftarrow P(x_2/x_5^0, x_9)$$
 Sample 1

. . .

$$x_2^2 \leftarrow P(x_2/x_5^1, x_9)$$
 Sample 2

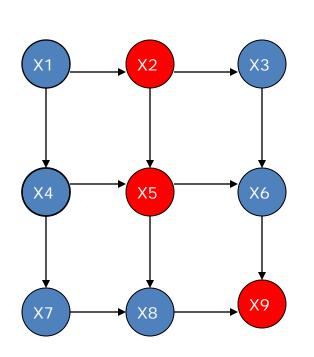
. .

$$x_2^3 \leftarrow P(x_2/x_5^2, x_9)$$
 Sample 3

$$\overline{P}(x_2 \mid x_9) = \frac{1}{3} \begin{bmatrix} P(x_2 \mid x_5^0, x_9) \\ + P(x_2 \mid x_5^1, x_9) \\ + P(x_2 \mid x_5^2, x_9) \end{bmatrix}$$

Cutset Sampling Example

Estimating $P(x_3 | e)$ for non-sampled node X_3 :



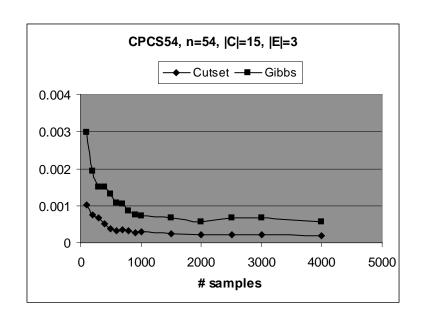
$$c^{1} = \{x_{2}^{1}, x_{5}^{1}\} \Rightarrow P(x_{3} \mid x_{2}^{1}, x_{5}^{1}, x_{9})$$

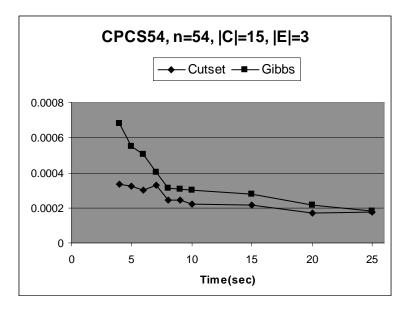
$$c^{2} = \{x_{2}^{2}, x_{5}^{2}\} \Rightarrow P(x_{3} \mid x_{2}^{2}, x_{5}^{2}, x_{9})$$

$$c^{3} = \{x_{2}^{3}, x_{5}^{3}\} \Rightarrow P(x_{3} \mid x_{2}^{3}, x_{5}^{3}, x_{9})$$

$$P(x_3 \mid x_9) = \frac{1}{3} \begin{bmatrix} P(x_3 \mid x_2^1, x_5^1, x_9) \\ + P(x_3 \mid x_2^2, x_5^2, x_9) \\ + P(x_3 \mid x_2^3, x_5^3, x_9) \end{bmatrix}$$

CPCS54 Test Results



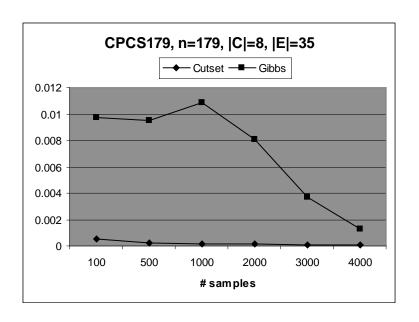


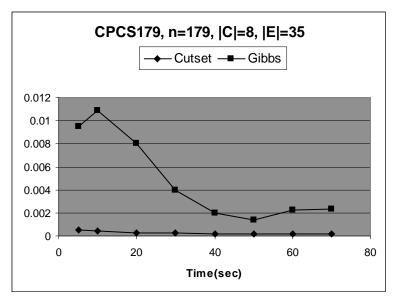
MSE vs. #samples (left) and time (right)

Ergodic, |X| = 54, $D(X_i) = 2$, |C| = 15, |E| = 3

Exact Time = 30 sec using Cutset Conditioning

CPCS179 Test Results

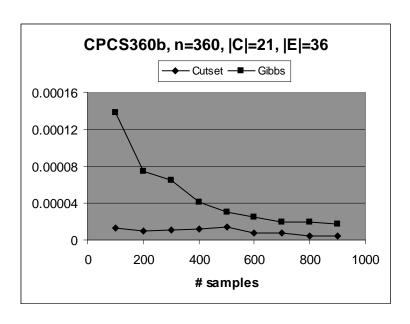


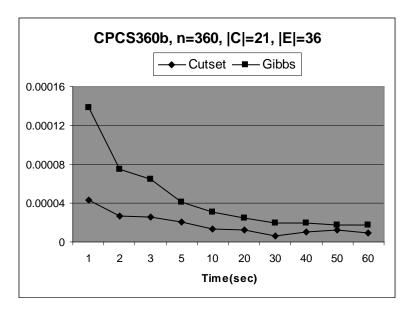


MSE vs. #samples (left) and time (right) Non-Ergodic (1 deterministic CPT entry) |X| = 179, |C| = 8, $2 <= D(X_i) <= 4$, |E| = 35

Exact Time = 122 sec using Cutset Conditioning

CPCS360b Test Results





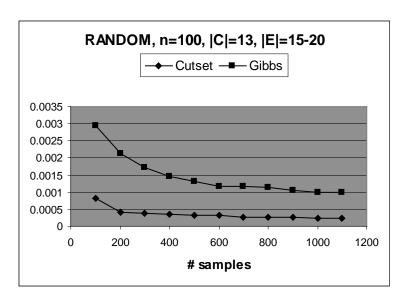
MSE vs. #samples (left) and time (right)

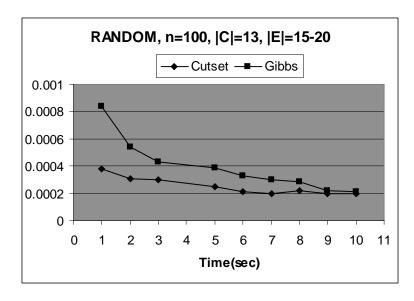
Ergodic, |X| = 360, $D(X_i) = 2$, |C| = 21, |E| = 36

Exact Time > 60 min using Cutset Conditioning

Exact Values obtained via Bucket Elimination

Random Networks





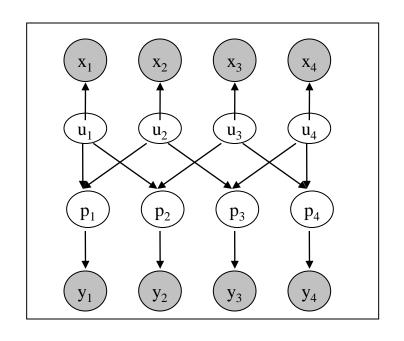
MSE vs. #samples (left) and time (right)

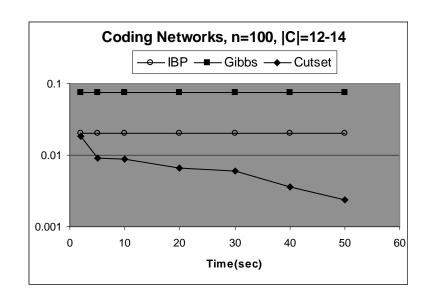
$$|X| = 100$$
, $D(X_i) = 2$, $|C| = 13$, $|E| = 15-20$

Exact Time = 30 sec using Cutset Conditioning

Coding Networks

Cutset Transforms Non-Ergodic Chain to Ergodic





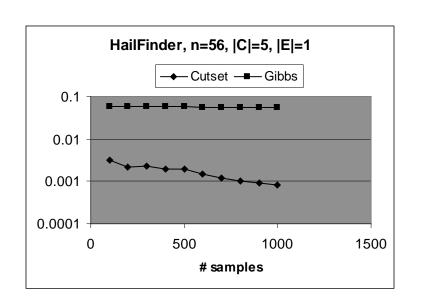
MSE vs. time (right)

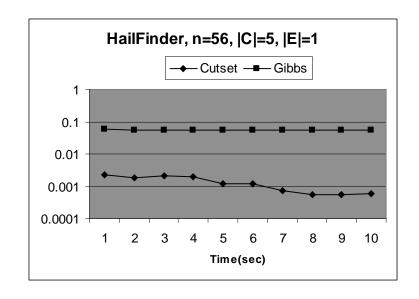
Non-Ergodic, |X| = 100, $D(X_i) = 2$, |C| = 13-16, |E| = 50

Sample Ergodic Subspace $U = \{U_1, U_2, ... U_k\}$

Exact Time = 50 sec using Cutset Conditioning

Non-Ergodic Hailfinder



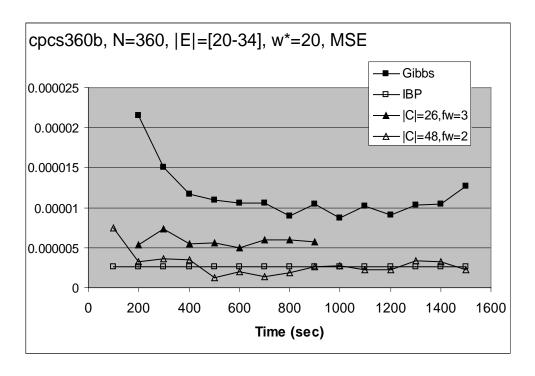


MSE vs. #samples (left) and time (right)

Non-Ergodic, |X| = 56, |C| = 5, $2 <= D(X_i) <= 11$, |E| = 0

Exact Time = 2 sec using Loop-Cutset Conditioning

CPCS360b - MSE



MSE vs. Time

Ergodic, |X| = 360, |C| = 26, $D(X_i) = 2$

Exact Time = 50 min using BTE

Cutset Importance Sampling

(Gogate & Dechter, 2005) and (Bidyuk & Dechter, 2006)

Apply Importance Sampling over cutset C

$$\hat{P}(e) = \frac{1}{T} \sum_{t=1}^{T} \frac{P(c^{t}, e)}{Q(c^{t})} = \frac{1}{T} \sum_{t=1}^{T} w^{t}$$

where $P(c^t,e)$ is computed using Bucket Elimination

$$\overline{P}(c_i \mid e) = \alpha \frac{1}{T} \sum_{t=1}^{T} \delta(c_i, c^t) w^t$$

$$\overline{P}(x_i \mid e) = \alpha \frac{1}{T} \sum_{t=1}^{T} P(x_i \mid c^t, e) w^t$$

Likelihood Cutset Weighting (LCS)

- Z=Topological Order{C,E}
- Generating sample t+1:

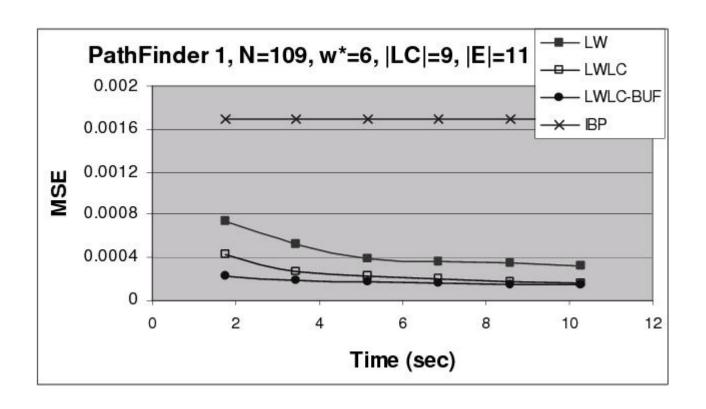
For
$$Z_i \in Z$$
 do: If $Z_i \in E$
$$z_i^{t+1} = z_i, z_i \in e$$
 Else
$$z_i^{t+1} \leftarrow P(Z_i \mid z_1^{t+1}, ..., z_{i-1}^{t+1})$$
 End If

- computed while generating sample t using bucket tree elimination
- can be memoized for some number of instances K
 (based on memory available

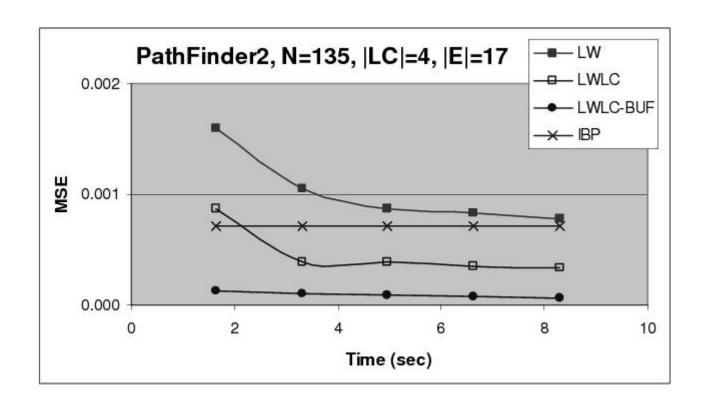
End For

 $KL[P(C|e), Q(C)] \leq KL[P(X|e), Q(X)]$

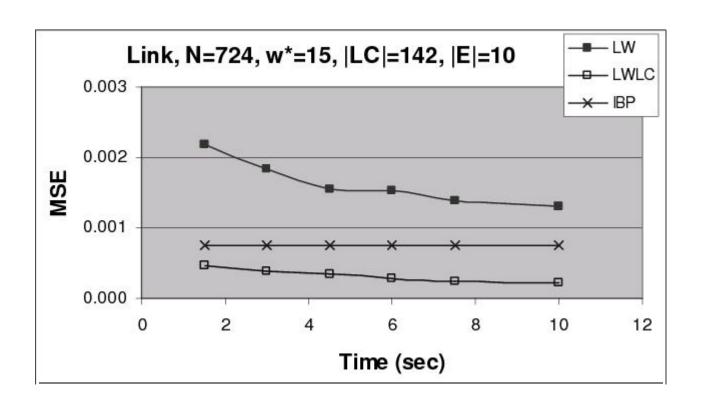
Pathfinder 1



Pathfinder 2



Link



Summary

Importance Sampling

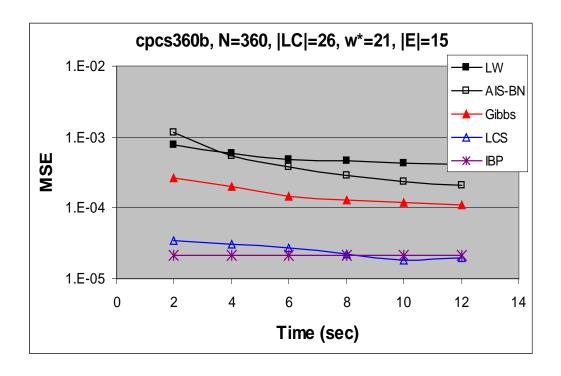
- i.i.d. samples
- Unbiased estimator
- Generates samples fast

- Samples from Q
- Reject samples with zero-weight
- Improves on cutset

Gibbs Sampling

- Dependent samples
- Biased estimator
- Generates samples slower
- Samples from P(X|e)
- Does not converge in presence of constraints
- Improves on cutset

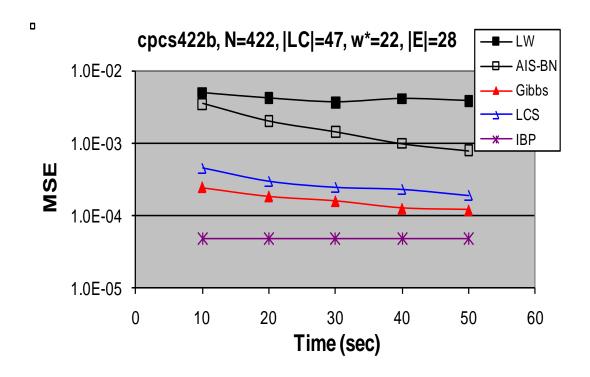
CPCS360b



LW – likelihood weighting

LCS – likelihood weighting on a cutset

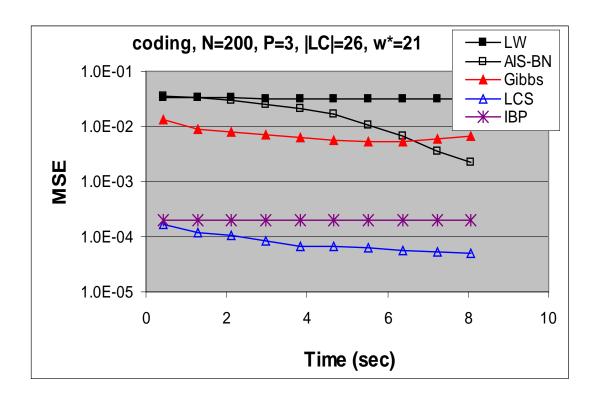
CPCS422b



LW – likelihood weighting

LCS – likelihood weighting on a cutset

Coding Networks



LW – likelihood weighting

LCS – likelihood weighting on a cutset