Sampling Techniques for Probabilistic and Deterministic Graphical models

ICS 276, Spring 2018

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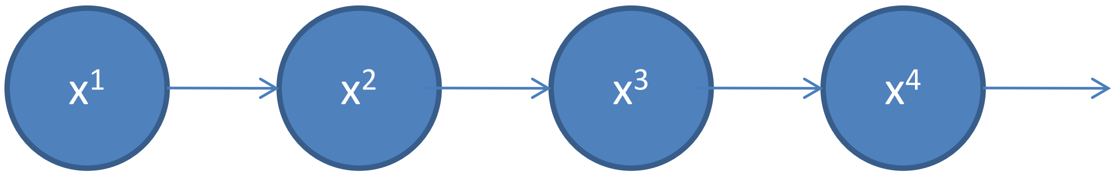
Reading" Darwiche chapter 15, related papers

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



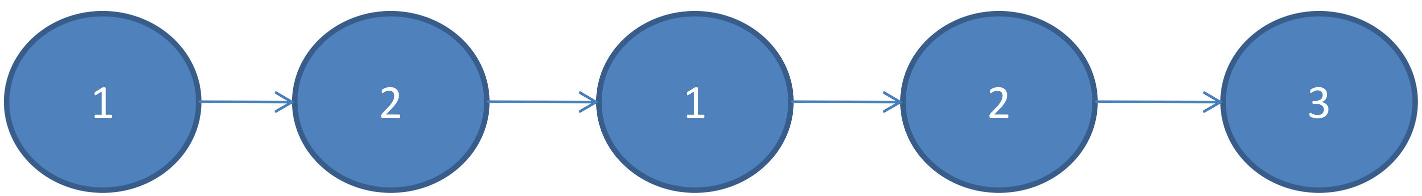
- A **Markov chain** is a discrete random process with the property that the next state depends only on the current state (**Markov Property**):

$$P(x^t \mid x^1, x^2, \ldots, x^{t-1}) = P(x^t \mid x^{t-1})$$

- 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**) $\sum_x P(X = x) = 1$

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

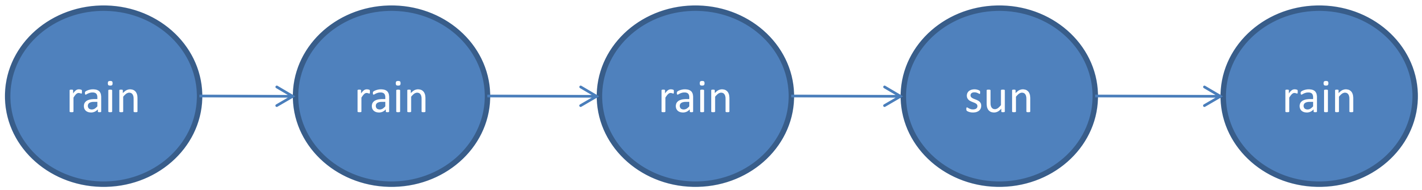


$$D(X) = \{0,1,2,\ldots\}$$

	$P(n-1)$	$P(n+1)$
n	0.5	0.5

transition matrix P(X)

Example: Weather Model



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

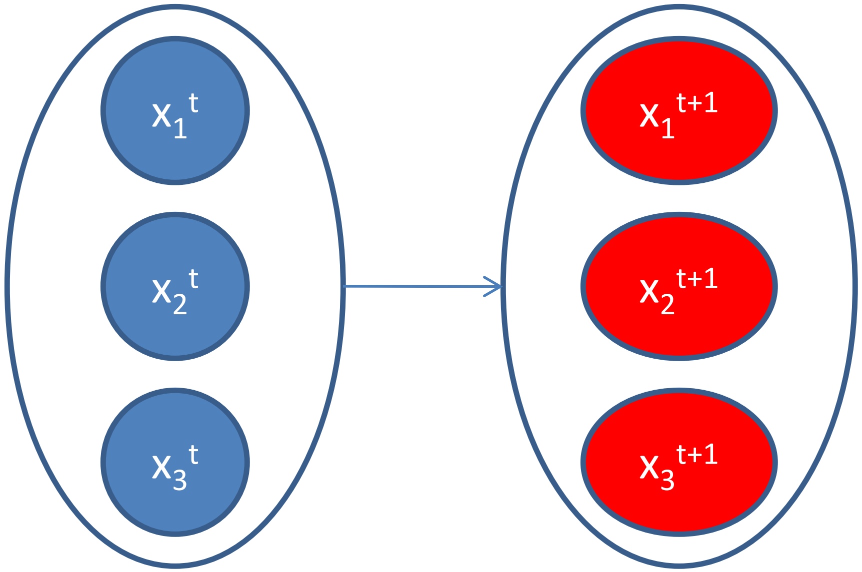
	$P(rainy)$	$P(sunny)$
$rainy$	0.9	0.1
$sunny$	0.5	0.5

transition matrix P(X)

Multi-Variable System

$$X = \{X_1, X_2, X_3\}, D(X_i) = discrete, finite$$

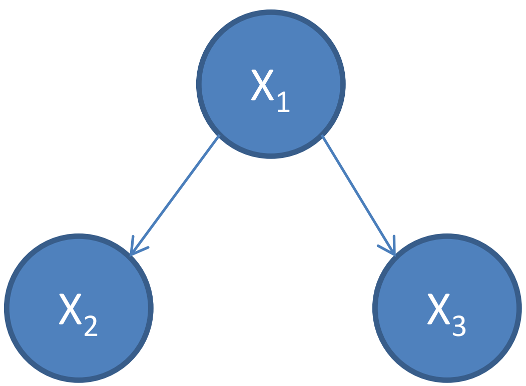
- state is an assignment of values to all the variables

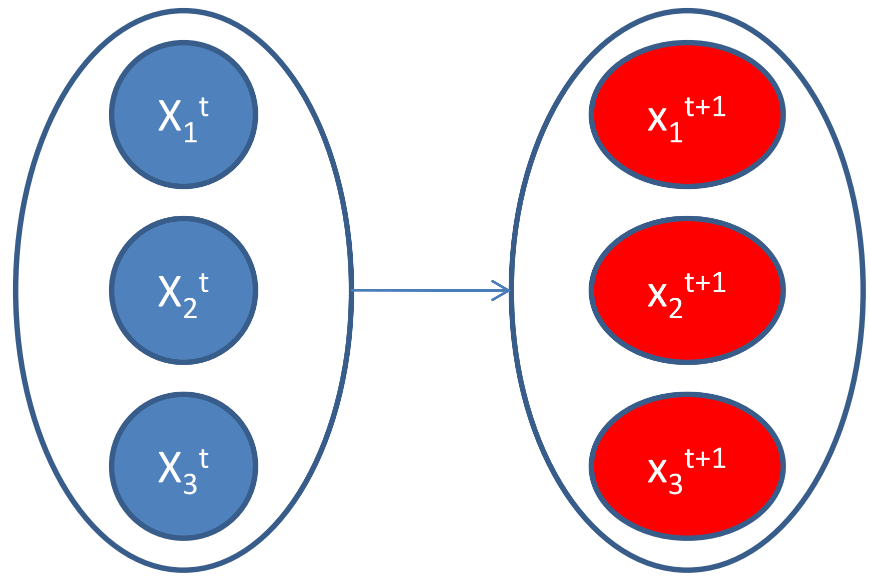


$$x^t = \{x_1^t, x_2^t, \ldots, x_n^t\}$$

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 π(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 x is *irreducible* if under the transition rule one has nonzero probability of moving from x 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 x is *recurrent* if the chain returns to x with probability 1
- Let M(x) be the expected number of steps to return to state x
- State x is *positive recurrent* if M(x) 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 $\forall i$, 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 $x^0,\dots,x^n$ can be viewed as "samples" from distribution π

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

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

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)

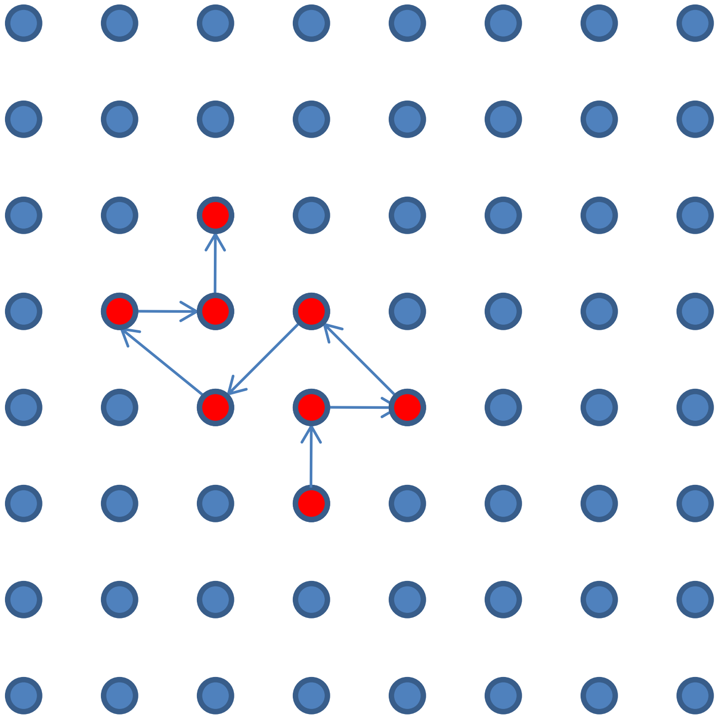
- Gibbs sampler is an algorithm to generate a sequence of samples from the **joint probability distribution** of two or more random variables
- Sample new variable value one variable at a time from the variable's conditional distribution:

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

- 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

$$X_1 = x_1^{t+1} \leftarrow P(X_1 \mid x_2^t, x_3^t, \ldots, x_N^t, e)$$

$$X_2 = x_2^{t+1} \leftarrow P(X_2 \mid x_1^{t+1}, x_3^t, \ldots, x_N^t, e)$$

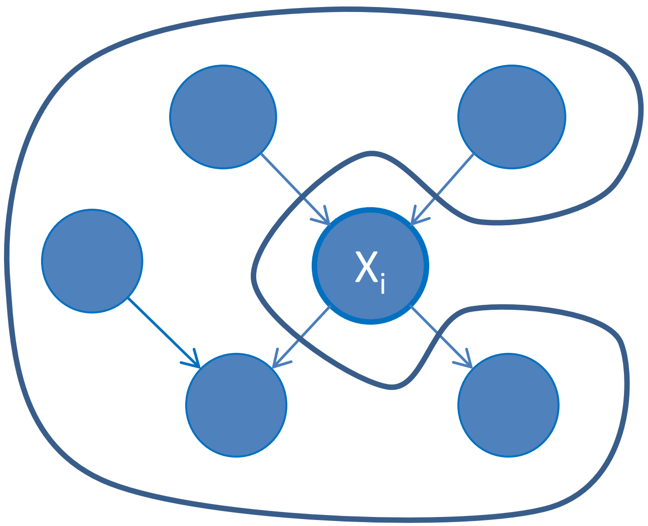
...

$$X_N = x_N^{t+1} \leftarrow P(X_N \mid x_1^{t+1}, x_2^{t+1}, \ldots, x_{N-1}^{t+1}, e)$$

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:

$$markov(X_i) = pa_i \cup ch_i \cup \left(\bigcup_{X_j \in ch_j} pa_j \right)$$

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

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

Computation is linear in the size of Markov blanket!

Ordered Gibbs Sampling Algorithm (Pearl,1988)

Input: *X, E=e*

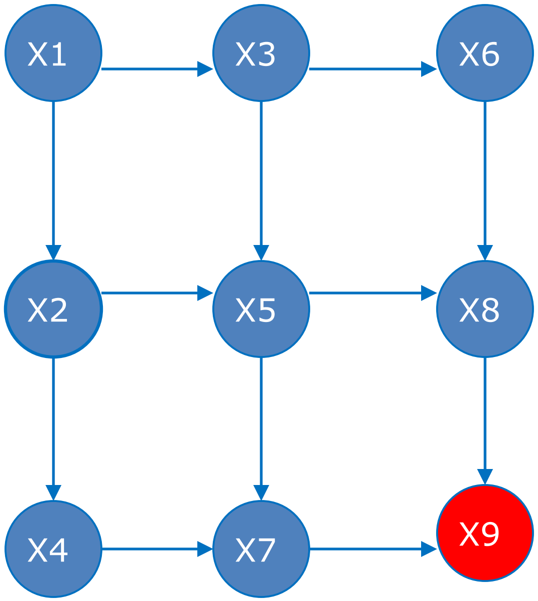
Output: *T* samples $\{x^t\}$

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

1. For t = 1 to T (compute samples)
2. 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

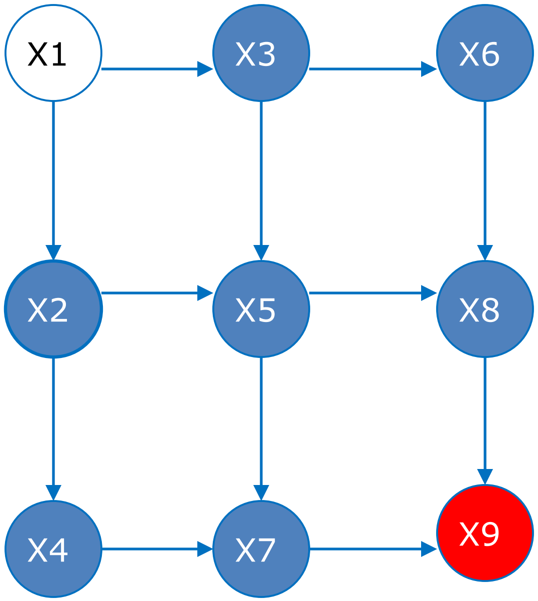
$$X = \{X_1, X_2, \ldots, X_9\}, E = \{X_9\}$$



$$X_1 = x_1^0$$
$$X_6 = x_6^0$$
$$X_2 = x_2^0$$
$$X_7 = x_7^0$$
$$X_3 = x_3^0$$
$$X_8 = x_8^0$$
$$X_4 = x_4^0$$
$$X_5 = x_5^0$$

Gibbs Sampling Example - BN

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



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

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

$$\ldots$$

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

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

Dirac delta f-n

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

- **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 π(R,L) and function g, the following result applies

$$Var[E\{g(R) \mid L\} \leq Var[g(R)]$$

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 on 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:

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

w_t

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

Gibbs Sampling: Convergence

- Sample from $\bar{P}(X|e) \rightarrow P(X|e)$
- Converges iff chain is irreducible and ergodic
- Intuition - must be able to explore all states:
  - if X_i and X_j are strongly correlated, $X_i=0 \leftrightarrow X_j=0$, 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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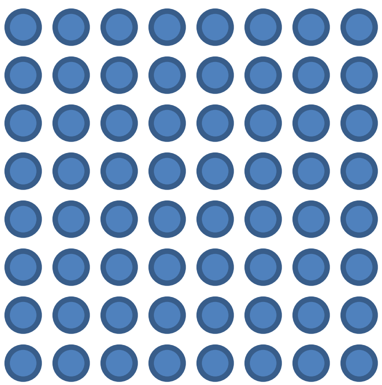
Sampling: Performance

- 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

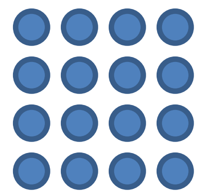
- Smaller state-space is easier to cover

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



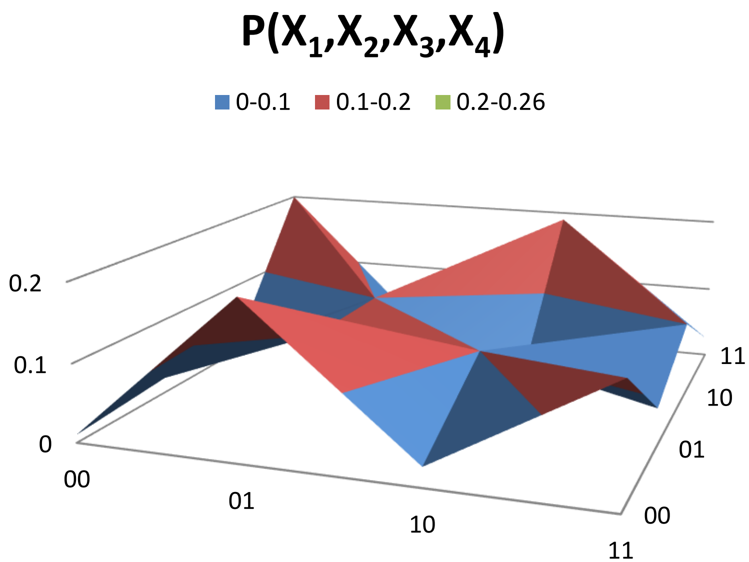
$$D(X) = 64$$

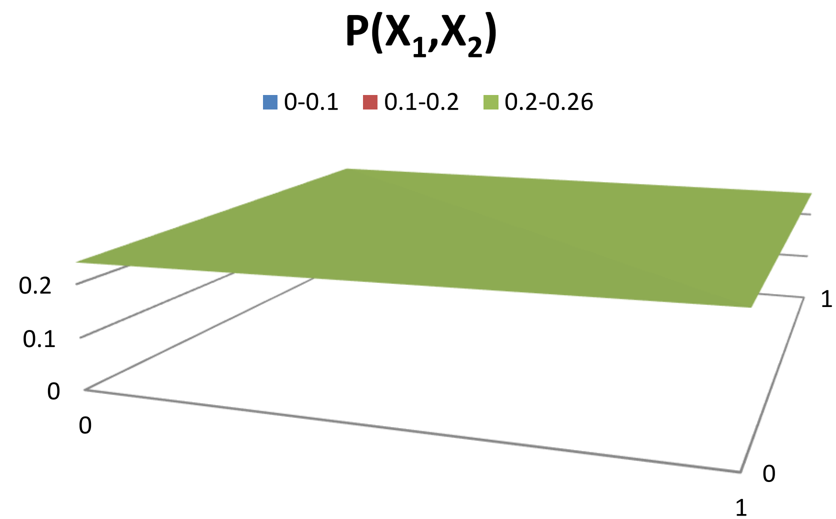
$$X = \{X_1, X_2\}$$



$$D(X) = 16$$

Smoother Distribution





Speeding Up Convergence

- Mean Squared Error of the estimator:

$$MSE_Q\left[\overline{P}\right] = BIAS^2 + Var_Q\left[\overline{P}\right]$$

- In case of unbiased estimator, BIAS=0

$$MSE_Q[\hat{P}] = Var_Q[\hat{P}] = \left(E_Q\left[\hat{P}\right]^2 - E_Q[P]^2 \right)$$

- Reduce variance $\Rightarrow$ speed up convergence !

Rao-Blackwellisation

$$X = R \cup L$$

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

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

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

$$Var\{g(x)\} \geq Var\{E[g(x) \mid l]\}$$

$$Var\{\hat{g}(x)\} = \frac{Var\{h(x)\}}{T} \geq \frac{Var\{E[h(x) \mid l]\}}{T} = Var\{\tilde{g}(x)\}$$

Liu, Ch.2.3

Rao-Blackwellisation

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

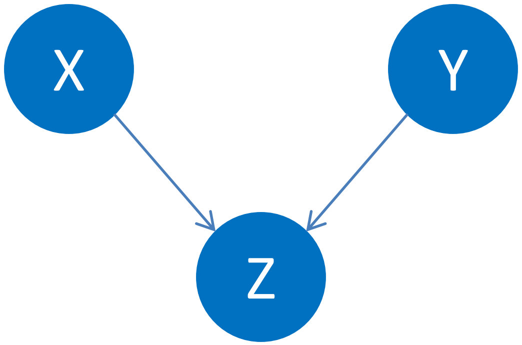
- X=R∪L
- Importance Sampling:

$$Var_Q\{\frac{P(R,L)}{Q(R,L)}\} \geq Var_Q\{\frac{P(R)}{Q(R)}\}$$

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:

$$P(x \mid y,z), P(y \mid x,z), P(z \mid x,y) \quad (1)$$

- Blocking:

$$P(x \mid y,z), P(y,z \mid x) \quad (2)$$

- Collapsed:

$$P(x \mid y), P(y \mid x) \quad (3)$$

Collapsed Gibbs Sampling

Generating Samples

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

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

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

...

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

In short, for i=1 to K:

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

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. $c_i^{t+1} \leftarrow P(C_i \mid c^t \backslash c_i)$
4. *End For*
5. *End For*

Calculation Time

- Computing $P(c_i | c^t \backslash c_i, e)$ 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 time-effective!

Exploiting Graph Properties

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

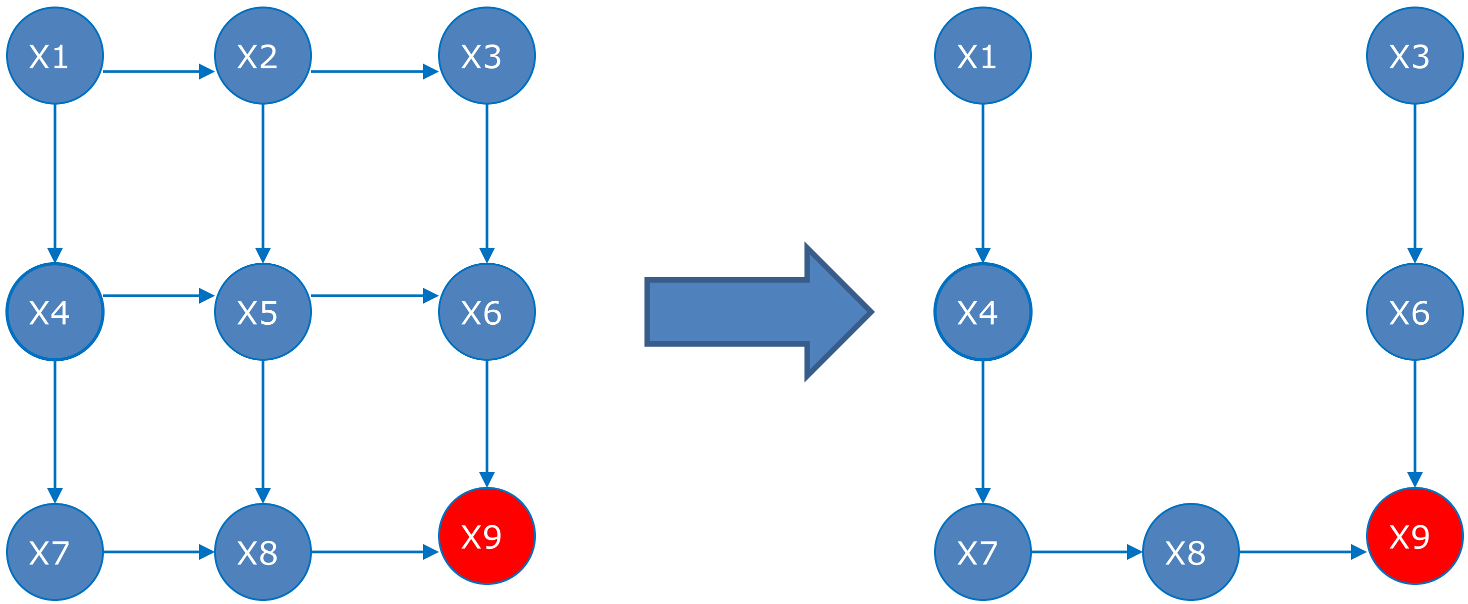
- **w-cutset** is a subset of variable s.t. when they are observed, induced width of the graph is w
- when sampled variables form a **w-cutset** , inference is exp(w) (e.g., using *Bucket Tree Elimination*)
- **cycle-cutset** is a special case of w-cutset

Sampling w-cutset $\Rightarrow$ **w-cutset sampling!**

What If C=Cycle-Cutset ?

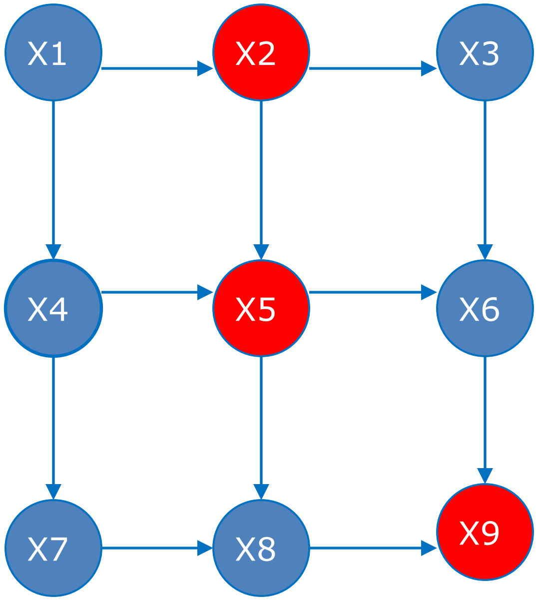
$$c^0 = \{x_2^0, x_5^0\}, E = \{X_9\}$$

$P(x_2,x_5,x_9)$ – 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

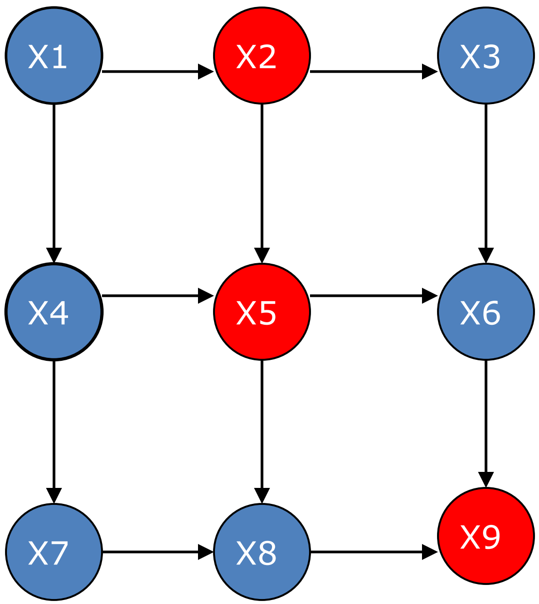
$$\overline{P}(x_i|e) = \frac{1}{T} \sum_{t=1}^{T} P(x_i \mid c^t, e)$$

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

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

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

$\ldots$

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

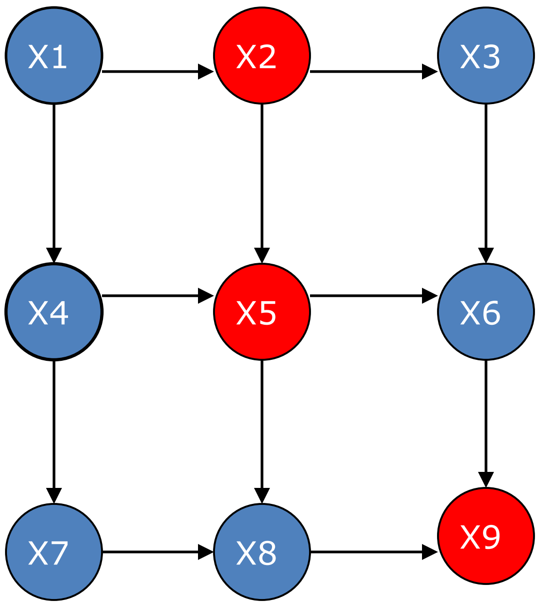
$\ldots$

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

$$\boxed{\overline{P}(x_2 | x_9) = \frac{1}{3}\left[\begin{array}{l} P(x_2 | x_5^0, x_9) \\ + P(x_2 | x_5^1, x_9) \\ + P(x_2 | x_5^2, x_9) \end{array}\right]}$$

Cutset Sampling Example

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



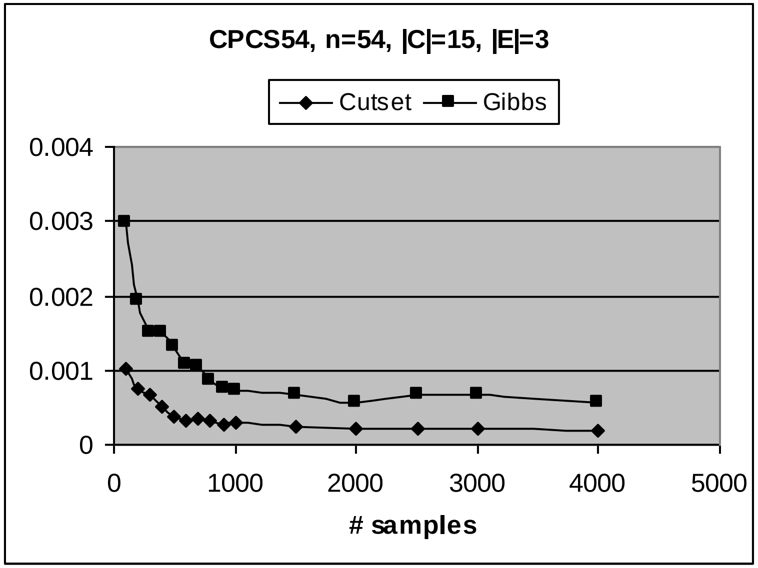
$$c^1 = \{x_2^1, x_5^1\} \Rightarrow P(x_3 \mid x_2^1, x_5^1, x_9)$$

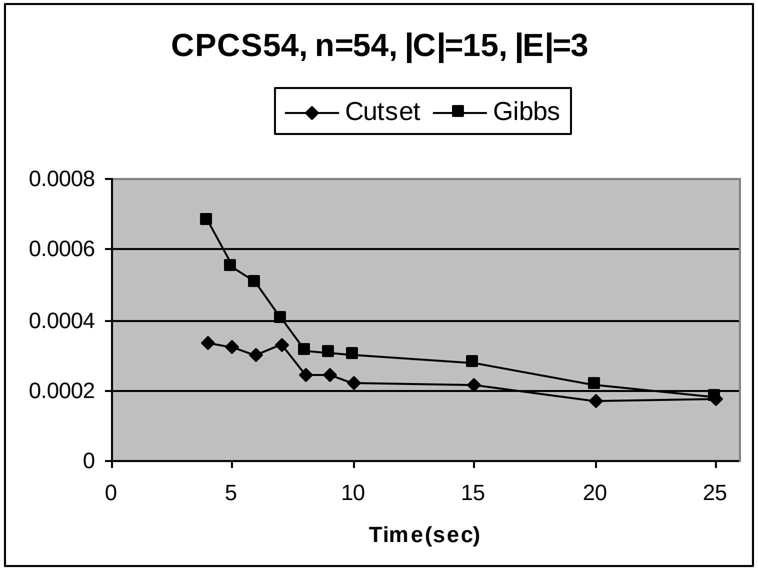
$$c^2 = \{x_2^2, x_5^2\} \Rightarrow P(x_3 \mid x_2^2, x_5^2, x_9)$$

$$c^3 = \{x_2^3, x_5^3\} \Rightarrow P(x_3 \mid x_2^3, x_5^3, x_9)$$

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

CPCS54 Test Results



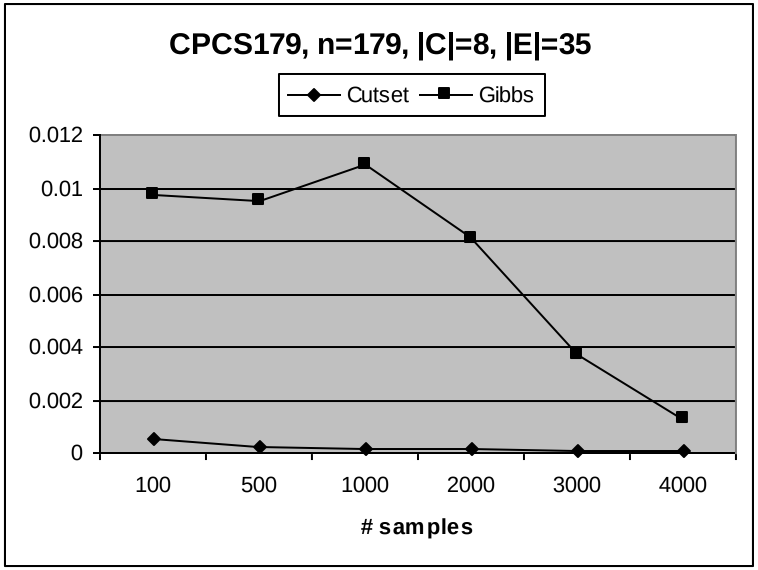


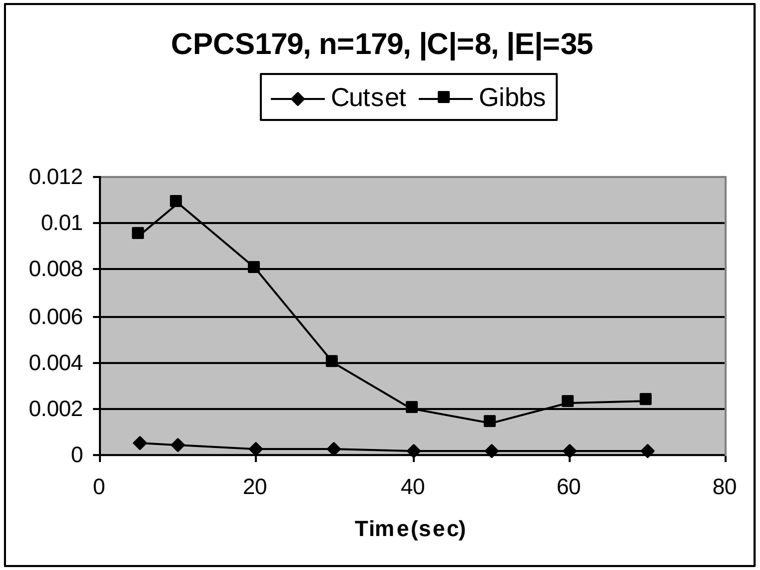
MSE vs. #samples (left) and time (right)

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

Exact Time = 30 sec using Cutset Conditioning

CPCS179 Test Results

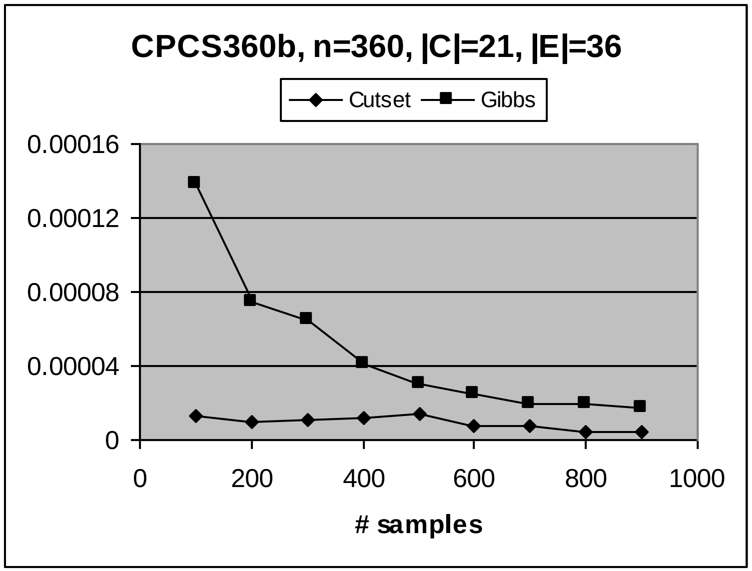


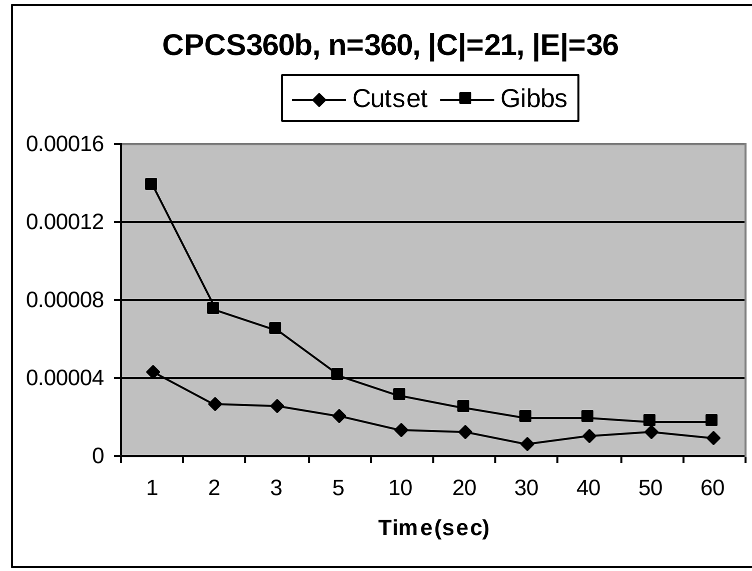


MSE vs. #samples (left) and time (right)
Non-Ergodic (1 deterministic CPT entry)
$|X| = 179$, $|C| = 8$, $2 <= D(X_i) <= 4$, $|E| = 35$

Exact Time = 122 sec using Cutset Conditioning

CPCS360b Test Results





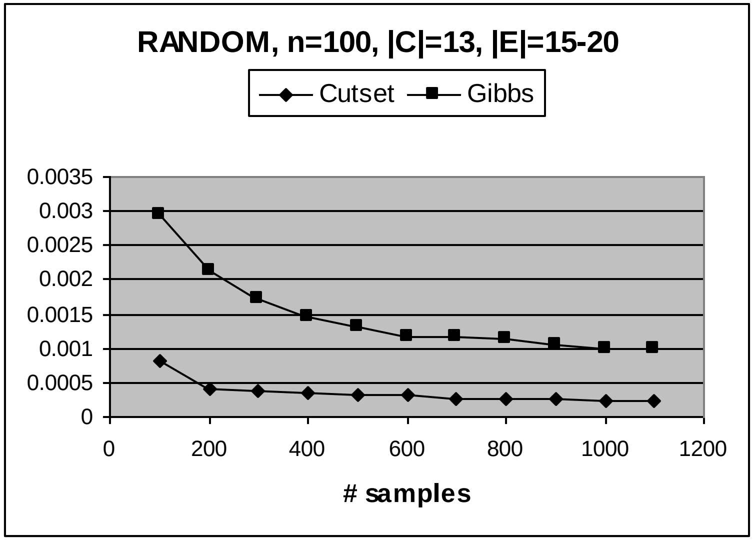
MSE vs. #samples (left) and time (right)

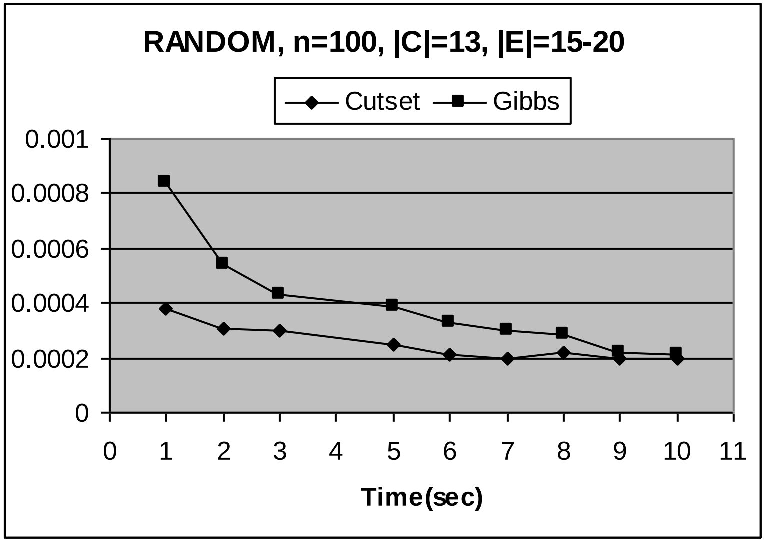
Ergodic, $|X| = 360$, $D(X_i)=2$, $|C| = 21$, $|E| = 36$

Exact Time > 60 min using Cutset Conditioning

Exact Values obtained via Bucket Elimination

Random Networks





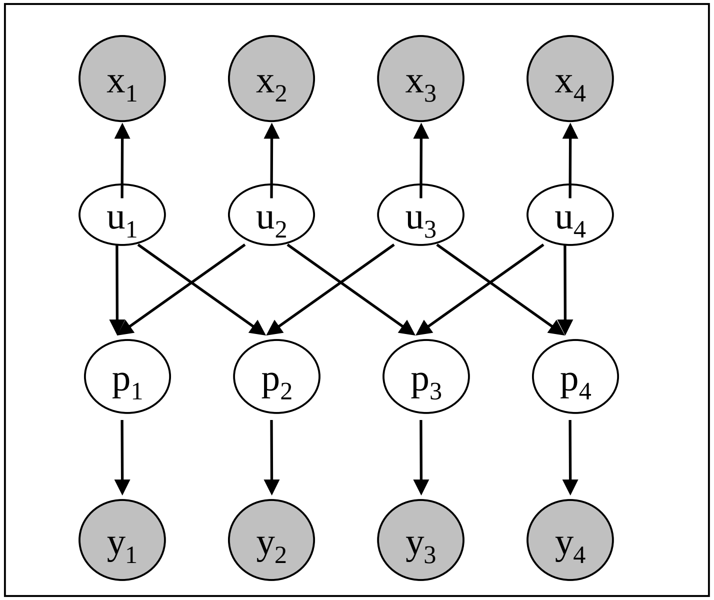
MSE vs. #samples (left) and time (right)

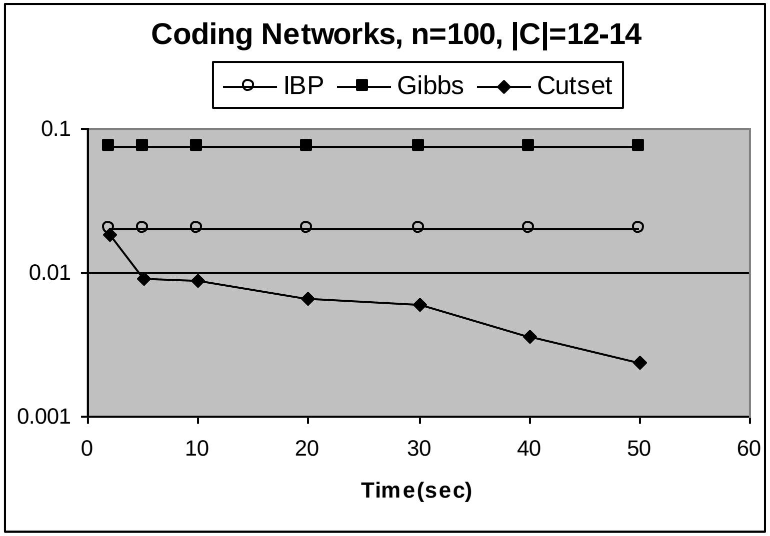
$|X| = 100$, $D(X_i) = 2$, $|C| = 13$, $|E| = 15\text{-}20$

Exact Time = 30 sec using Cutset Conditioning

Coding Networks

Cutset Transforms Non-Ergodic Chain to Ergodic





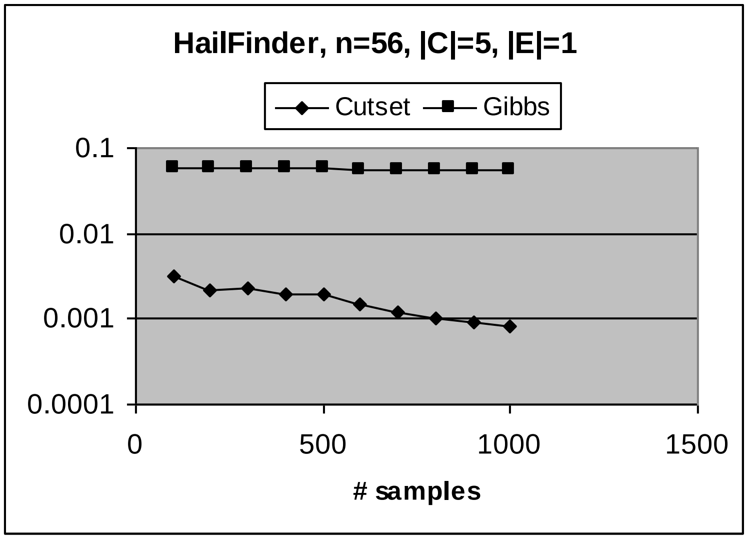
MSE vs. time (right)

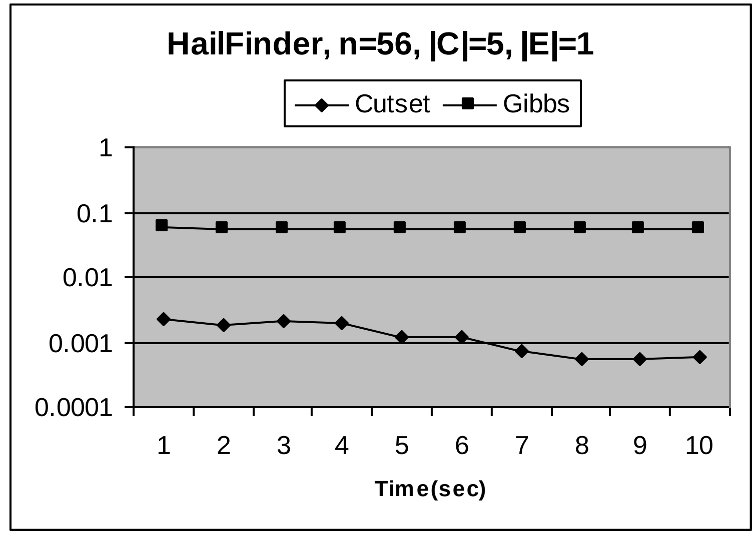
Non-Ergodic, |X| = 100, $D(X_i)$=2, |C| = 13-16, |E| = 50

Sample Ergodic Subspace U={U_1, U_2,…U_k}

Exact Time = 50 sec using Cutset Conditioning

Non-Ergodic Hailfinder



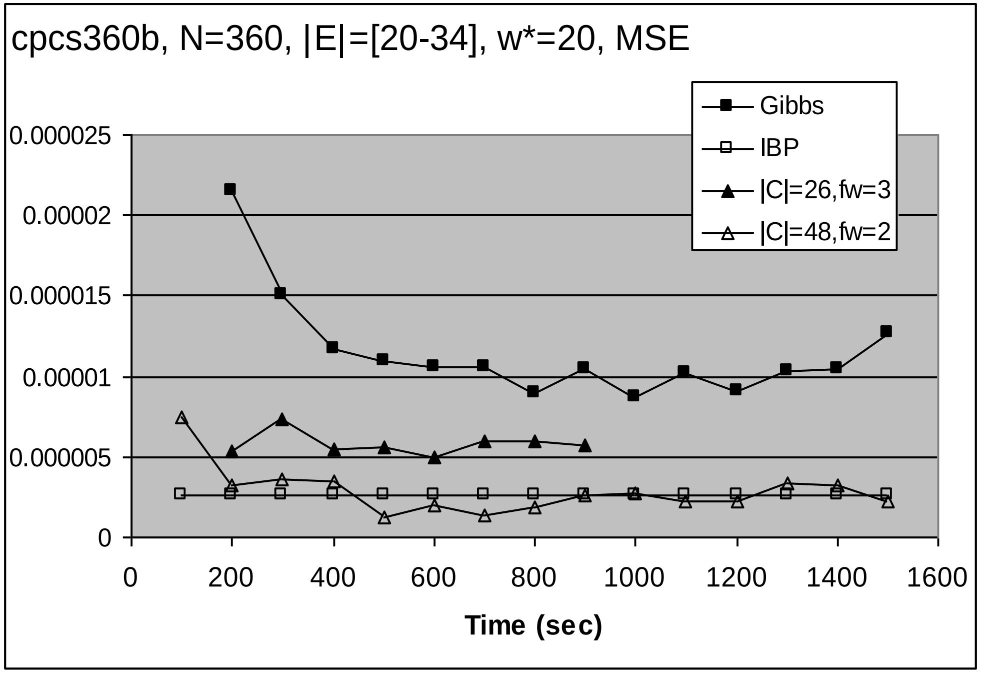


MSE vs. #samples (left) and time (right)

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:

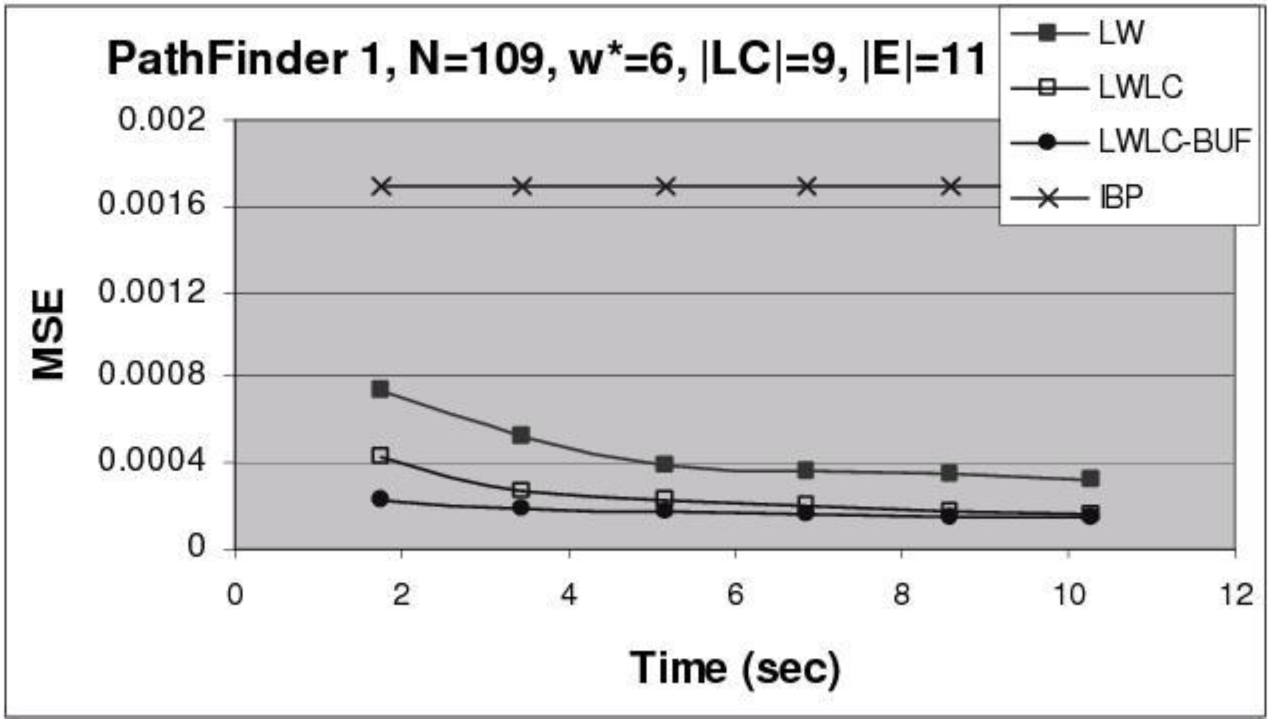
$$
\begin{array}{l}
\text{For } Z_i \in Z \text{ do}: \\
\quad \text{If } Z_i \in E \\
\qquad z_i^{t+1} = z_i, z_i \in e \\
\quad \text{Else} \\
\qquad z_i^{t+1} \leftarrow P(Z_i \mid z_1^{t+1}, \ldots, z_{i-1}^{t+1}) \\
\quad \text{End If} \\
\text{End For}
\end{array}
$$

- computed while generating sample t using bucket tree elimination

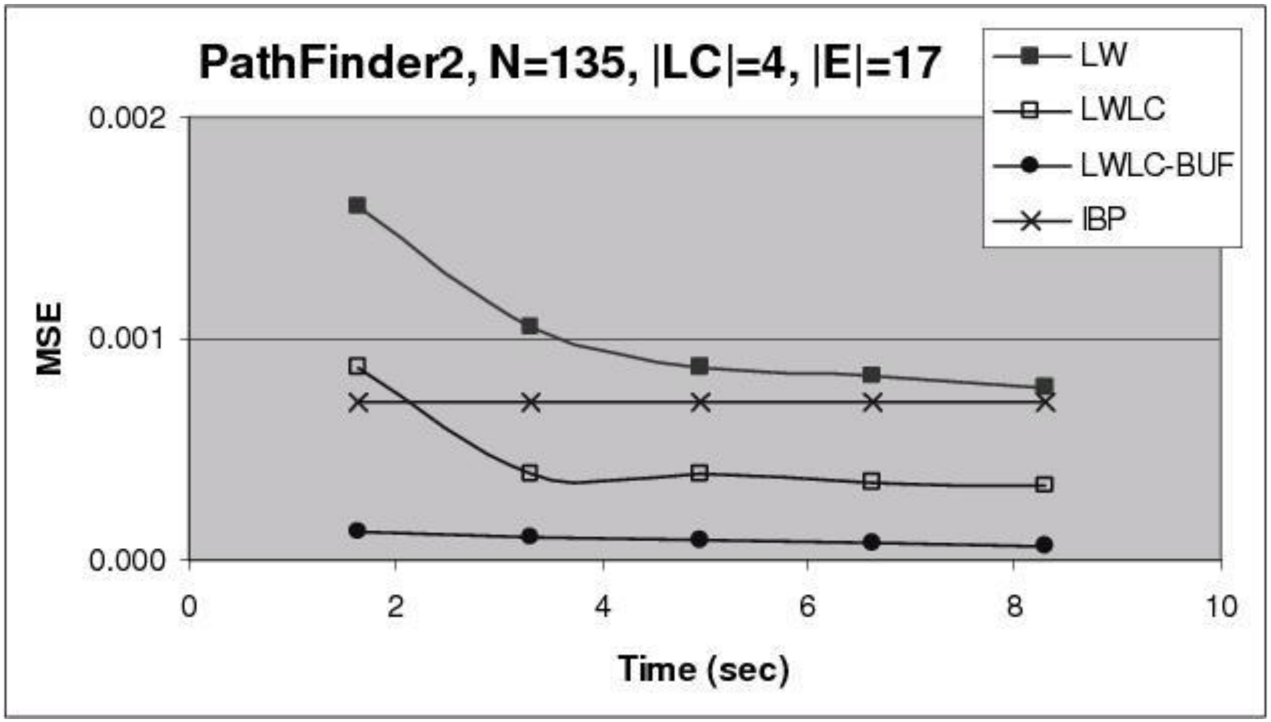
- can be memoized for some number of instances K (based on memory available

KL[P(C|e), Q(C)] ≤ KL[P(X|e), Q(X)]

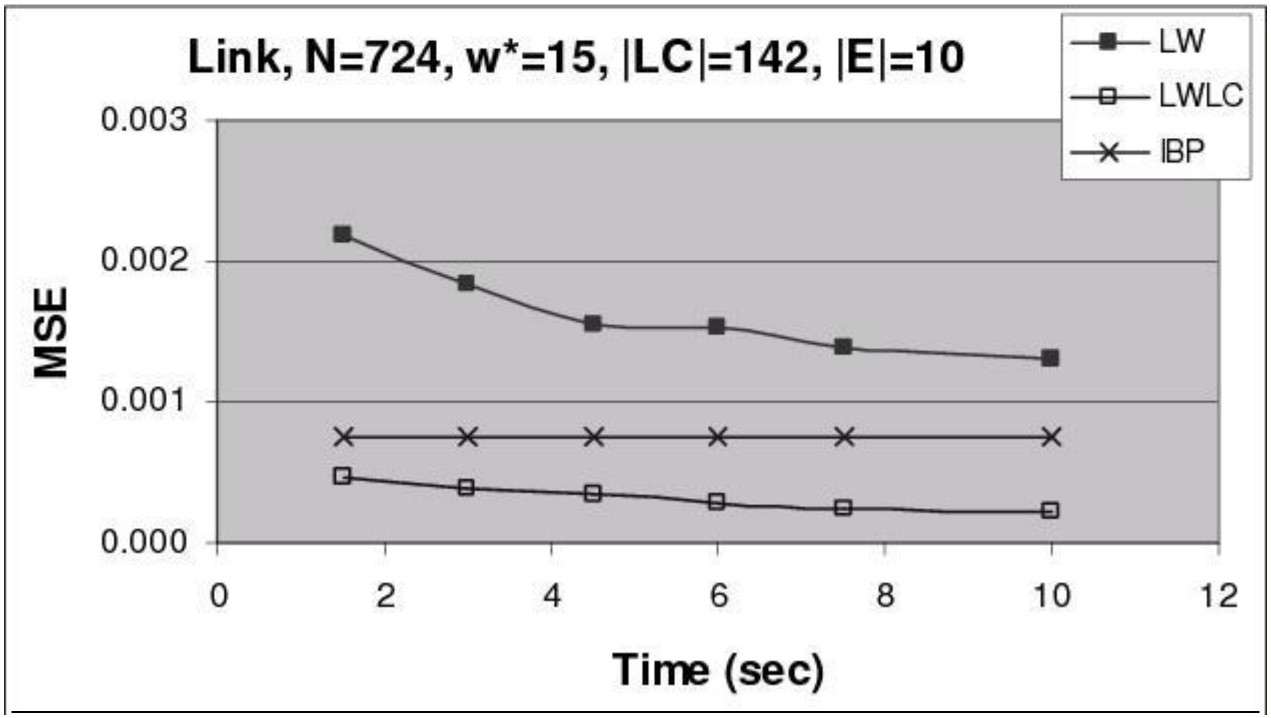
Pathfinder 1



Pathfinder 2



Link



Link, N=724, w*=15, |LC|=142, |E|=10
LW
LWLC
IBP
MSE
0.003
0.002
0.001
0.000
0
2
4
6
8
10
12
Time (sec)

Summary

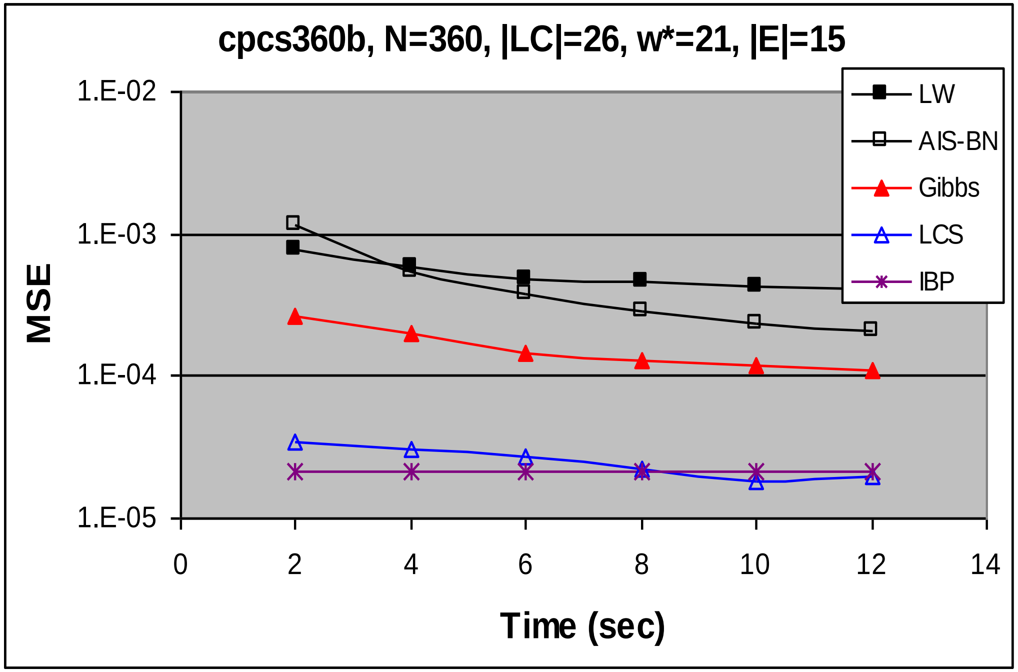
Importance Sampling

- i.i.d. samples
- Unbiased estimator
- Generates samples fast
- Samples from Q
- Reject samples with zero-weight
- Improves on cutset

Gibbs Sampling

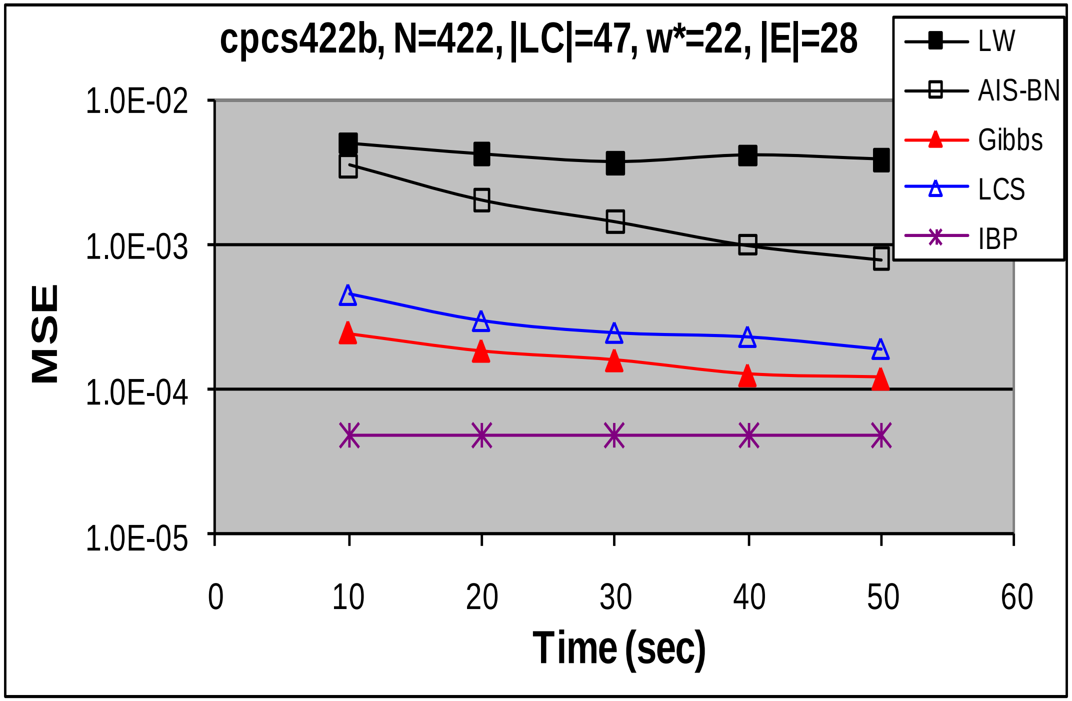
- Dependent samples
- Biased estimator
- Generates samples slower
- Samples from $\bar{P}(X|e)$
- Does not converge in presence of constraints
- Improves on cutset

CPCS360b



LW – likelihood weighting
LCS – likelihood weighting on a cutset

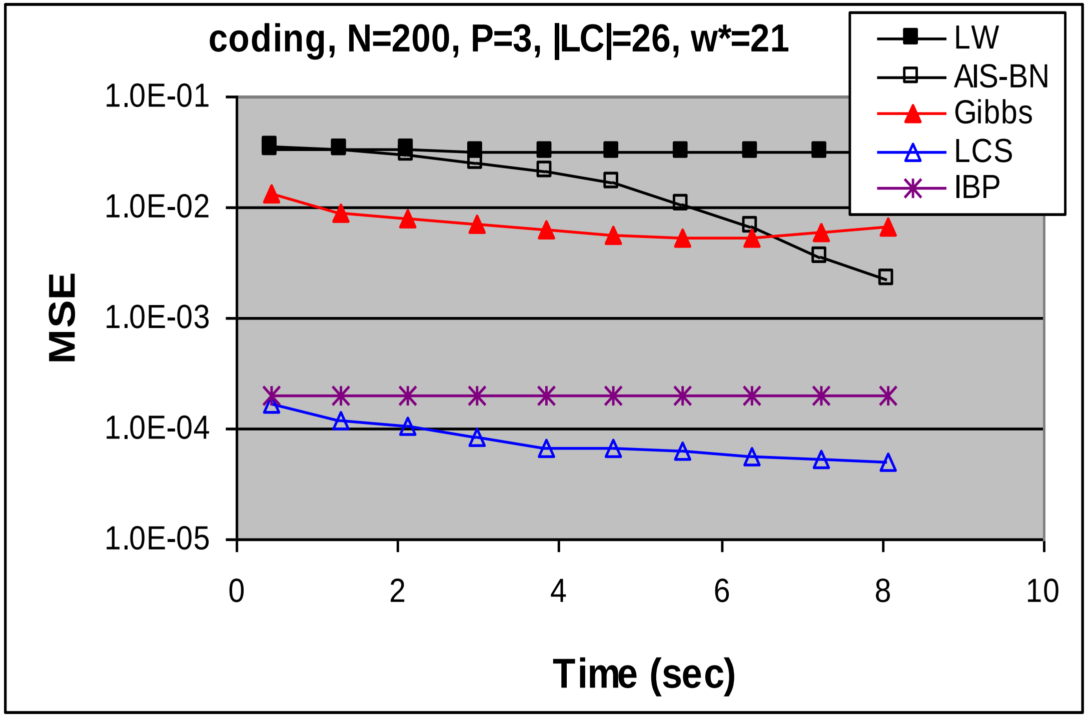
CPCS422b



LW – likelihood weighting

LCS – likelihood weighting on a cutset

Coding Networks



LW – likelihood weighting
LCS – likelihood weighting on a cutset