Lecture : Inference in Graphical Models

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Exact Inference

Variable Elimination and Belief Propagation

Inference

Inference corresponds to using the distribution to answers questions about the environment.

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examples

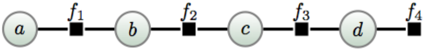
- What is the probability $p(x = 4|y = 1, z = 2)$?
- What is the most likely joint state of the distribution $p(x, y)$?
- What is the entropy of the distribution $p(x, y, z)$?
- What is the probability that this example is in class 1?
- What is the probability the stock market will do down tomorrow?

Computational Efficiency

- Inference can be computationally very expensive and we wish to characterise situations in which inferences can be computed efficiently.
- For singly-connected graphical models, and certain inference questions, there exist efficient algorithms based on the concept of message passing.
- In general, the case of multiply-connected models is computationally inefficient.

Sum-Product Algorithm

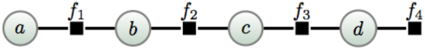
$p(a,b,c,d) \propto f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d)$ $\quad a,b,c,d$ binary variables



$$
\begin{aligned}
p(a) &= \sum_{b,c,d} p(a,b,c,d) \\
&\propto \sum_{b,c,d} f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d) \Rightarrow 2^3 \text{ sums}
\end{aligned}
$$

Sum-Product Algorithm

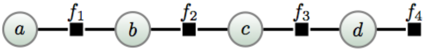
$p(a,b,c,d) \propto f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d)$ $\quad a,b,c,d$ binary variables



$$
\begin{aligned}
p(a) &= \sum_{b,c,d} p(a,b,c,d) \\
&\propto \sum_{b,c,d} f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d) \Rightarrow 2^3 \text{ sums} \\
&= \sum_{b} f_1(a,b) \sum_{c} f_2(b,c) \sum_{d} f_3(c,d)\, f_4(d) \Rightarrow 2 \times 3 \text{ sums}
\end{aligned}
$$

Sum-Product Algorithm

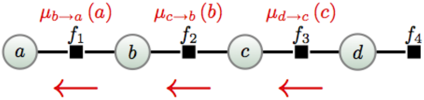
$$p(a,b,c,d) \propto f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d) \qquad a,b,c,d \text{ binary variables}$$



$$\begin{aligned}
p(a) &= \sum_{b,c,d} p(a,b,c,d) \\
&\propto \sum_{b,c,d} f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d) \\
&= \underbrace{\sum_b f_1(a,b) \underbrace{\sum_c f_2(b,c) \underbrace{\sum_d f_3(c,d)\, f_4(d)}_{\mu_{d\to c}(c)}}_{\mu_{c\to b}(b)}}_{\mu_{b\to a}(a)}
\end{aligned}$$

Sum-Product Algorithm

$p(a,b,c,d) \propto f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d)$ $\quad a, b, c, d$ binary variables

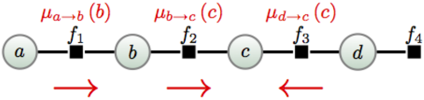


Passing variable-to-variable messages from d up to a

$$
\begin{aligned}
p(a) &= \sum_{b,c,d} p(a,b,c,d) \\
&\propto \sum_{b,c,d} f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d) \\
&= \underbrace{\sum_b f_1(a,b) \underbrace{\sum_c f_2(b,c) \underbrace{\sum_d f_3(c,d)\, f_4(d)}_{\mu_{d\to c}(c)}}_{\mu_{c\to b}(b)}}_{\mu_{b\to a}(a)}
\end{aligned}
$$

Sum-Product Algorithm

For $p(c)$ need to send messages in both directions

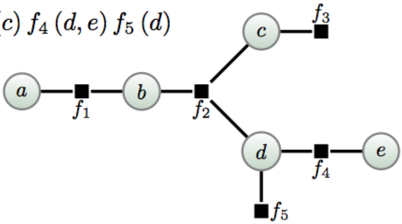


$$p(c) \propto \sum_{a,b,d} f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d)$$

$$= \underbrace{\sum_b \underbrace{\sum_a f_1(a,b)}_{\mu_{a\to b}(b)} f_2(b,c)}_{\mu_{b\to c}(c)} \underbrace{\sum_d f_3(c,d)\, f_4(d)}_{\mu_{d\to c}(c)}$$

Sum-Product Algorithm

$$p(a,b,c,d,e) \propto f_1(a,b)\, f_2(b,c,d)\, f_3(c)\, f_4(d,e)\, f_5(d)$$



Need to define factor-to-variable messages and variable-to-factor messages

$$p(a) \propto \underbrace{f_1(a,b) \underbrace{\sum_{c,d} f_2(b,c,d)\, \underbrace{f_3(c)}_{\mu_{c\to f_2}(c)=\mu_{f_3\to c}(c)}\, \underbrace{\underbrace{f_5(d)}_{\mu_{f_5\to d}(d)}\, \underbrace{\sum_{e} f_4(d,e)}_{\mu_{f_4\to d}(d)}}_{\mu_{d\to f_2}(d)}}_{\mu_{b\to f_1}(b)=\mu_{f_2\to b}(b)}}_{\mu_{f_1\to a}(a)}$$

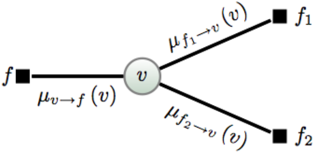
$\Rightarrow$ **Marginal inference for a singly-connected structure is easy.**

Sum-Product Algorithm for Factor Graphs

Variable to factor message

$\mu_{v\to f}(v) = \prod_{f_i \sim v \setminus f} \mu_{f_i \to v}(v)$

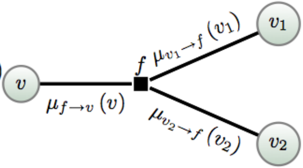
Messages from extremal variables are set to 1



Factor to variable message

$\mu_{f\to v}(v) = \sum_{\{v_i\}} f(v, \{v_i\}) \prod_{v_i \sim f \setminus v} \mu_{v_i \to f}(v_i)$

Messages from extremal factors are set to the factor

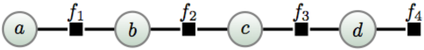


Marginal

$p(v) \propto \prod_{f_i \sim v} \mu_{f_i \to v}(v)$

Max Product Algorithm

$$p(a,b,c,d) \propto f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d) \qquad a,b,c,d \text{ binary variables}$$

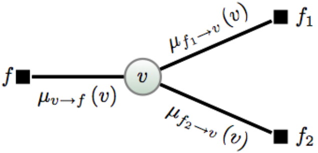


$$\begin{aligned}
\max_{a,b,c,d} p(a,b,c,d) &= \max_{a,b,c,d} f_1(a,b)\, f_2(b,c)\, f_3(c,d)\, f_4(d) \\
&= \max_a \underbrace{\max_b f_1(a,b) \underbrace{\max_c f_2(b,c) \underbrace{\max_d f_3(c,d)\, f_4(d)}_{\mu_{d\to c}(c)}}_{\mu_{c\to b}(b)}}_{\mu_{b\to a}(a)}
\end{aligned}$$

Max Product Algorithm

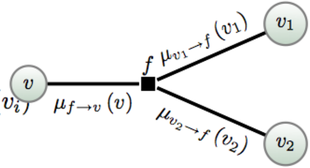
Variable to factor message

$\mu_{v\to f}(v) = \prod_{f_i \sim v \setminus f} \mu_{f_i \to v}(v)$



Factor to variable message

$\mu_{f\to v}(v) = \max_{\{v_i\}} f(v,\{v_i\}) \prod_{v_i \sim f \setminus v} \mu_{v_i \to f}(v_i)$



Marginal

$v^* = \underset{v}{\operatorname{argmax}} \prod_{f_i \sim v} \mu_{f_i \to v}(v)$

Message Passing

- Also known as **belief propagation** or **dynamic programming**
- Note that for non-branching graphs (they look like lines), only variable to variable messages are required.
- For message passing to work we need to be able to distribute the operator over the factors (which means that the operator algebra is a semiring) and that the graph is singly-connected.
- Provided the above conditions hold, marginal inference scales linearly with the number of nodes in the graph.

Approximate Inference

Sampling Methods

Inference for Graphical Models

Before we looked into **Exact Inference :**

- Can be slow in many cases!

Approximate Inference : Sampling Methods represent desired distribution with a set of samples $\rightarrow$ as more samples are used, obtain more accurate representation

Sampling

Fundamental problem we address:

- How to obtain samples from a probability distribution $p(\mathbf{z})$
- This could be a conditional distribtion $p(\mathbf{z}|\mathbf{e})$

We wish to evaluate expectations such as

$$\mathbb{E}[f] = \int f(z)p(z)dz \tag{1}$$

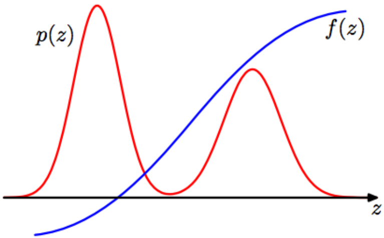
- e.g mean when $f(z) = z$

For complicated p(z), this is difficult to do exactly, so approximate as

$$\hat{f} = \frac{1}{Z}\sum_{l=1}^{L} f(z^{(l)}) \tag{2}$$

where $\{z^{(l)}|l = 1, ...L\}$ are independent samples from p($\mathbf{z}$)

Sampling



- Approximate

$$\hat{f} = \frac{1}{L}\sum_{l=1}^{L} f(\mathbf{z}^{(l)})$$

where $\{\mathbf{z}^{(l)} | l = 1, \ldots, L\}$ are independent samples from $p(\mathbf{z})$

Simple Monte Carlo

Statistical sampling can be applied to any expectation:

In general:

$$\int f(x)P(x)\,\mathrm{d}x \approx \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)}), \quad x^{(s)} \sim P(x)$$

Example: making predictions

$$\begin{aligned} p(x|\mathcal{D}) &= \int P(x|\theta,\mathcal{D})P(\theta|\mathcal{D})\,\mathrm{d}\theta \\ &\approx \frac{1}{S}\sum_{s=1}^{S} P(x|\theta^{(s)},\mathcal{D}), \quad \theta^{(s)} \sim P(\theta|\mathcal{D}) \end{aligned}$$

Properties of Monte Carlo

Estimator: $$\int f(x)P(x)\,\mathrm{d}x \approx \hat{f} \equiv \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)}), \quad x^{(s)} \sim P(x)$$

Estimator is unbiased:

$$\mathbb{E}_{P(\{x^{(s)}\})}\left[\hat{f}\right] = \frac{1}{S}\sum_{s=1}^{S}\mathbb{E}_{P(x)}[f(x)] = \mathbb{E}_{P(x)}[f(x)]$$

Variance shrinks $\propto 1/S$:

$$\mathrm{var}_{P(\{x^{(s)}\})}\left[\hat{f}\right] = \frac{1}{S^2}\sum_{s=1}^{S}\mathrm{var}_{P(x)}[f(x)] = \mathrm{var}_{P(x)}[f(x)]\,/S$$

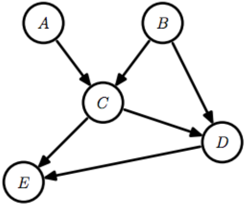
"Error bars" shrink like $\sqrt{S}$

Sampling from a Bayesian Network

Ancestral pass for directed graphical models:

— sample each top level variable from its marginal

— sample each other node from its conditional
once its parents have been sampled



Sample:

$A \sim P(A)$
$B \sim P(B)$
$C \sim P(C \mid A, B)$
$D \sim P(D \mid B, C)$
$E \sim P(D \mid C, D)$

$$P(A,B,C,D,E) = P(A)\,P(B)\,P(C \mid A,B)\,P(D \mid B,C)\,P(E \mid C,D)$$

Sampling from Bayesian Networks

- Sampling from discrete Bayesian networks with no observations is straight-forward, using ancestral sampling
- Bayesian network specifies factorization of joint distribution

$$P(z_1, \ldots, z_n) = \prod_{i=1}^{n} P(z_i | pa(z_i))$$

- Sample in-order, sample parents before children
  - Possible because graph is a DAG
- Choose value for z_i from $p(z_i | pa(z_i))$

Ancestral Sampling

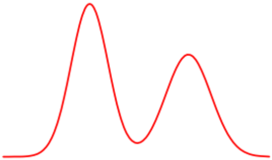
Given a DAG model

- Start by sampling from $P(x_1)$
- Then sample from $P(x_2|x_1)$
- Then sample from $P(x_3|x_2)$
- Finally sample from $P(x_4|x_3)$

$\{x_1, x_2, x_3, x_4\}$ is a sample from the joint distribution

Basic Sampling Algorithm

How to generate samples from simple non-uniform distributions assuming we can generate samples from uniform distribution.



Define: $h(y) = \int_{-\infty}^{y} p(\hat{y}) d\hat{y}$

Sample: $z \sim U[0, 1]$.

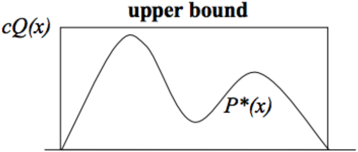
Then: $y = h^{-1}(z)$ is a sample from $p(y)$.

Problem: Computing cumulative $h(y)$ is just as hard!

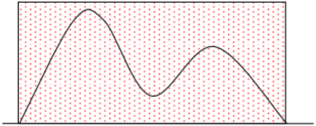
Rejection Sampling

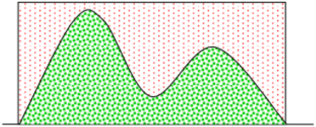
Need a proposal density Q(x) [e.g. uniform or Gaussian], and a constant c such that c(Qx) is an upper bound for P*(x)

Example with Q(x) uniform



generate uniform random samples in upper bound volume





accept samples that fall below the P*(x) curve

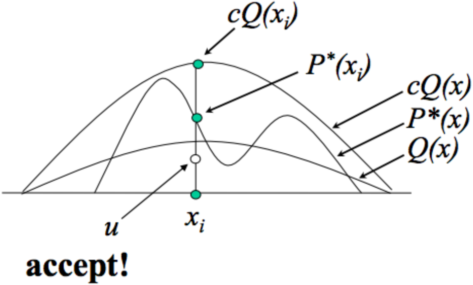
the marginal density of the x coordinates of the points is then proportional to P*(x)

Note the relationship to Monte Carlo integration.

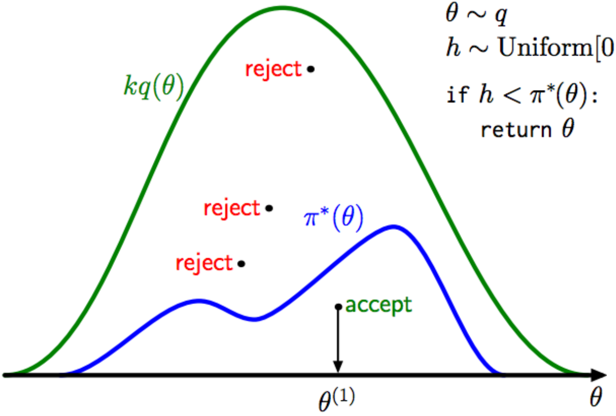
Rejection Sampling

More generally:

1) generate sample x_i from a proposal density $Q(x)$
2) generate sample u from uniform $[0, cQ(x_i)]$
3) if $u <= P^*(x_i)$ accept x_i; else reject



Rejection Sampling



while true:

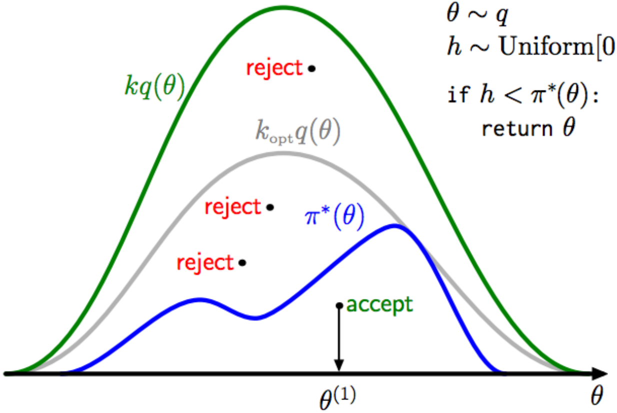
  $\theta \sim q$

  $h \sim \mathrm{Uniform}[0, kq(\theta)]$

  if $h < \pi^*(\theta)$:

    return θ

Rejection Sampling




```
while true:
    θ ~ q
    h ~ Uniform[0, kq(θ)]
    if h < π*(θ):
        return θ
```

Importance Sampling

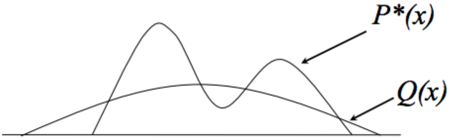
Not for generating samples. It is a method to estimate the expected value of a function $f(x_i)$ directly

- Generate x_i directly from $Q(x)$
- An empirical estimate of $\mathbb{E}_Q(f(x))$, the expected value of $f(x)$ under the distribution $Q(x)$ is then

$$\mathbb{E}_Q(f(x)) = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \tag{3}$$

- However, we want $\mathbb{E}_P(f(x))$ which is the expected value of $f(x)$ under the distribution $P(x)$

Importance Sampling



When we generate from Q(x), values of x where Q(x) is greater than P*(x) are overrepresented, and values where Q(x) is less than P*(x) are underrepresented.

To mitigate this effect, introduce a weighting term

$$w_i = \frac{P^*(x_i)}{Q(x_i)}$$

Importance Sampling

New procedure to estimate $E_P(f(x))$:

1) Generate N samples x_i from $Q(x)$

2) form importance weights

$$w_i = \frac{P^*(x_i)}{Q(x_i)}$$

3) compute empirical estimate of $E_P(f(x))$, the expected value of $f(x)$ under distribution $P(x)$, as

$$\hat{E}_P(f(x)) = \frac{\sum w_i f(x_i)}{\sum w_i}$$

Importance Sampling

Computing $\tilde{P}(x)$ and $\tilde{Q}(x)$, then *throwing* x *away* seems wasteful
Instead rewrite the integral as an expectation under Q:

$$\int f(x)P(x)\,\mathrm{d}x = \int f(x)\frac{P(x)}{Q(x)}Q(x)\,\mathrm{d}x, \qquad (Q(x) > 0 \text{ if } P(x) > 0)$$
$$\approx \frac{1}{S}\sum_{s=1}^{S} f(x^{(s)})\frac{P(x^{(s)})}{Q(x^{(s)})}, \quad x^{(s)} \sim Q(x)$$

This is just simple Monte Carlo again, so it is unbiased.

Importance sampling applies when the integral is not an expectation.
Divide and multiply any integrand by a convenient distribution.

Importance Sampling

Previous slide assumed we could evaluate $P(x) = \tilde{P}(x)/\mathcal{Z}_P$

$$\int f(x)P(x)\,\mathrm{d}x \approx \frac{\mathcal{Z}_Q}{\mathcal{Z}_P}\frac{1}{S}\sum_{s=1}^{S} f(x^{(s)}) \underbrace{\frac{\tilde{P}(x^{(s)})}{\tilde{Q}(x^{(s)})}}_{\tilde{r}^{(s)}}, \quad x^{(s)} \sim Q(x)$$

$$\approx \cancel{\frac{1}{S}}\sum_{s=1}^{S} f(x^{(s)}) \frac{\tilde{r}^{(s)}}{\cancel{\frac{1}{S}}\sum_{s'} \tilde{r}^{(s')}} \equiv \sum_{s=1}^{S} f(x^{(s)}) w^{(s)}$$

This estimator is **consistent** but **biased**

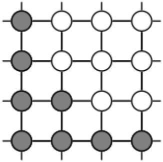
Summary so far

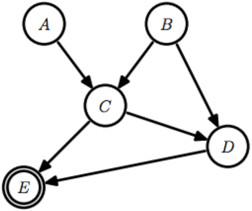
- Sums and integrals, often expectations, occur frequently in statistics
- **Monte Carlo** approximates expectations with a sample average
- **Rejection sampling** draws samples from complex distributions
- **Importance sampling** applies Monte Carlo to 'any' sum/integral

Application to Large Problems

We often can't decompose $P(X)$ into low-dimensional conditionals

Undirected graphical models: $P(x) = \frac{1}{\mathcal{Z}} \prod_i f_i(x)$





Posterior of a directed graphical model

$$P(A, B, C, D \,|\, E) = \frac{P(A, B, C, D, E)}{P(E)}$$

We often don't know $\mathcal{Z}$ or $P(E)$

Gibbs Sampling

For large graphical models, given a multivariate distribution, it is simpler to sample from a conditional distribution than to marginalize by integrating over a joint distribution

- We want samples approximate the joint distribution of all variables
- The marginal distribution of any subset of variables can be approximated by simply considering the samples for that subset of variables (Markov Blanket in Bayes Nets!)
- The expected value of any variable can be approximated by averaging over all the samples

Gibbs Sampling

A method with no rejections:

- Initialize $\mathbf{x}$ to some value
- Pick each variable in turn or randomly and resample $P(x_i|\mathbf{x}_{j\neq i})$

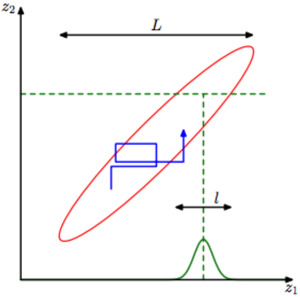
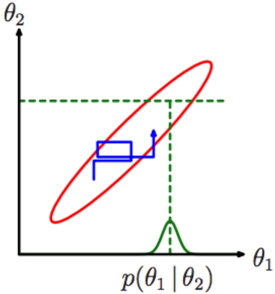


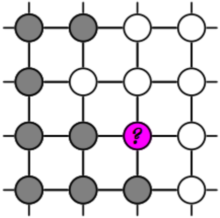
Figure from PRML, Bishop (2006)

Gibbs Sampling

Pick variables in turn or randomly,

and resample $p(\theta_i \,|\, \theta_{j\neq i})$



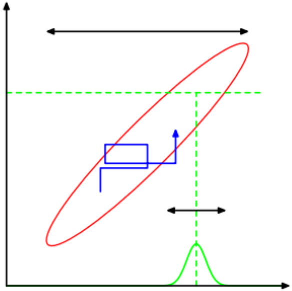


$$T_i(\theta' \leftarrow \theta) = p(\theta'_i \,|\, \theta_{j\neq i})\, \delta(\theta'_{j\neq i} - \theta_{j\neq i})$$

LHS adapted from Fig 11.11 Bishop PRML

Gibbs Sampler

Consider sampling from $p(z_1, ..., z_N)$.



Initialize z_i, $i = 1, ..., N$

For t=1,...,T

Sample $z_1^{t+1} \sim p(z_1 | z_2^t, ..., z_N^t)$

Sample $z_2^{t+1} \sim p(z_2 | z_1^{t+1}, x_3^t, ..., z_N^t)$

...

Sample $z_N^{t+1} \sim p(z_N | z_1^{t+1}, ..., z_{N-1}^{t+1})$

Gibbs sampler is a particular instance of M-H algorithm with proposals $p(z_n | \mathbf{z}_{i \neq n}) \rightarrow$ accept with probability 1. Apply a series (component-wise) of these operators.

Gibbs Sampling for Bayes Nets

1. Initialization
   - Set evidence variables E, to the observed values e
   - Set all other variables to random values (e.g. by forward sampling)

   This gives us a sample $x_1, \ldots, x_n$.
2. Repeat (as much as wanted)
   - Pick a non-evidence variable X_i uniformly randomly)
   - Sample x'_i from $P(X_i | x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$.
   - Keep all other values: $x'_j = x_j, \forall j \neq i$
   - The new sample is $x'_1, \ldots, x'_n$
3. Alternatively, you can march through the variables in some predefined order

Why Gibbs works in Bayes Nets

- The key step is sampling according to $P(X_i|x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$. How do we compute this?
- In Bayes nets, we know that a variable is conditionally independent of all others given its Markov blanket (parents, children, spouses)

$$P(X_i|x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) = P(X_i|\text{MarkovBlanket}(X_i))$$

- So we need to sample from $P(X_i|\text{MarkovBlanket}(X_i))$
- Let $Y_j, j = 1, \ldots, k$ be the children of X_i. It is easy to show that:

$$\begin{aligned} P(X_i = x_i|\text{MarkovBlanket}(X_i)) \quad \propto \quad & P(X_i = x_i|\text{Parents}(X_i)) \cdot \\ & \cdot \prod_{j=1}^{k} P(Y_j = y_j|\text{Parents}(Y_j)) \end{aligned}$$

Summary

Ways of doing inference in graphical models...

Exact Inference

- Message Passing algorithms

Approximate Inference (Sampling Methods)

- Monte-Carlo Sampling
- Importance Sampling
- Gibbs Sampling in Bayesian Networks

Note : We will cover Sampling Methods in more details when we talk about Approximate Inference and Variational Methods (later...)