NUS National University of Singapore | School of Computing

CS5340
Uncertainty Modeling in AI

Lecture 9:
Monte Carlo Inference (Sampling)

Assoc. Prof. Lee Gim Hee

AY 2022/23

Semester 1

Course Schedule

Week	Date	Topic	Remarks
1	10 Aug	Introduction to probabilistic reasoning	**Assignment 0:** Python Numpy Tutorial (Ungraded)
2	17 Aug	Bayesian networks (Directed graphical models)	
3	24 Aug	Markov random Fields (Undirected graphical models)	
4	31 Aug	Variable elimination and belief propagation	**Assignment 1:** Belief propagation and maximal probability (15%)
5	07 Sep	Factor graph and the junction tree algorithm	
6	14 Sep	Parameter learning with complete data	**Assignment 1:** Due **Assignment 2:** Junction tree and parameter learning (15%)
-	21 Sep	Recess week	**No lecture**
7	28 Sep	Mixture models and the EM algorithm	**Assignment 2:** Due
8	05 Oct	Hidden Markov Models (HMM)	**Assignment 3:** Hidden Markov model (15%)
9	12 Oct	Monte Carlo inference (Sampling)	
*	15 Oct	Variational inference	Makeup Lecture (LT15) Time: 9.30am – 12.30pm (Saturday)
10	19 Oct	Variational Auto-Encoder and Mixture Density Networks	**Assignment 3:** Due **Assignment 4:** MCMC Sampling (15%)
11	26 Oct	No Lecture	I will be traveling
12	02 Nov	Graph-cut and alpha expansion	**Assignment 4:** Due
13	09 Nov	-	

Acknowledgements

- A lot of slides and content of this lecture are adopted from:

1. "An introduction to MCMC for Machine Learning", Christophe Andrieu et. al.
   http://www.cs.bham.ac.uk/~axk/mcmc1.pdf

2. "Pattern Recognition and Machine Learning", Christopher Bishop, Chapter 11.

3. http://www.cs.cmu.edu/~epxing/Class/10708/lectures/lecture16-MC.pdf
   http://www.cs.cmu.edu/~epxing/Class/10708/lectures/lecture17-MCMC.pdf, Eric Xing, CMU.

4. "Machine Learning – A Probabilistic Perspective", Kevin Murphy, Chapter 23.

5. "Probabilistic Graphical Models", Daphne Koller and Nir Friedman, chapter 12.

Learning Outcomes

- Students should be able to:

1. Explain the Monte Carlo principle and its justification for sampling methods.

2. Apply Rejection, Importance, Metropolis-Hasting, Metropolis and Gibbs sampling methods to do maximal probability, approximate inference, and expectation.

3. Use Markov chain properties, i.e. homogenous, stationary distribution, irreducibility, aperiod, egordic and detail balance, to show validity of MH algorithm.

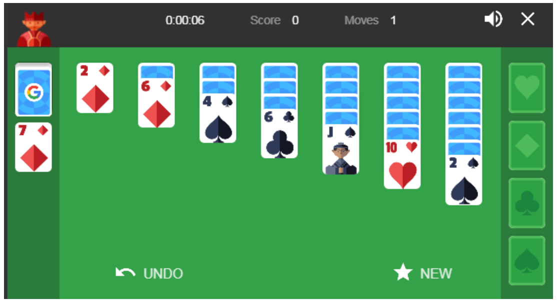
History of Monte Carlo Sampling

Metropolis algorithm is selected as one of the top 10 algorithms that had the greatest influence on science and engineering in the 20th century.

[Beichl & Sullivan 2000]

History of Monte Carlo Sampling

- Invented by Stan Ulam in 1946 when he was playing solitaire, while convalescing from an illness.



- Occurred to him to try to compute the chances that a particular solitaire laid out with 52 cards would come out successfully.


Stanislaw Ulam
1909-1984

- He attempted exhaustive combinatorial calculations, but decided to lay out several solitaires at random and then observing and counting the number of successful plays.

Image source: https://en.wikipedia.org/wiki/Stanislaw_Ulam

Idea Behind Monte Carlo Sampling

Ulam's idea of selecting a statistical sample to approximate a hard combinatorial problem by a much simpler problem is at the heart of modern Monte Carlo simulation.

Pioneers of Monte Carlo Sampling

Stanislaw Ulam
1909-1984

John von Neumann
1903-1957

Nicholas Metropolis
1915-1999

Marshall Rosenbluth
1927-2003

Edward Teller
1908-2003

Augusta H. Teller
1909-2000

Why Do We Need Sampling?

Bayesian inference and learning:

Given some unknown variables $X \in \mathcal{X}$ and data $Y \in \mathcal{Y}$, the following typically intractable integration problems are central to Bayesian statistics.

1. **Normalization**. To obtain the posterior $p(x \mid y)$ given the prior $p(x)$ and likelihood $p(y \mid x)$, the normalizing factor in Bayes' theorem needs to be computed

$$p(x \mid y) = \frac{p(y \mid x)p(x)}{\int_{\mathcal{X}} p(y \mid x')p(x')\,dx'}$$

Intractable to compute in large dimensional space

Why Do We Need Sampling?

2. **Marginalization**: Given the joint posterior of $(X, Z) \in \mathcal{X} \times \mathcal{Z}$, we may often be interested in the marginal posterior.

$$p(x \mid y) = \int_{\mathcal{Z}} p(x, z \mid y)\, dz$$

Intractable to compute in large dimensional space

3. **Expectation**: The objective of the analysis is often to obtain summary statistics of the form

$$\mathbb{E}_{p(x|y)}(f(x)) = \int_{\mathcal{X}} f(x) p(x \mid y)\, dx$$

Intractable to compute in large dimensional space

for some function of interest $f : \mathcal{X} \rightarrow \mathbb{R}^{n_f}$ integrable with respect to $p(x \mid y)$.

Why Do We Need Sampling?

Optimization:

- The goal of optimization is to extract the solution that minimizes some objective function from a large set of feasible solutions.
- This set can be continuous and unbounded.
- In general, it is too computationally expensive to compare all the solutions to find out which one is optimal.

The Monte Carlo Principle

- Draw an i.i.d. set of samples $\{x^{(i)}\}_{i=1}^{N}$ from a target density $p(x)$ defined on a high-dimensional space $\mathcal{X}$.

- E.g. the set of possible configurations of a system, the space on which the posterior is defined, or the combinatorial set of feasible solutions.

- These N samples can be used to approximate the target density with the following empirical point-mass function:

$$p_N(x) = \frac{1}{N} \sum_{i=1}^{N} \delta_{x^{(i)}}(x)$$

Delta-Dirac mass located at $x(i)$

Weak vs Strong Law of Large Numbers

- **Weak law of large numbers:** the sample average, $\bar{X}$ converges in probability towards the expected value, μ, i.e.,

$$\overline{X}_n \xrightarrow{P} \mu \qquad \text{when } n \to \infty.$$

- That is, for any positive number ε,

$$\lim_{n\to\infty} \Pr\left(|\overline{X}_n - \mu| > \varepsilon \right) = 0.$$

where

$$\bar{X} = \frac{1}{N} \sum_n X_n \quad \text{and} \quad \mu = \int X p(X) dX$$

Weak vs Strong Law of Large Numbers

- **Strong law of large numbers**: the sample average, $\bar{X}$ converges almost surely to the expected value, μ, i.e.,

$$\bar{X}_n \xrightarrow{\text{a.s.}} \mu \qquad \text{when } n \to \infty.$$

- That is,

$$\Pr\left(\lim_{n\to\infty} \bar{X}_n = \mu\right) = 1.$$

where

$$\bar{X} = \frac{1}{N}\sum_n X_n \quad \text{and} \quad \mu = \int Xp(X)dX$$

The Monte Carlo Principle

- Consequently, we can approximate the integrals (or very large sums) $I(f)$ with tractable sums $I_N(f)$ that converge as follows:

$$\underbrace{I_N(f) = \frac{1}{N}\sum_{i=1}^{N} f\left(x^{(i)}\right)}_{\text{Similar to } \bar{X}} \xrightarrow[N\to\infty]{a.s.} \underbrace{I(f) = \int_{\mathcal{X}} f(x)p(x)\,dx}_{\text{Similar to } \mu}$$

- That is, the estimate $I_N(f)$ is unbiased and by the strong law of large numbers, it will almost surely converge to $I(f)$.

The Monte Carlo Principle

- If the variance (in the univariate case for simplicity) of $f(x)$ satisfies:

$$\sigma_f^2 \triangleq \mathbb{E}_{p(x)}\big(f^2(x)\big) - I^2(f) < \infty,$$

- Then the variance of the estimator $I_N(f)$ is equal to:

$$\operatorname{var}\big(I_N(f)\big) = \frac{\sigma_f^2}{N},$$

The Monte Carlo Principle

Proof:

$$Var(X) = \mathbb{E}[(X - \mathbb{E}[X])^2] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$$

$$\Longrightarrow Var(f) = \mathbb{E}_{p(x)}\left[\left(f - \mathbb{E}_{p(x)}[f]\right)^2\right]$$

$$= \mathbb{E}_{p(x)}[f^2] - \mathbb{E}_{p(x)}[f]^2 = \mathbb{E}_{p(x)}[f^2] - I(f)^2 = \sigma_f^2$$

$$Var(\bar{X}) = Var\left(\frac{1}{N}\sum_n X_n\right) = \frac{1}{N^2}\sum_n Var(X_n) = \frac{\sigma^2}{N}$$

Let $\bar{X} \coloneqq I_N(f)$ and $X \coloneqq f$, we get:

$$Var(I_N(f)) = Var\left(\frac{1}{N}\sum_n f_n\right) = \frac{1}{N^2}\sum_n Var(f_n) = \frac{\sigma_f^2}{N}$$

$\square$

The Monte Carlo Principle

- and a central limit theorem yields convergence in distribution of the error:

Convergence in distribution

$$\sqrt{N}(I_N(f) - I(f)) \underset{N\to\infty}{\Longrightarrow} \mathcal{N}(0, \sigma_f^2) \quad .$$

- The N samples can also be used to obtain a maximum of the objective function $p(x)$ as follows:

$$\hat{x} = \underset{x^{(i)}; i=1,\ldots,N}{\arg\max} \; p\left(x^{(i)}\right)$$

Non-Parametric Representation

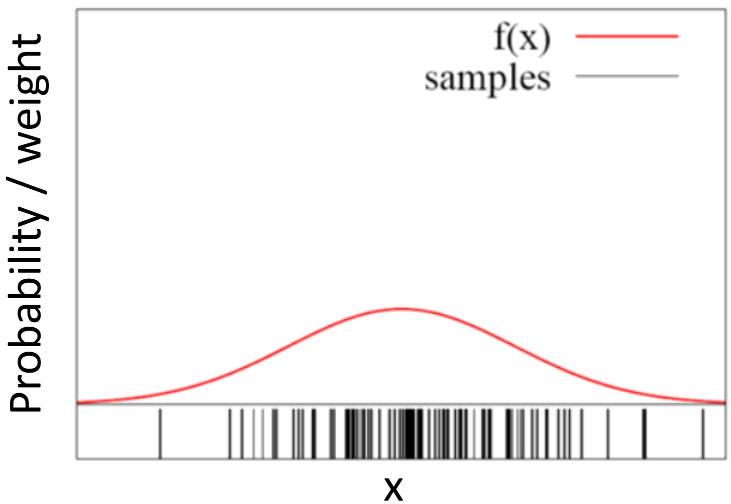
Probability distributions can be represented:

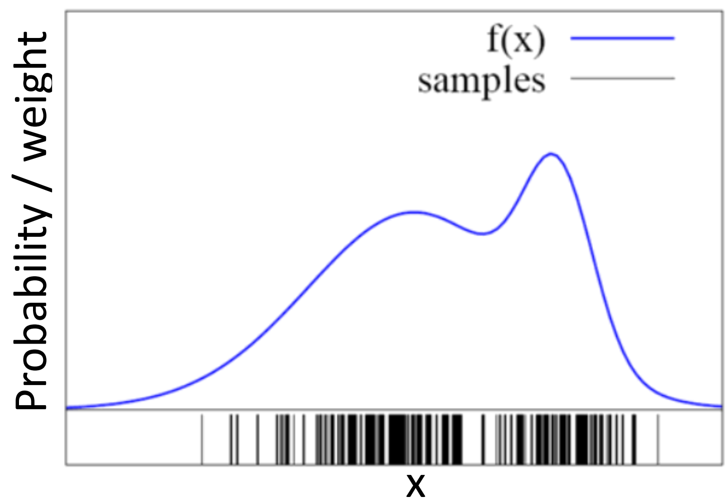
1. Parametrically: e.g. using mean and covariance of a Gaussian, or
2. Non-parametrically: using a set of *hypotheses* (samples) drawn from the distribution.

Advantage of non-parametric representation:

- No restriction on the *type* of distribution (e.g. can be multi-modal, non-Gaussian, etc)

Non-Parametric Representation





The more samples are in an interval, the higher the probability of that interval.

But:

How to draw samples from a function/distribution?

Rejection Sampling

- Suppose we wish to sample from a distribution $p(z)$, where direct sampling is difficult.

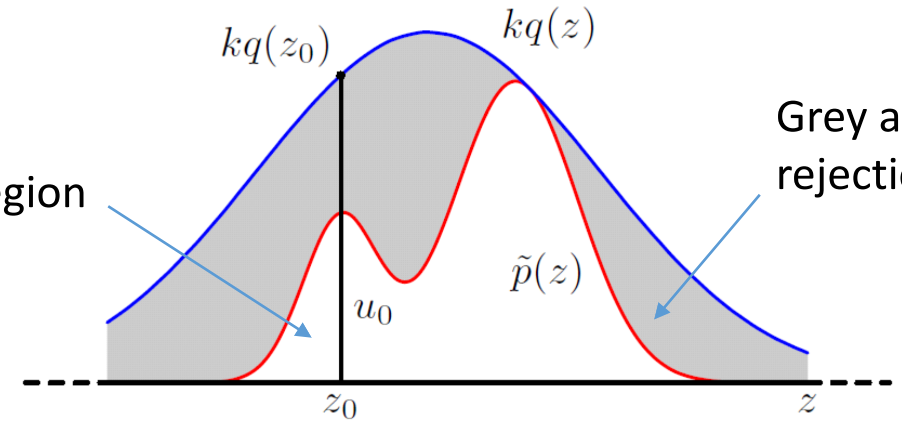
- Furthermore, suppose that we are unable to easily evaluate $p(z)$ due to an unknown normalizing constant Z_p, so that:

$$p(z) = \frac{1}{Z_p}\widetilde{p}(z)$$

- Where $\tilde{p}(z)$ can readily be evaluated.

Rejection Sampling

White area: acceptance region



Grey area: rejection region

Algorithm : Rejection Sampling

Set $i = 1$
Repeat until $i = N$ // draw N samples

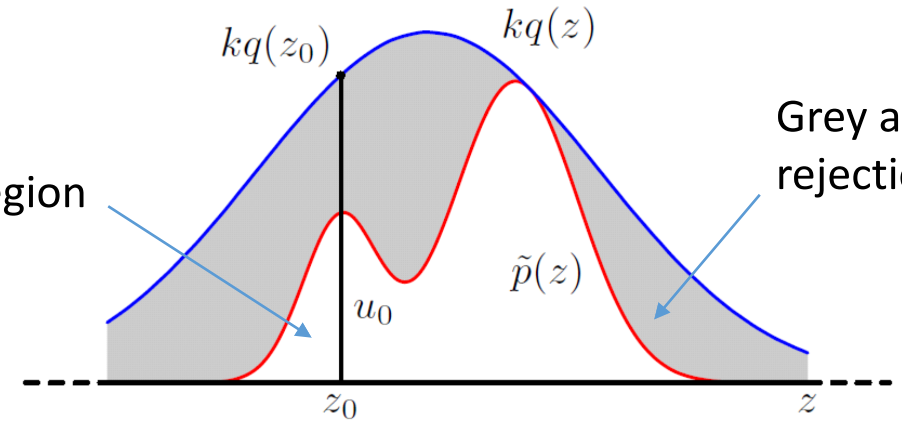
Proposal distribution $q(z)$ is an easier-to-sample distribution e.g. Gaussian!

1. Sample $z^{(i)} \sim q(z)$ and $u \sim U_{(0,1)}$ // sample from proposal distribution $q(z)$ // sample from uniform distribution $U_{(0,1)}$
2. If $u < \frac{\tilde{p}(z^{(i)})}{kq(z^{(i)})}$, then accept $z^{(i)}$ and increment the counter i by 1.
3. Otherwise, reject.

Image source: "Machine Learning and Pattern Recognition", Christopher Bishop

Rejection Sampling

White area: acceptance region



Grey area: rejection region

Algorithm : Rejection Sampling

Set $i = 1$
Repeat until $i = N$ // draw N samples

Accept proposal $z^{(i)}$ when u falls in the acceptance region.

1. Sample $z^{(i)} \sim q(z)$ and $u \sim U_{(0,1)}$ // sample from proposal distribution $q(z)$ // sample from uniform distribution $U_{(0,1)}$
2. If $u < \frac{\tilde{p}(z^{(i)})}{kq(z^{(i)})}$, then accept $z^{(i)}$ and increment the counter i by 1.
3. Otherwise, reject.

// accept proposal $z^{(i)}$ if $u < \frac{\tilde{p}(z^{(i)})}{kq(z^{(i)})}$,
// constant k is chosen such that $\tilde{p}(z^{(i)}) \leq kq(z)$ for all values of z

Image source: "Machine Learning and Pattern Recognition", Christopher Bishop

Rejection Sampling: Limitations

- It is not always possible to bound $\frac{\tilde{p}(z)}{q(z)}$ with a reasonable constant k over the whole space $\mathcal{Z}$.

- If k is too large, the acceptance probability:

$$\Pr(z \text{ accepted}) = \Pr\left(u < \frac{\tilde{p}(z)}{kq(z)}\right) = \frac{1}{k},$$

  will be too small.

- This makes the method impractical in high dimensional space scenarios.

Importance Sampling

- Given a target distribution $p(z)$ which is difficult to draw samples directly.

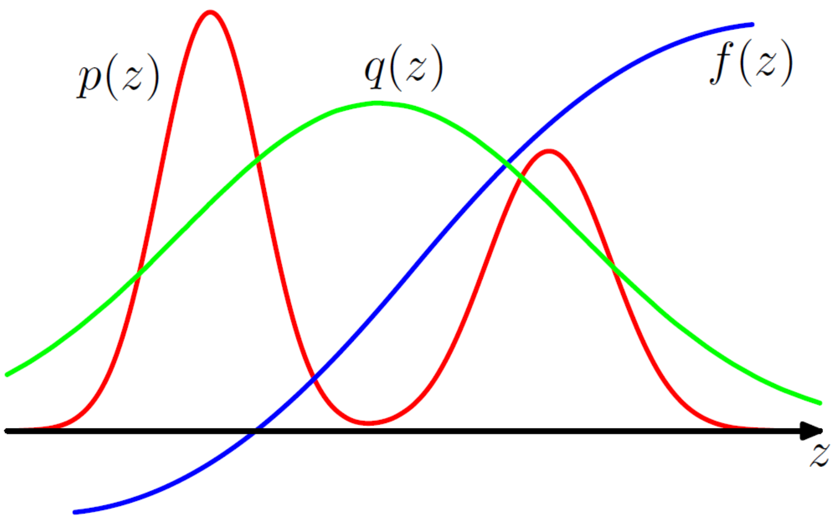
- Importance sampling provides a framework for approximating expectations of a function $f(z)$ w.r.t. $p(z)$.

- Samples $\{z^{(l)}\}$ are drawn from a simpler distribution $q(z)$, i.e. proposal distribution.

Importance Sampling

- Express expectation in the form of a finite sum over samples $\{z^{(l)}\}$ weighted by the ratios $p(z^{(l)})/q(z^{(l)})$:

$$\begin{aligned}\mathbb{E}[f] &= \int f(\mathbf{z})p(\mathbf{z})\,\mathrm{d}\mathbf{z} \\ &= \int f(\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}q(\mathbf{z})\,\mathrm{d}\mathbf{z} \\ &\simeq \frac{1}{L}\sum_{l=1}^{L}\frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})}f(\mathbf{z}^{(l)}).\end{aligned}$$



Recall:

$$I_N(f) = \frac{1}{N}\sum_{i=1}^{N} f\left(x^{(i)}\right) \xrightarrow[N\to\infty]{a.s.} I(f) = \int_{\mathcal{X}} f(x)p(x)\,dx$$

Image source: "Machine Learning and Pattern Recognition", Christopher Bishop

Importance Sampling

- The quantities $r_l = p(z^{(l)})/q(z^{(l)})$ are known as importance weights.

- And they correct the bias introduced by sampling from the wrong distribution.

- Note that, unlike rejection sampling, all the samples generated are retained.

Importance Sampling

- Often the case that $\tilde{p}(z)$ can be evaluated easily, but not $p(z) = \tilde{p}(z)/Z_p$, where Z_p is unknown.

- Let us define the proposal distribution in similar form, i.e. $q(z) = \tilde{q}(z)/Z_q$.

- We then have:

$$\begin{aligned}\mathbb{E}[f] &= \int f(\mathbf{z})p(\mathbf{z})\,\mathrm{d}\mathbf{z} \\ &= \frac{Z_q}{Z_p}\int f(\mathbf{z})\frac{\widetilde{p}(\mathbf{z})}{\widetilde{q}(\mathbf{z})}q(\mathbf{z})\,\mathrm{d}\mathbf{z} \\ &\simeq \frac{Z_q}{Z_p}\frac{1}{L}\sum_{l=1}^{L}\widetilde{r}_l f(\mathbf{z}^{(l)}),\end{aligned}$$

where $\widetilde{r}_l = \dfrac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})}$.

Importance Sampling

- We can use the same sample set to evaluate the ratio Z_p/Z_q with the result:

$$\frac{Z_p}{Z_q} = \frac{1}{Z_q}\int \widetilde{p}(\mathbf{z})\,\mathrm{d}\mathbf{z} = \int \frac{\widetilde{p}(\mathbf{z})}{\widetilde{q}(\mathbf{z})} q(\mathbf{z})\,\mathrm{d}\mathbf{z}$$

$$\simeq \frac{1}{L}\sum_{l=1}^{L} \widetilde{r}_l \qquad \text{where} \quad \widetilde{r}_l = \frac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})}.$$

- And hence

$$\mathbb{E}[f] \simeq \sum_{l=1}^{L} w_l f(\mathbf{z}^{(l)})$$

where

$$w_l = \frac{\widetilde{r}_l}{\sum_m \widetilde{r}_m} = \frac{\widetilde{p}(\mathbf{z}^{(l)})/q(\mathbf{z}^{(l)})}{\sum_m \widetilde{p}(\mathbf{z}^{(m)})/q(\mathbf{z}^{(m)})}.$$

Important weight which is easy to compute!

Importance Sampling

Proof:

Substituting $\frac{Z_p}{Zq} = \frac{1}{L}\sum_m \tilde{r}_m$ into $\mathbb{E}[f] = \frac{Z_q}{Z_p}\frac{1}{L}\sum_l \tilde{r}_l f\left(z^{(l)}\right)$,

we get:

$$\mathbb{E}[f] = \frac{L}{\sum_m \tilde{r}_m}\frac{1}{L}\sum_l \tilde{r}_l f\left(z^{(l)}\right)$$

$$= \sum_l \frac{\tilde{r}_l}{\sum_m \tilde{r}_m} f\left(z^{(l)}\right)$$

$$= \sum_l w_l f\left(z^{(l)}\right)$$

□

Importance Sampling: Limitations

- Success of the importance sampling approach depends crucially on how well $q(z)$ matches $p(z)$.
- A strongly varying $p(z)f(z)$ has a significant proportion of its mass concentrated over relatively small regions of z space.
- Set of importance weights $\{r_l\}$ may be dominated by a few weights having large values, with the remaining weights being relatively insignificant.

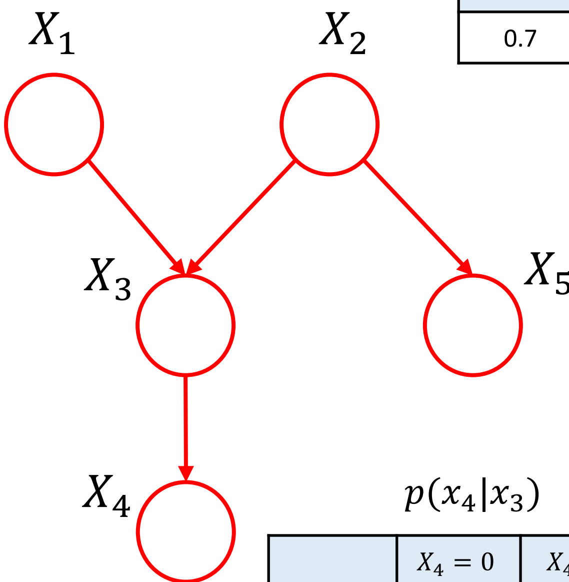
Importance Sampling: Example on a Bayesian Network

$p(x_1)$

$X_1 = 0$	$X_1 = 1$
0.6	0.4

$p(x_2)$

$X_2 = 0$	$X_2 = 1$
0.7	0.3



$p(x_3|x_1,x_2)$

	$X_3 = 0$	$X_3 = 1$	$X_3 = 2$
$X_1 = 0, X_2 = 0$	0.3	0.4	0.3
$X_1 = 0, X_2 = 1$	0.05	0.25	0.7
$X_1 = 1, X_2 = 0$	0.9	0.08	0.02
$X_1 = 1, X_2 = 1$	0.5	0.3	0.2

$p(x_5|x_2)$

	$X_5 = 0$	$X_5 = 1$
$X_2 = 0$	0.95	0.05
$X_2 = 1$	0.2	0.8

$p(x_4|x_3)$

	$X_4 = 0$	$X_4 = 1$
$X_3 = 0$	0.1	0.9
$X_3 = 1$	0.4	0.6
$X_3 = 2$	0.99	0.01

How do we compute $p(x_1, x_4, x_5 \mid x_2 = 1, x_3 = 1)$?

X_1: Difficulty, X_2: Intelligence, X_3: Grade, X_4: Letter, X_5: SAT score

Importance Sampling: Example on a Bayesian Network

- How do we compute $p(x_1, x_4, x_5 \,|x_2 = 1, x_3 = 1)$?

Importance Sampling!!!

$$p(x_1, x_4, x_5 \,|x_2 = 1, x_3 = 1) = \frac{p(x_1, x_4, x_5, x_2 = 1, x_3 = 1)}{p(x_2 = 1, x_3 = 1)}$$

$$= \frac{p(x_F, x_E)}{p(x_E)}$$

$$= \frac{1}{Z_p}\tilde{p}(x)$$

We don't want to evaluate Z_p

Target distribution

- What should we use as the proposal distribution $q(x)$?

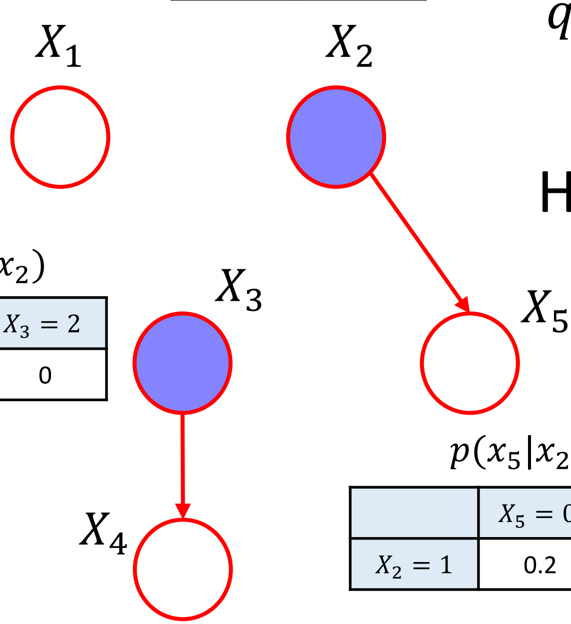
Importance Sampling: Example on a Bayesian Network

$p(x_1)$

$X_1 = 0$	$X_1 = 1$
0.6	0.4

$p(x_2 = 1)$

$X_2 = 0$	$X_2 = 1$
0	1



$p(x_3 = 1|x_1, x_2)$

$X_3 = 0$	$X_3 = 1$	$X_3 = 2$
0	1	0

$p(x_5|x_2 = 1)$

	$X_5 = 0$	$X_5 = 1$
$X_2 = 1$	0.2	0.8

$p(x_4|x_3 = 1)$

	$X_4 = 0$	$X_4 = 1$
$X_3 = 1$	0.4	0.6

Proposal distribution:

$$q(x_1, x_4, x_5) = p(x_1)p(x_4|x_3 = 1)p(x_5|x_2 = 1)$$

How do we sample from $q(x_1, x_4, x_5)$?

$$x_1 \sim p(x_1)$$

$$x_4 \sim p(x_4|x_3 = 1)$$

$$x_5 \sim p(x_5|x_2 = 1)$$

e.g. randomly generate a number within [0,1] (uniform distribution), i.e. $n = \text{rand}$; $x_1 = 0$ if $n < 0.6$, $x_1 = 1$ otherwise.

Importance Sampling: Example on a Bayesian Network

- For each sample $x^{(l)}$, we evaluate the weight as:

$$w_l = \frac{\tilde{r}_l}{\sum_m \tilde{r}_m} = \frac{\tilde{p}\big(x^{(l)}\big)/q\big(x^{(l)}\big)}{\sum_m \tilde{p}\big(x^{(m)}\big)/q\big(x^{(m)}\big)}.$$

- Example:

$x^{(l)}$: $\{x_1 = 0, x_4 = 1, x_5 = 1\}$ obtained from sampling, we have

$$\begin{aligned}\tilde{p}\big(x^{(l)}\big) &= p(x_1 = 0, x_4 = 1, x_5 = 1, x_2 = 1, x_3 = 1)\\ &= p(x_1 = 0)p(x_2 = 1)p(x_3 = 1 | x_2 = 1, x_1 = 0)\\ &\qquad p(x_4 = 1 \mid x_3 = 1)p(x_5 = 1 \mid x_2 = 1)\\ &= (0.6)(0.3)(0.25)(0.6)(0.8)\\ &= 0.0216\end{aligned}$$

Importance Sampling: Example on a Bayesian Network

- For each sample $x^{(l)}$, we evaluate the weight as:

$$w_l = \frac{\tilde{r}_l}{\sum_m \tilde{r}_m} = \frac{\tilde{p}\left(x^{(l)}\right)/q\left(x^{(l)}\right)}{\sum_m \tilde{p}\left(x^{(m)}\right)/q\left(x^{(m)}\right)}.$$

- Example:

$x^{(l)}: \{x_1 = 0, x_4 = 1, x_5 = 1\}$ obtained from sampling, we have

$$q\left(x^{(l)}\right) = p(x_1 = 0)p(x_4 = 1|x_3 = 1)p(x_5 = 1|x_2 = 1)$$

$$= (0.6)(0.6)(0.8) = 0.288$$

$$\Rightarrow \frac{\tilde{p}\left(x^{(l)}\right)}{q\left(x^{(l)}\right)} = \frac{0.0216}{0.288} = 0.075$$

- Finally, denominator (hence each weight w_l) can be computed from all M samples.

Importance Sampling: Example on a Bayesian Network

- We can compute $p(x_1, x_4, x_5 \,|x_2 = 1, x_3 = 1)$ from all the weights and samples:

Sum of all weights from samples at $\{x_1 = 0, x_4 = 0, x_5 = 0\,\}$

$$p(x_1 = 0, x_4 = 0, x_5 = 0 \,|x_2 = 1, x_3 = 1) = \frac{\boxed{\sum_m w_m \delta(x^{(m)} = \{x_1 = 0, x_4 = 0, x_5 = 0\})}}{\boxed{\sum_m w_m}}$$

normalizer: ensure probability sums to 1

$$\vdots$$

$$p(x_1 = 1, x_4 = 1, x_5 = 1 \,|x_2 = 1, x_3 = 1) = \frac{\sum_m w_m \delta(x^{(m)} = \{x_1 = 1, x_4 = 1, x_5 = 1\})}{\sum_m w_m}$$

- In summary, we get:

$$p(x_F \,|x_E) = \frac{\sum_m w_m \delta(x^{(m)})}{\sum_m w_m}$$

Sampling and the EM Algorithm

- Sampling methods can be used to approximate the E step of the EM algorithm for models in which the E step cannot be performed analytically.

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \int \underbrace{p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})}_{\text{Cannot be computed analytically!}} \ln p(\mathbf{Z}, \mathbf{X}|\boldsymbol{\theta}) \, \mathrm{d}\mathbf{Z}$$

Sampling and the EM Algorithm

- Approximate integral by a finite sum over samples $\{Z^l\}$, which are drawn from the current estimate for $p(Z \mid X, \theta^{old})$, so that:

$$Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) \simeq \frac{1}{L} \sum_{l=1}^{L} \ln p(\mathbf{Z}^{(l)}, \mathbf{X} | \boldsymbol{\theta})$$

- The Q function is then optimized in the usual way in the M step.

- This procedure is called the Monte Carlo EM algorithm.

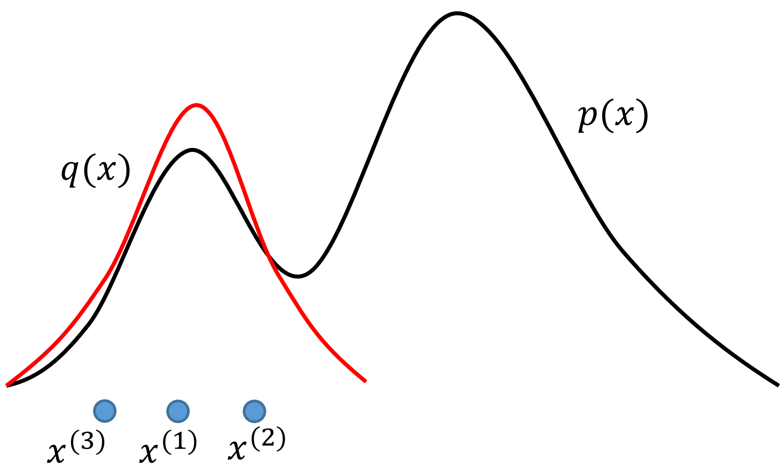
Markov Chain Monte Carlo (MCMC)

- MCMC is a strategy for generating samples $x^{(i)}$ while exploring the state space $\mathcal{X}$ using a Markov chain.
- The chain is constructed to spend more time in the most important regions.
- In particular, it is constructed so that the samples $x^{(i)}$ mimic samples drawn from the target distribution $p(x)$.

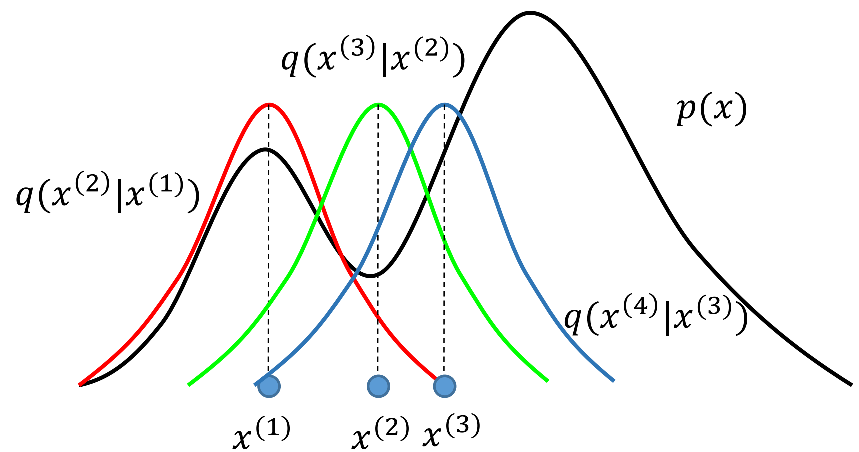
Markov Chain Monte Carlo (MCMC)

- MCMC algorithms feature adaptive proposals:
  - Instead of $q(x')$, we use $q(x'|x)$ where x' is the new state being sampled, and x is the previous sample.
  - As x changes, $q(x'|x)$ can also change (as a function of x').

Importance sampling with bad proposal $q(x)$



MCMC with adaptive proposal $q(x'|x)$



MCMC: Metropolis-Hasting Algorithm

Algorithm : Metropolis-Hasting

1. Initialize $x^{(0)}$
2. For $i = 0$ to $N - 1$
3. Sample $u \sim \mathcal{U}_{[0,1]}$ // draw acceptance threshold
4. Sample $x' \sim q(x' | \, x^{(i)})$ // draw from proposal
5. If $u < \mathcal{A}\left(x', x^{(i)}\right) = \min\left\{1, \frac{\tilde{p}(x')q(x^{(i)}|x')}{\tilde{p}(x^{(i)})q(x'|x^{(i)})}\right\}$ // acceptance probability
6. $x^{(i+1)} = x'$ // new sample is accepted
7. else
8. $x^{(i+1)} = x^{(i)}$ // new sample is rejected
// we create a duplicate of the previous sample

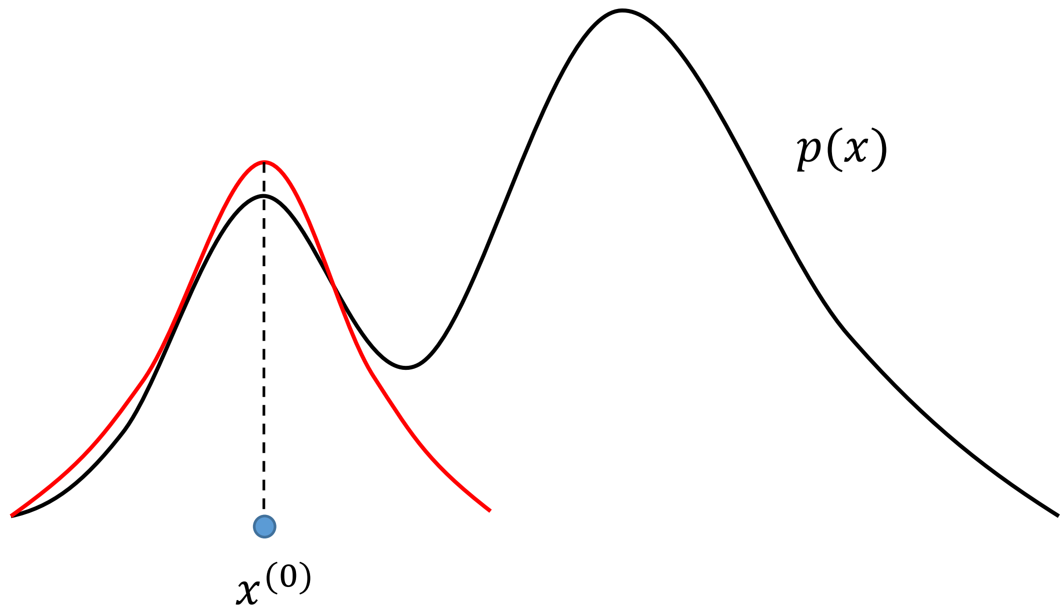
MCMC: Metropolis-Hasting Algorithm

Example:

- Our goal is to sample from a bimodal distribution $p(x)$.
- Let $q(x'|x)$ be a Gaussian centered on x.

$$\boxed{\mathcal{A}(x', x^{(i)}) = \min\left\{1, \frac{\tilde{p}(x')q(x^{(i)}|x')}{\tilde{p}(x^{(i)})q(x'|x^{(i)})}\right\}}$$

Initialize $x^{(0)}$



MCMC: Metropolis-Hasting Algorithm

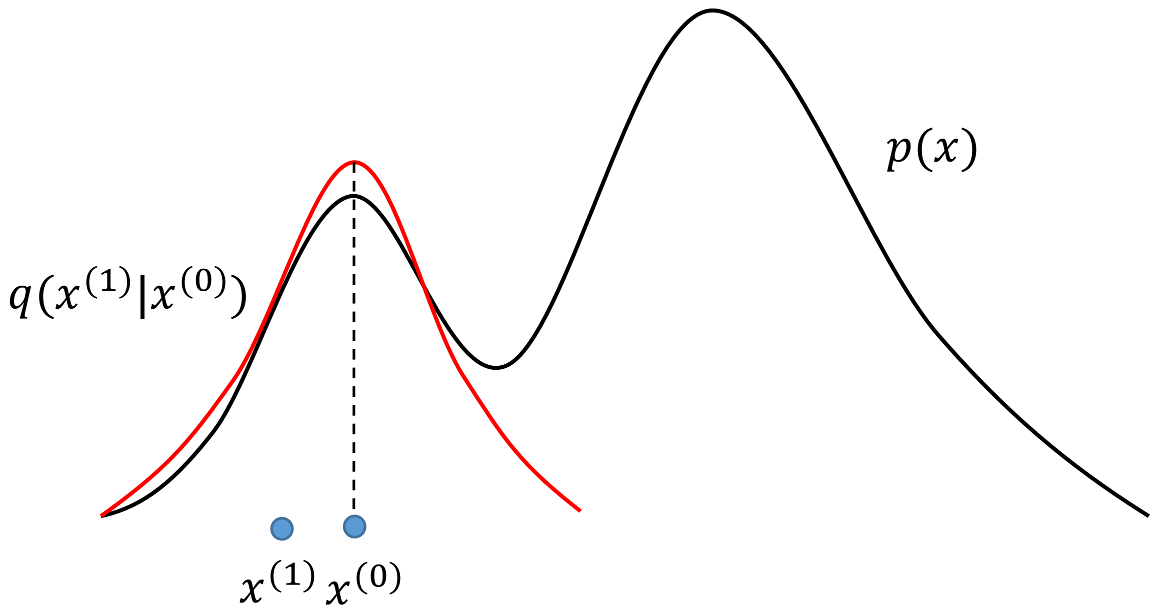
Example:

- Our goal is to sample from a bimodal distribution $p(x)$.
- Let $q(x'|x)$ be a Gaussian centered on x.

Initialize $x^{(0)}$

Draw, accept $x^{(1)}$

$$\mathcal{A}(x', x^{(i)}) = \min\left\{1, \frac{\tilde{p}(x')q(x^{(i)}|x')}{\tilde{p}(x^{(i)})q(x'|x^{(i)})}\right\}$$



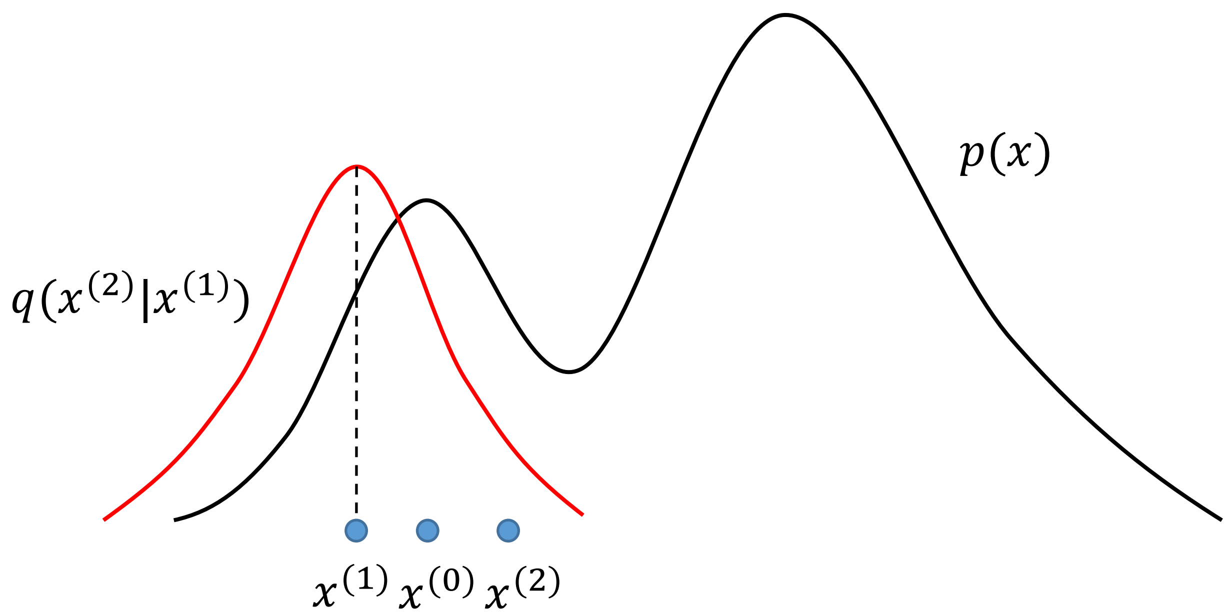
MCMC: Metropolis-Hasting Algorithm

Example:

- Our goal is to sample from a bimodal distribution $p(x)$.
- Let $q(x'|x)$ be a Gaussian centered on x.

$$\mathcal{A}\left(x', x^{(i)}\right) = \min\left\{1, \frac{\tilde{p}(x')q(x^{(i)}|x')}{\tilde{p}(x^{(i)})q(x'|x^{(i)})}\right\}$$

Initialize $x^{(0)}$
Draw, accept $x^{(1)}$
Draw, accept $x^{(2)}$



MCMC: Metropolis-Hasting Algorithm

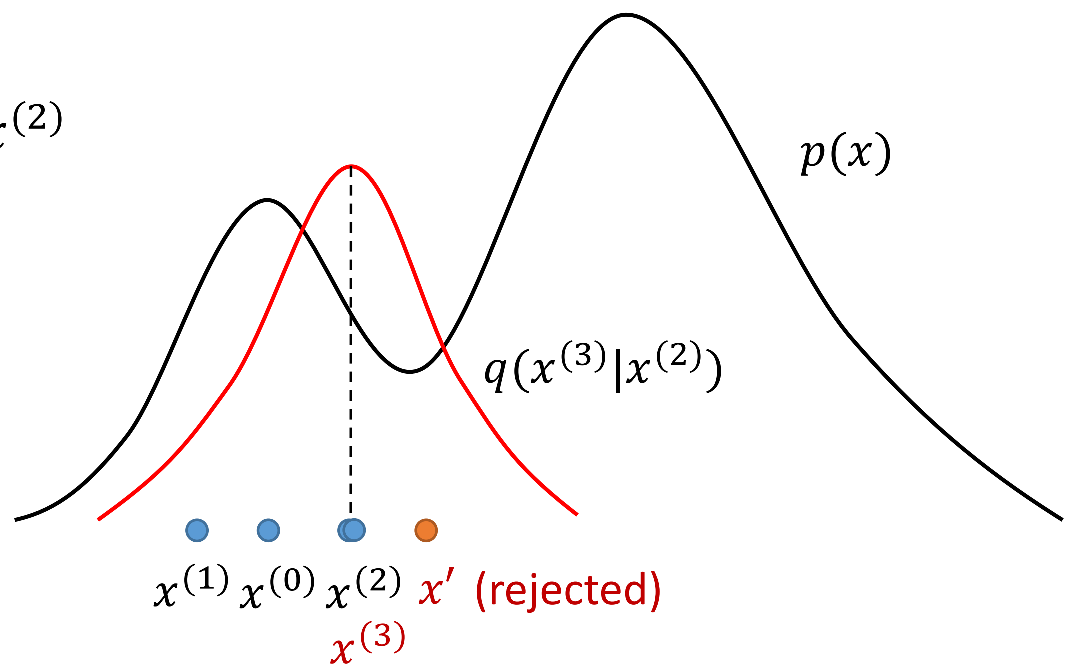
Example:

- Our goal is to sample from a bimodal distribution $p(x)$.
- Let $q(x'|x)$ be a Gaussian centered on x.

$$\mathcal{A}(x', x^{(i)}) = \min\left\{1, \frac{\tilde{p}(x')q(x^{(i)}|x')}{\tilde{p}(x^{(i)})q(x'|x^{(i)})}\right\}$$

Initialize $x^{(0)}$
Draw, accept $x^{(1)}$
Draw, accept $x^{(2)}$
Draw but reject; set $x^{(3)} = x^{(2)}$

Reject because $\frac{\tilde{p}(x')}{q(x'|x^{(2)})} < 1$ and $\frac{\tilde{p}(x^{(2)})}{q(x^{(2)}|x')} > 1$, hence $\mathcal{A}(x', x^{(2)})$ is close to zero!



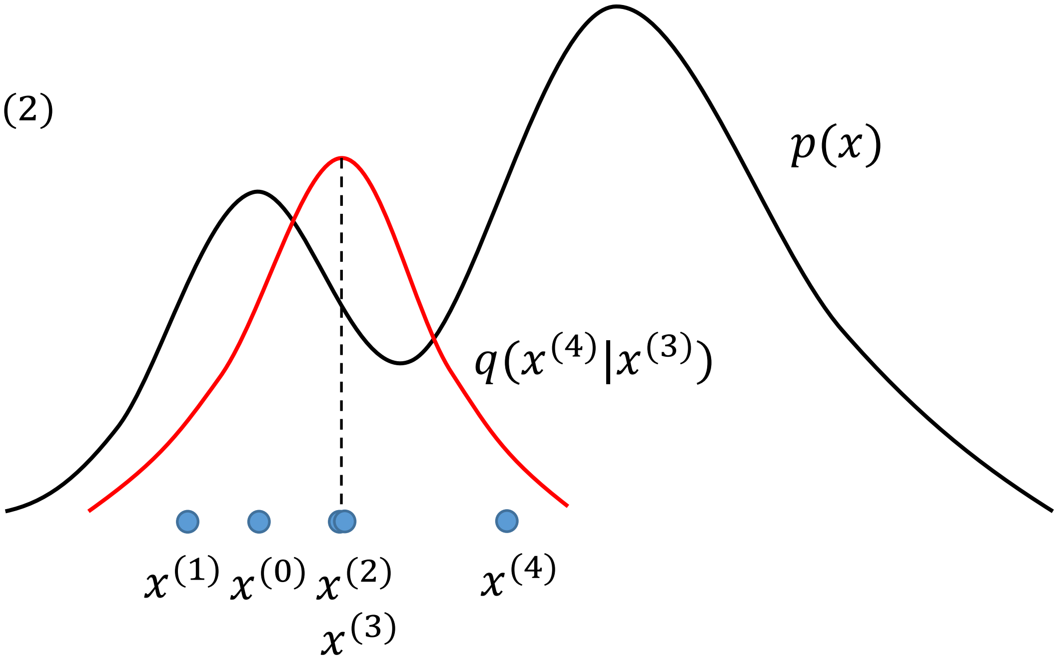
MCMC: Metropolis-Hasting Algorithm

Example:

- Our goal is to sample from a bimodal distribution $p(x)$.
- Let $q(x'|x)$ be a Gaussian centered on x.

$$\mathcal{A}(x', x^{(i)}) = \min\left\{1, \frac{\tilde{p}(x')q(x^{(i)}|x')}{\tilde{p}(x^{(i)})q(x'|x^{(i)})}\right\}$$

Initialize $x^{(0)}$
Draw, accept $x^{(1)}$
Draw, accept $x^{(2)}$
Draw but reject; set $x^{(3)} = x^{(2)}$
Draw, accept $x^{(4)}$



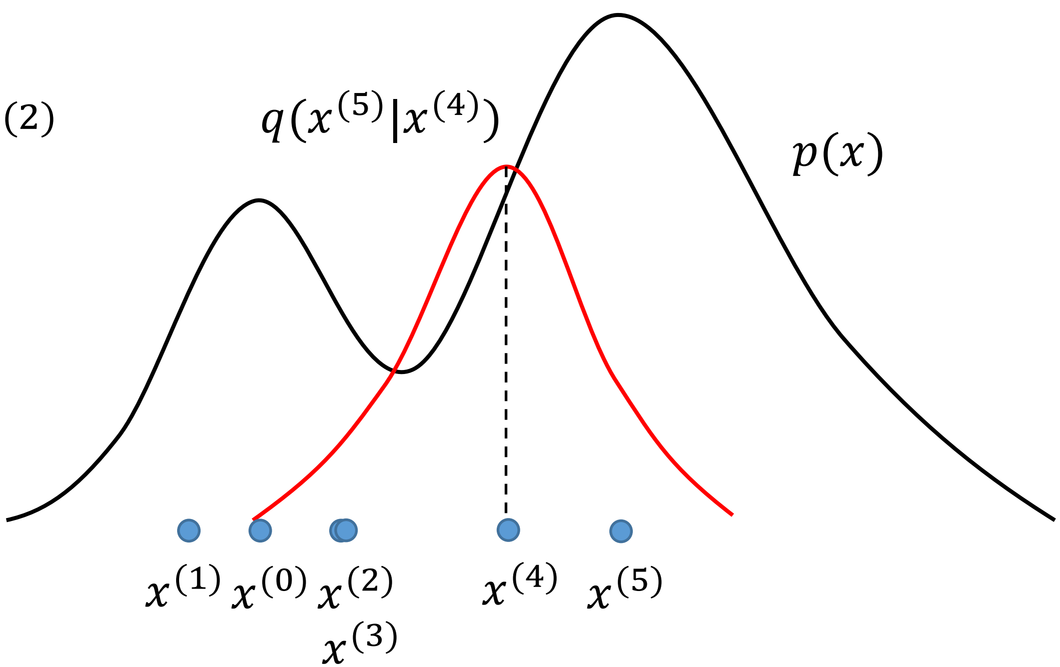
MCMC: Metropolis-Hasting Algorithm

Example:

- Our goal is to sample from a bimodal distribution $p(x)$.
- Let $q(x'|x)$ be a Gaussian centered on x.

$$\mathcal{A}(x', x^{(i)}) = \min\left\{1, \frac{\tilde{p}(x')q(x^{(i)}|x')}{\tilde{p}(x^{(i)})q(x'|x^{(i)})}\right\}$$

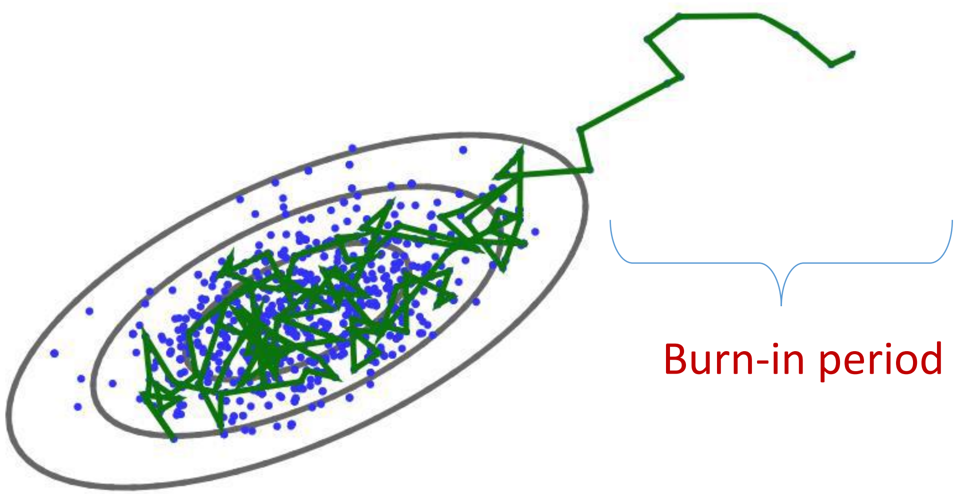
Initialize $x^{(0)}$
Draw, accept $x^{(1)}$
Draw, accept $x^{(2)}$
Draw but reject; set $x^{(3)} = x^{(2)}$
Draw, accept $x^{(4)}$
Draw, accept $x^{(5)}$



The adaptive proposal $q(x'|x^{(i)})$ allows us to sample both modes of $p(x)$!

Burn-In Period

- The initial samples may follow a very different distribution, especially if the starting point is in a region of low density.
- As a result, a burn-in period is typically necessary, where an initial number of samples (e.g. the first 1,000 or so) are thrown away.



Burn-in period

Image source: http://wiki.ubc.ca/Course:CPSC522/MCMC

What is the connection between Markov chains and MCMC?

Why does the Metropolis-Hasting algorithm work?

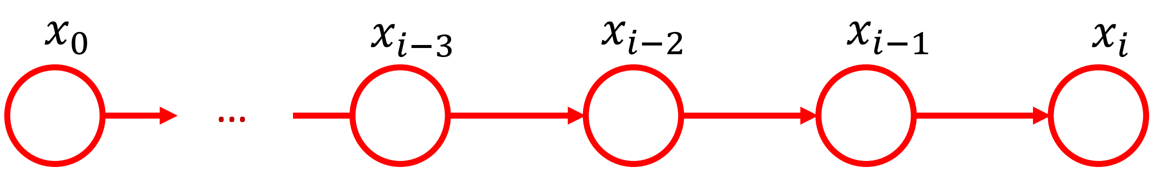
What is a Markov Chain?

- Intuitive to introduce Markov chains on finite state spaces, where $x^{(i)}$ can only take s discrete values $x^{(i)} \in \mathcal{X} = \{x_1, x_2, \dots, x_s\}$.

- The stochastic process $x^{(i)}$ is called a Markov chain if:

$$p\left(x^{(i)} \,\middle|\, x^{(i-1)}, \dots, x^{(1)}\right) = T\left(x^{(i)} \,\middle|\, x^{(i-1)}\right)$$

$s \times s$ matrix



- Current state $x^{(i)}$ is conditionally independent of all previous states given most recent state $x^{(i-1)}$.

Properties of a Markov Chain

1. **Homogeneous chain**:

- Chain is homogeneous if $T \triangleq T\left(x^{(i)} \mid x^{(i-1)}\right)$ remains invariant $\forall\, i$, with $\underbrace{\sum_{x^{(i)}} T\left(x^{(i)} \mid x^{(i-1)}\right) = 1}_{\text{Sum of each row in } T \text{ equals to } 1}$ for any i.

- That is, the evolution of the chain in a space $\mathcal{X}$ depends solely on the current state of the chain and a fixed transition matrix.

Properties of a Markov Chain

2. Stationary and limiting distributions:

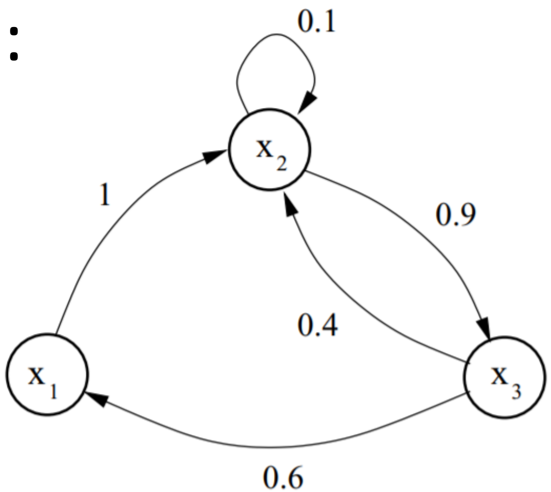
- A probability vector $\pi = p(x)$ defined on $\mathcal{X}$ is a stationary (invariant) distribution (w.r.t T) if

$$\pi T = \pi.$$

- A limiting distribution π, is a distribution over the states such that whatever the starting distribution π_0, the Markov chain converges to π.

Properties of a Markov Chain

Example:



Transition graph for the Markov chain example with $\mathcal{X} = \{x_1, x_2, x_3\}$.

$$T = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0.1 & 0.9 \\ 0.6 & 0.4 & 0 \end{bmatrix}$$

If initial state is $\mu\left(x^{(1)}\right) = (0.5, 0.2, 0.3)$ (can be any state), it follows that:

$$\mu\left(x^{(2)}\right) = \mu\left(x^{(1)}\right)T = (0.18, 0.64, 0.18)$$

$$\vdots$$

$$\mu\left(x^{(t)}\right) = \mu\left(x^{(t-1)}\right)T = (0.2213, 0.4098, 0.3689)$$

$$\mu\left(x^{(t+1)}\right) = \mu\left(x^{(t+2)}\right)T = (0.2213, 0.4098, 0.3689)$$

Converges to stationary distribution!

Image source: “An introduction to MCMC for Machine Learning”, Christophe Andrieu at. al.

Properties of a Markov Chain

3. Irreducibility:

- A Markov chain is irreducible if for any state of the Markov chain, there is a positive probability of visiting all other states, i.e.

$$if \quad \forall a, b \in \mathcal{X}, \qquad \exists\, t \geq 0$$

$$s.t. \quad p(x_t = b \mid x_0 = a) > 0$$

Properties of a Markov Chain

4. Aperiodicity:

- The Markov chain should not get trapped in cycles, i.e.

$$\gcd\{t : p(x_t = a \mid x_0 = a) > 0\} = 1, \quad \forall\, a \in \mathcal{X}$$

greatest common divisor

Ergodic Theorem for Markov Chains

- A Markov chain is ergodic if it is irreducible and aperiodic.
- **Ergodicity is important**: it implies we can reach the stationary/limiting distribution π, no matter the initial distribution π_0.
- All good MCMC algorithms must satisfy ergodicity, so that we cannot initialize in a way that will never converge.

Detailed Balance (Reversibility)

- A probability vector $\pi = p(x)$ defined on $\mathcal{X}$ satisfies detailed balance w.r.t T if:

$$\pi_a T_{ab} = \pi_b T_{ba}, \qquad \forall a, b \in x$$

Remark 1: Detailed balance $\Longrightarrow$ stationary distribution, i.e. $\pi T = \pi$.

Proof:

$$\begin{aligned}
\pi_b &= \textstyle\sum_a \pi_a T_{ab} \\
&= \textstyle\sum_a \pi_b T_{ba} && \text{(detailed balance)} \\
&= \pi_b \boxed{\textstyle\sum_a T_{ba}} = 1 && \text{(sum over row of } T_{ba}\text{)} \\
&= \pi_b, \qquad \forall b \in x && \text{(stationary distribution)}
\end{aligned}$$

Detailed Balance (Reversibility)

- A probability vector $\pi = p(x)$ defined on $\mathcal{X}$ satisfies detailed balance w.r.t T if:

$$\pi_a T_{ab} = \pi_b T_{ba}, \qquad \forall a, b \in \mathcal{x}$$

Remark 2: Detailed balance = "reversibility"

- Just a terminology: we say that a Markov chain is "reversible" if it had a stationary distribution π that satisfies detailed balance w.r.t T.

Why does Metropolis-Hastings work?

- Recall that we draw a sample x' according to $q(x'|x)$, and then accept/reject according to $\mathcal{A}(x', x)$.

- In other words, the transition kernel is:

$$T(\, x' \mid x \,) = \; q(\, x' \mid x \,)\mathcal{A}(\, x' \mid x \,)$$

- We shall prove that the Metropolis-Hasting algorithm satisfies detailed balance!

Why does Metropolis-Hastings work?

- Recall that:

$$\mathcal{A}(x', x) = \min\left\{1, \frac{\tilde{p}(x')q(x|x')}{\tilde{p}(x)q(x'|x)}\right\}$$

- Notice this implies the following:

if $\mathcal{A}(x', x) \leq 1$, then $\dfrac{\tilde{p}(x)q(x'|x)}{\tilde{p}(x')q(x|x')} \geq 1$

and thus $\mathcal{A}(x, x') = 1$

Why does Metropolis-Hastings work?

- Now suppose $\mathcal{A}(x', x) < 1$ and $\mathcal{A}(x, x') = 1$, we have:

$$\mathcal{A}(x', x) = \frac{\tilde{p}(x')q(x|x')}{\tilde{p}(x)q(x'|x)}$$

$$\mathcal{A}(x', x)\tilde{p}(x)q(x'|x) = \tilde{p}(x')q(x|x')$$

$$\mathcal{A}(x', x)\tilde{p}(x)q(x'|x) = \mathcal{A}(x, x')\tilde{p}(x')q(x|x')$$

$$\tilde{p}(x)T(\, x' \mid x \,) = \tilde{p}(x')T(x \mid x')$$

This is the detailed balance condition!

Why does Metropolis-Hastings work?

$$\tilde{p}(x)T(\,x' \mid x\,) = \tilde{p}(x')T(x \mid x')$$

- In other words, the Metropolis-Hasting algorithm leads to a stationary distribution $\tilde{p}(x)$!
- Recall we defined $\tilde{p}(x)$ to be the (un-normalized) true distribution of x!
- Thus, the Metropolis-Hasting eventually converges to the true distribution!

Metropolis Algorithm

- Metropolis algorithm is a special case of the Metropolis-Hasting algorithm.

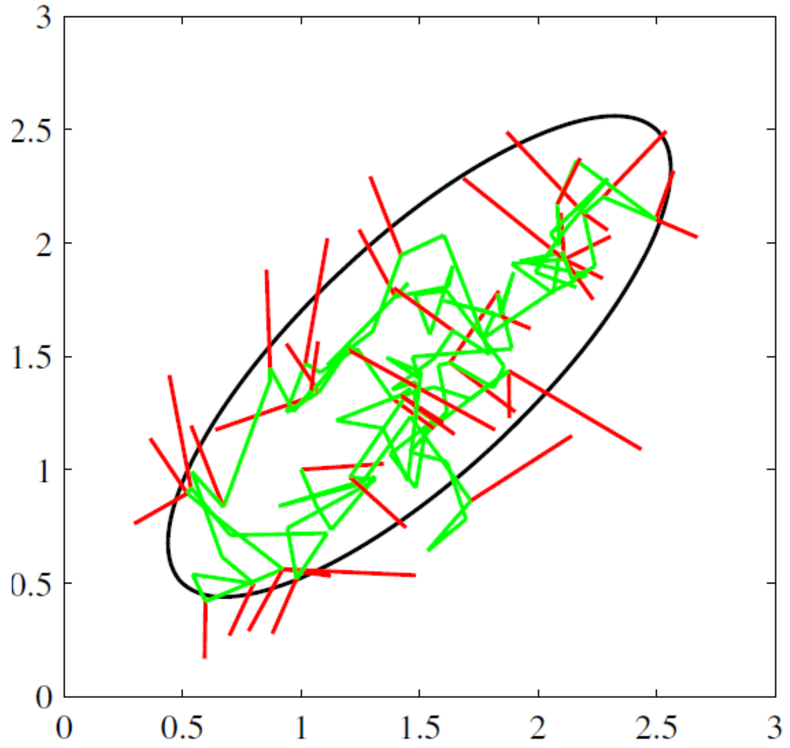
- Proposal distribution is a random walk, i.e. $q(x|x')$= $q(x'|x)$, e.g. an isotropic Gaussian distribution.

- Acceptance probability of Metropolis algorithm is given by:

$$\mathcal{A}(x', x) = \min\left\{1, \frac{\tilde{p}(x')\cancel{q(x|x')}}{\tilde{p}(x)\cancel{q(x'|x)}}\right\} = \min\left\{1, \frac{\tilde{p}(x')}{\tilde{p}(x)}\right\}$$

Metropolis Algorithm

- Illustration of using Metropolis algorithm (proposal distribution: isotropic Gaussian) to sample from a Gaussian distribution:



Accepted sample

Rejected sample

150 candidate samples are generated, 43 are rejected.

Image Source: "Pattern Recognition and Machine Learning", Christopher Bishop

Gibbs Sampling

- Suppose we have an N-dimensional vector x and the expressions for the full conditionals:

$$p(\,x_j\,|x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_N).$$

- In this case, we use the following proposal distribution for $j = 1, \dots, N$:

$$q\left(x' \middle| x^{(i)}\right) = \begin{cases} p(x_j' \mid x_{\setminus j}^{(i)}) & \text{if } x_{\setminus j}' = x_{\setminus j}^{(i)} \\ 0 & \text{Otherwise} \end{cases}$$

Gibbs Sampling

- Gibbs sampling is a special case of the Metropolis-Hasting algorithm where the acceptance probability is always one.

Proof: $\mathcal{A}(x', x) = \min\left\{1, \dfrac{p(x')q(x|x')}{p(x)q(x'|x)}\right\}$, where $\begin{aligned} p(x) &= p\left(x_j \middle| x_{\setminus j}\right)p(x_{\setminus j}) \\ p(x') &= p\left(x'_j \middle| x'_{\setminus j}\right)p(x'_{\setminus j}) \end{aligned}$

$$= \min\left\{1, \frac{p\left(x'_j \middle| x'_{\setminus j}\right)p(x'_{\setminus j})p(x_j \mid x'_{\setminus j})}{p\left(x_j \middle| x_{\setminus j}\right)p\left(x_{\setminus j}\right)p\left(x'_j \mid x_{\setminus j}\right)}\right\}$$

We use $x'_{\setminus j} = x_{\setminus j}$ because these components are kept fixed during the sampling step:

$$\Longrightarrow \mathcal{A}(x', x) = \min\left\{1, \frac{p\left(x'_j \middle| x'_{\setminus j}\right)p\left(x_{\setminus j}\right)p\left(x_j \mid x_{\setminus j}\right)}{p\left(x_j \middle| x_{\setminus j}\right)p\left(x_{\setminus j}\right)p\left(x'_j \mid x'_{\setminus j}\right)}\right\} = 1$$

1

$\square$

Gibbs Sampling

Algorithm : Gibbs Sampling

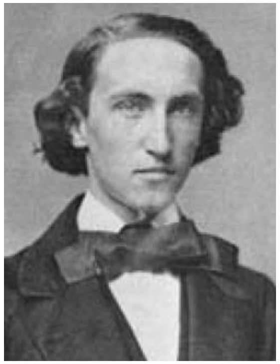
1. Initialize $\{x_i : i = 1, \ldots, M\}$
2. For $\tau = 1, \ldots, T$:
3. Sample $x_1^{\tau+1} \sim p(x_1 | x_2^{(\tau)}, x_3^{(\tau)}, \ldots, x_M^{(\tau)})$.
4. Sample $x_2^{\tau+1} \sim p(x_2 | x_1^{(\tau+1)}, x_3^{(\tau)}, \ldots, x_M^{(\tau)})$.

$$\vdots$$

5. Sample $x_j^{\tau+1} \sim p\left(x_j \middle| x_1^{(\tau+1)}, \ldots, x_{j-1}^{(\tau+1)}, x_{j+1}^{(\tau)}, \ldots, x_M^{(\tau)}\right)$.

$$\vdots$$

6. Sample $x_M^{\tau+1} \sim p(x_M | x_1^{(\tau+1)}, x_2^{(\tau+1)}, \ldots, x_{M-1}^{(\tau+1)})$



Josiah Willard Gibbs
1839–1903

Image Source: “Pattern Recognition and Machine Learning”, Christopher Bishop

Gibbs Sampling: Markov Blankets

- The conditional $p(\,x_j\,|x_1,\dots,x_{j-1},x_{j+1},\dots,x_N)$ looks intimidating, but recall Markov Blankets:

$$p\left(\,x_j\,\middle|x_1,\dots,x_{j-1},x_{j+1},\dots,x_N\right) = p(\,x_j\mid \underbrace{\mathrm{MB}(x_j)}_{\text{Markov blanket of } x_j}\,)\,.$$

- Bayesian network: the Markov blanket of X_j is the set containing its parents, children, and co-parents.

- MRF: the Markov Blanket of X_j is its immediate neighbors.

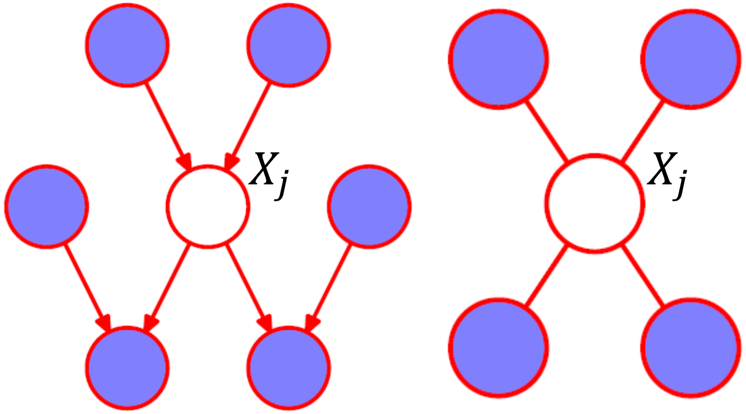


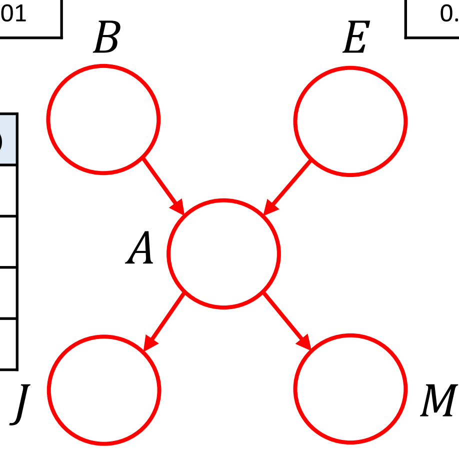
Image Source: “Pattern Recognition and Machine Learning”, Christopher Bishop

Gibbs Sampling: Example on a Bayesian Network

B: Burglary, E: Earthquake, A: Alarm, J: John Calls, M: Mary Calls

$p(B)$
0.001

$p(E)$
0.002



B	E	$p(A \mid B, E)$
T	T	0.95
T	F	0.94
F	T	0.29
F	F	0.01

A	$p(J \mid A)$
T	0.90
F	0.05

A	$p(M \mid A)$
T	0.70
F	0.01

- Assume we sample variables in the order B, E, A, J, M.
- Initialize all variables at $t = 0$ to False.

t	B	E	A	J	M
0	F	F	F	F	F
1					
2					
3					
4					

Gibbs Sampling: Example on a Bayesian Network

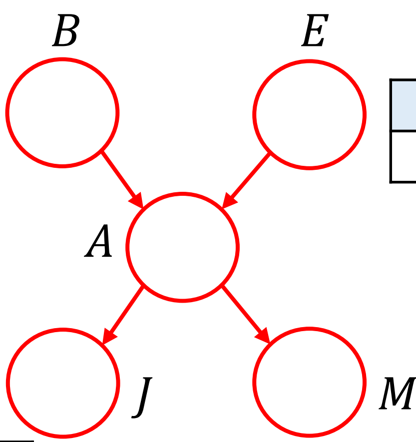
- Sampling $p(B|\, A, E)$ at $t = 1$: using Bayes rule, we have

$$p(\, B \mid A, E \,) \propto p(\, A \mid B, E \,)\, p(\, B \,)$$

- $(A, E) = (F, F)$, we compute the following, and sample $B = F$

$$p(\, B = T \mid A = F, E = F \,) \propto (0.06)(0.001) = 0.00006$$
$$p(\, B = F \mid A = F, E = F \,) \propto (0.99)(0.999) = 0.98901$$

$p(B)$
0.001



$p(E)$
0.002

B	E	$p(A \mid B, E)$
T	T	0.95
T	F	0.94
F	T	0.29
F	F	0.01

A	$p(J \mid A)$
T	0.90
F	0.05

A	$p(M \mid A)$
T	0.70
F	0.01

t	B	E	A	J	M
0	F	F	F	F	F
1	F				
2					
3					
4					

Gibbs Sampling: Example on a Bayesian Network

- Sampling $p(E|A,B)$ at $t = 1$: using Bayes rule, we have

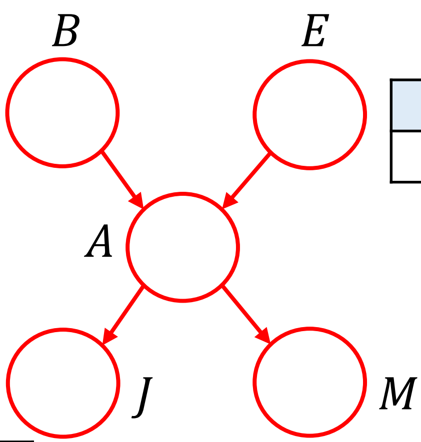
$$p(\,E \mid A, B\,) \propto p(\,A \mid B, E\,)\,p(\,E\,)$$

- $(A, B) = (F, F)$, we compute the following, and sample $E = T$

$$p(\,E = T\;|A = F, B = F\,) \propto (0.71)(0.002) = 0.00142$$
$$p(\,E = F\;|A = F, B = F\,) \propto (0.99)(0.998) = 0.98802$$

$p(B)$
0.001

$p(E)$
0.002



B	E	$p(A \mid B, E)$
T	T	0.95
T	F	0.94
F	T	0.29
F	F	0.01

A	$p(J \mid A)$
T	0.90
F	0.05

A	$p(M \mid A)$
T	0.70
F	0.01

t	B	E	A	J	M
0	F	F	F	F	F
1	F	T			
2					
3					
4					

Gibbs Sampling: Example on a Bayesian Network

- Sampling $p(A|B,E,J,M)$ at $t = 1$: using Bayes rule

$$p(A \mid B,E,J,M) \propto p(J|A)p(M|A)p(A|B,E)$$

- $(B,E,J,M) = (F,T,F,F)$, we compute the following, and sample $A = F$

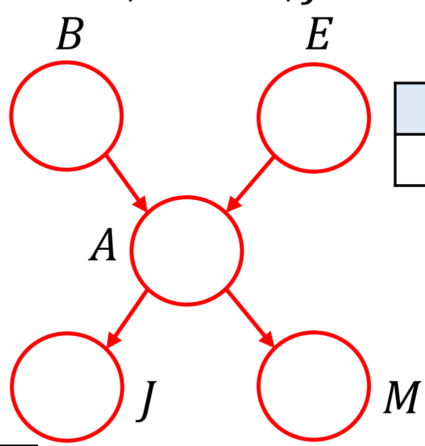
$$p(A = T|B = F,E = T,J = F,M = F) \propto (0.1)(0.3)(0.29) = 0.0087$$

$$p(A = F|B = F,E = T,J = F,M = F) \propto (0.95)(0.99)(0.71) = 0.6678$$

$p(B)$
0.001

$p(E)$
0.002

B	E	$p(A \mid B,E)$
T	T	0.95
T	F	0.94
F	T	0.29
F	F	0.01



A	$p(J \mid A)$
T	0.90
F	0.05

A	$p(M \mid A)$
T	0.70
F	0.01

t	B	E	A	J	M
0	F	F	F	F	F
1	F	T	F		
2					
3					
4					

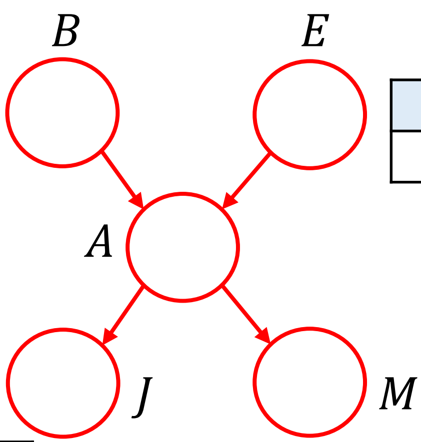
Gibbs Sampling: Example on a Bayesian Network

- Sampling $p(J|A)$ at $t = 1$: no need to apply Bayes rule
- $A = F$, we compute the following, and sample $J = T$

$$p(J = T|A = F) \propto 0.05$$
$$p(J = F|A = F) \propto 0.95$$

$p(B)$
0.001

B	E	$p(A \mid B, E)$
T	T	0.95
T	F	0.94
F	T	0.29
F	F	0.01



$p(E)$
0.002

A	$p(J \mid A)$
T	0.90
F	0.05

A	$p(M \mid A)$
T	0.70
F	0.01

t	B	E	A	J	M
0	F	F	F	F	F
1	F	T	F	T	
2					
3					
4					

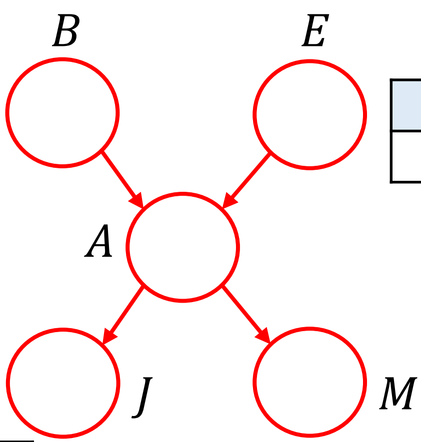
Gibbs Sampling: Example on a Bayesian Network

- Sampling $p(M|A)$ at $t = 1$: no need to apply Bayes rule
- $A = F$, we compute the following, and sample $M = F$

$$p(M = T|A = F) \propto 0.01$$
$$p(M = F|A = F) \propto 0.99$$

$p(B)$
0.001

B	E	$p(A \mid B, E)$
T	T	0.95
T	F	0.94
F	T	0.29
F	F	0.01



$p(E)$
0.002

A	$p(J \mid A)$
T	0.90
F	0.05

A	$p(M \mid A)$
T	0.70
F	0.01

t	B	E	A	J	M
0	F	F	F	F	F
1	F	T	F	T	F
2					
3					
4					

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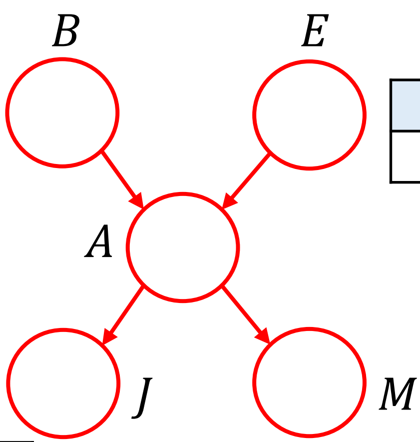
- Now $t = 2$, and we repeat the procedure to sample new values of B, E, A, J, M …
- And similarly for $t = 3, 4$, etc.

$p(B)$
0.001

$p(E)$
0.002



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T	T	0.95
T	F	0.94
F	T	0.29
F	F	0.01

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T	0.90
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A	$p(M \mid A)$
T	0.70
F	0.01

t	B	E	A	J	M
0	F	F	F	F	F
1	F	T	F	T	F
2	F	T	T	T	T
3	T	F	T	F	T
4	T	F	T	F	F

Gibbs Sampling: Illustration

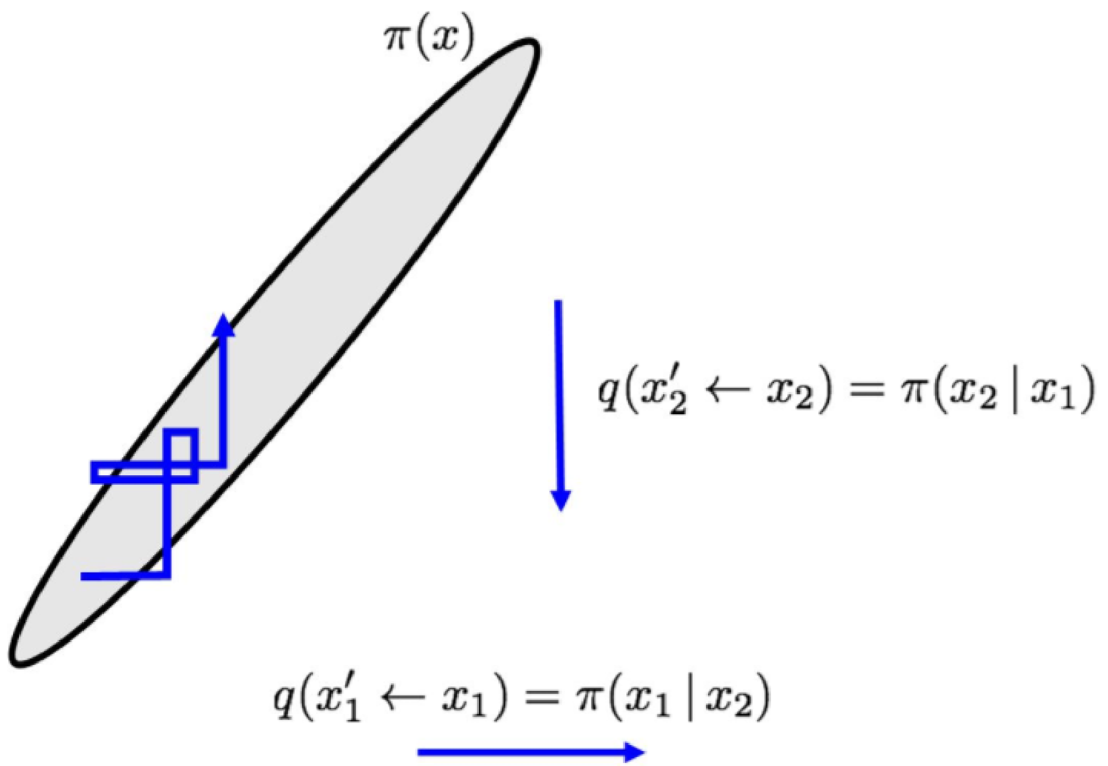

Image source: http://slideplayer.com/slide/4261639/

Summary

- We have looked at how to:

1. Explain the Monte Carlo principle and its justification for sampling methods.

2. Apply Rejection, Importance, Metropolis-Hasting, Metropolis and Gibbs sampling methods to do maximal probability, approximate inference, and expectation.

3. Use Markov chain properties, i.e. homogenous, stationary distribution, irreducibility, aperiod, egordic and detail balance, to show validity of MH algorithm.