School of Computer Science
Carnegie Mellon

Probabilistic Graphical Models

Approximate Inference: Markov Chain Monte Carlo

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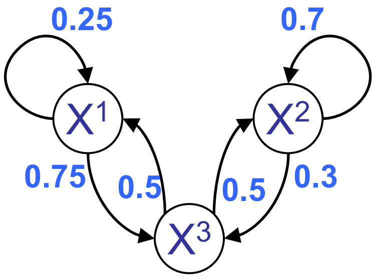
Lecture 17, March 19, 2014



Recap of Monte Carlo

- Monte Carlo methods are algorithms that:
  - Generate samples from a given probability distribution $p(x)$
  - Estimate expectations of functions $E[f(x)]$ under a distribution $p(x)$

- Why is this useful?
  - Can use samples of $p(x)$ to approximate $p(x)$ itself
    - Allows us to do graphical model inference when we can't compute $p(x)$
  - Expectations $E[f(x)]$ reveal interesting properties about $p(x)$
    - e.g. means and variances of $p(x)$

Limitations of Monte Carlo

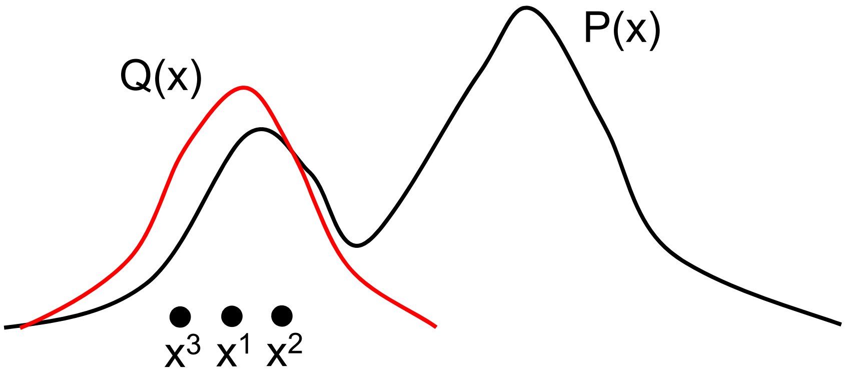
- Direct sampling
  - Hard to get rare events in high-dimensional spaces
  - Infeasible for MRFs, unless we know the normalizer Z
- Rejection sampling, Importance sampling
  - Do not work well if the proposal Q(x) is very different from P(x)
  - Yet constructing a Q(x) similar to P(x) can be difficult
    - Making a good proposal usually requires knowledge of the analytic form of P(x) – but if we had that, we wouldn't even need to sample!

- Intuition: instead of a fixed proposal Q(x), what if we could use an adaptive proposal?

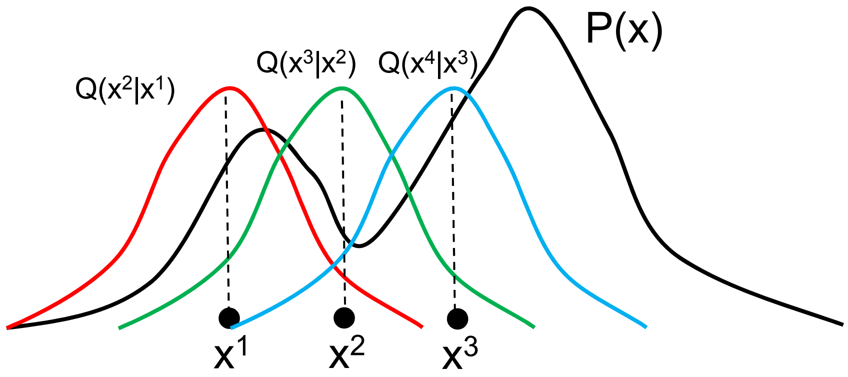
Markov Chain Monte Carlo

- MCMC algorithms feature adaptive proposals
  - Instead of Q(x’), they 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 a (bad) proposal Q(x)



MCMC with adaptive proposal Q(x’|x)



Metropolis-Hastings

- Let's see how MCMC works in practice
  - Later, we'll look at the theoretical aspects
- Metropolis-Hastings algorithm
  - Draws a sample x' from Q(x'|x), where x is the previous sample
  - The new sample x' is accepted or rejected with some probability A(x'|x)
    - This acceptance probability is $A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$
    - A(x'|x) is like a ratio of importance sampling weights
      - P(x')/Q(x'|x) is the importance weight for x', P(x)/Q(x|x') is the importance weight for x
      - We divide the importance weight for x' by that of x
      - Notice that we only need to compute P(x')/P(x) rather than P(x') or P(x) separately
    - A(x'|x) ensures that, after sufficiently many draws, our samples will come from the true distribution P(x) – we shall learn why later in this lecture

The MH Algorithm

```
1. Initialize starting state $x^{(0)}$, set $t$ =0
2. Burn-in: while samples have “not converged”
    - $x=x^{(t)}$
    - $t=t+1$,
    - sample $x^* \sim Q(x^*|x)$   // draw from proposal
    - sample $u \sim \mathrm{Uniform}(0,1)$ // draw acceptance threshold
        - if   $u < A(x^* | x) = \min\left(1, \frac{P(x^*)Q(x | x^*)}{P(x)Q(x^* | x)}\right)$
            - $x^{(t)} = x^*$          // transition
        - else
            - $x^{(t)} = x$            // stay in current state
```

Function
Draw sample (x(t))

- Take samples from P(x) = : Reset t=0, for t =1:N
  - x(t+1) ← Draw sample (x(t))

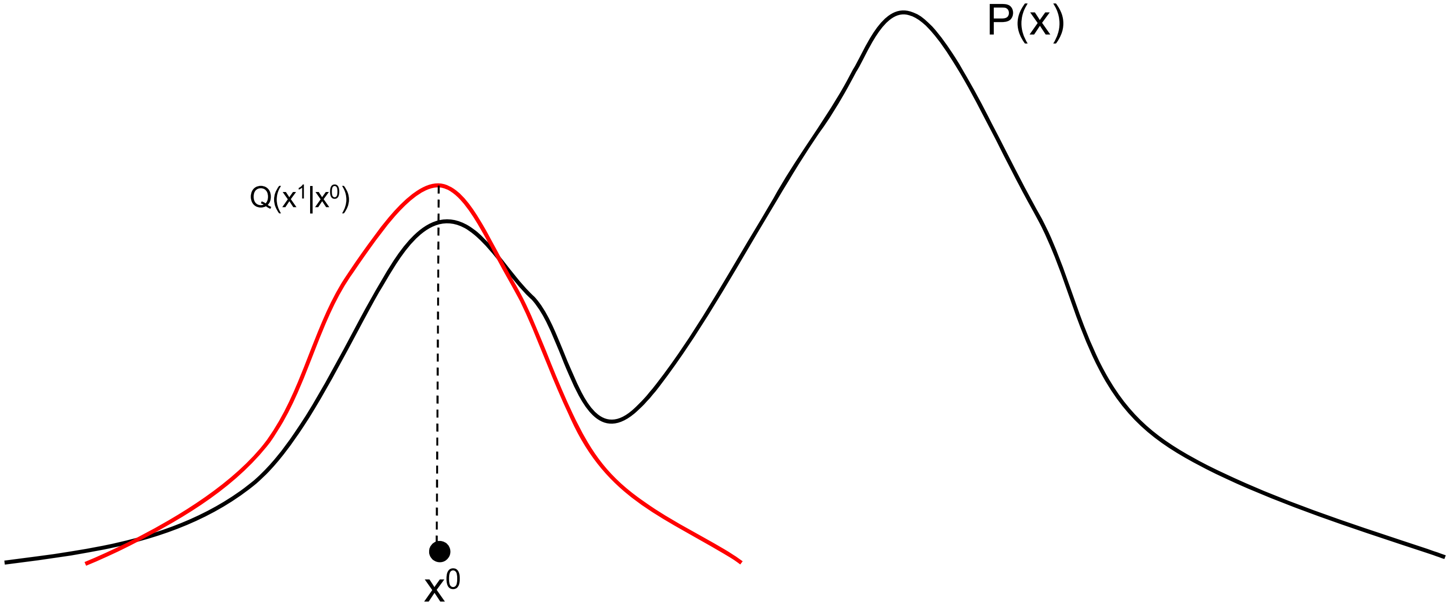
The MH Algorithm

$$\boxed{A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)}$$

- Example:
  - Let Q(x'|x) be a Gaussian centered on x
  - We're trying to sample from a bimodal distribution P(x)

Initialize $x^{(0)}$

…

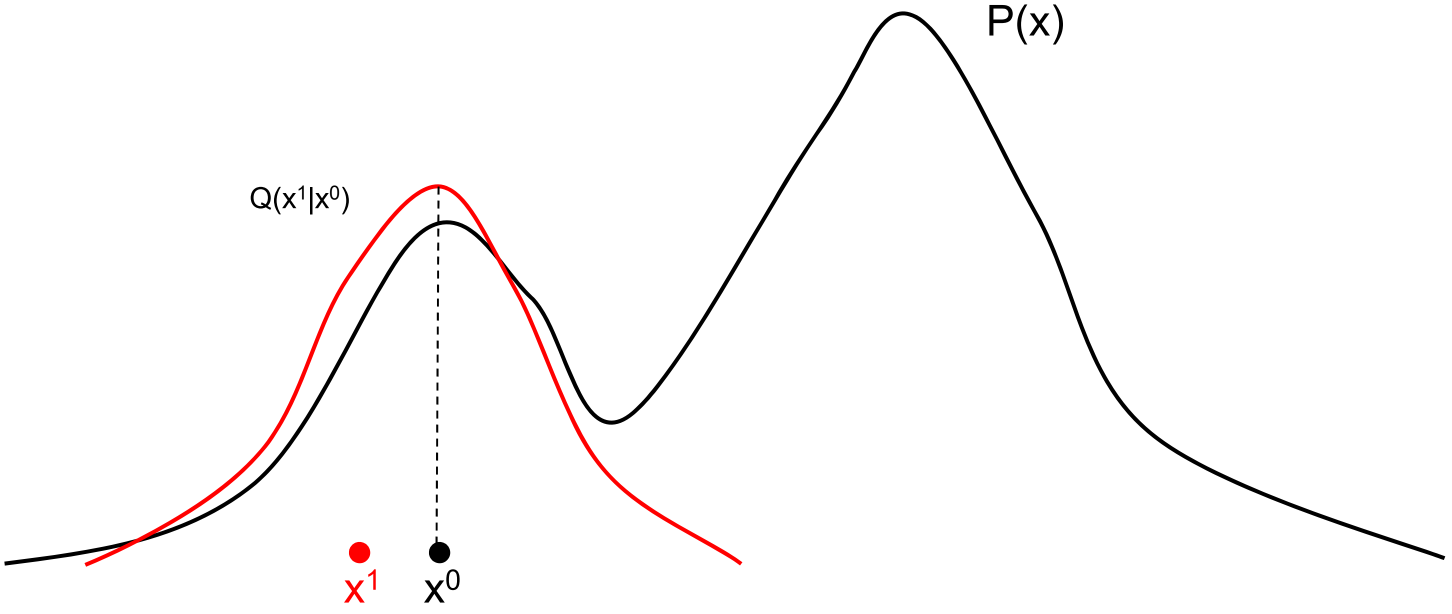


The MH Algorithm

$$A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$$

- Example:
  - Let Q(x'|x) be a Gaussian centered on x
  - We're trying to sample from a bimodal distribution P(x)

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

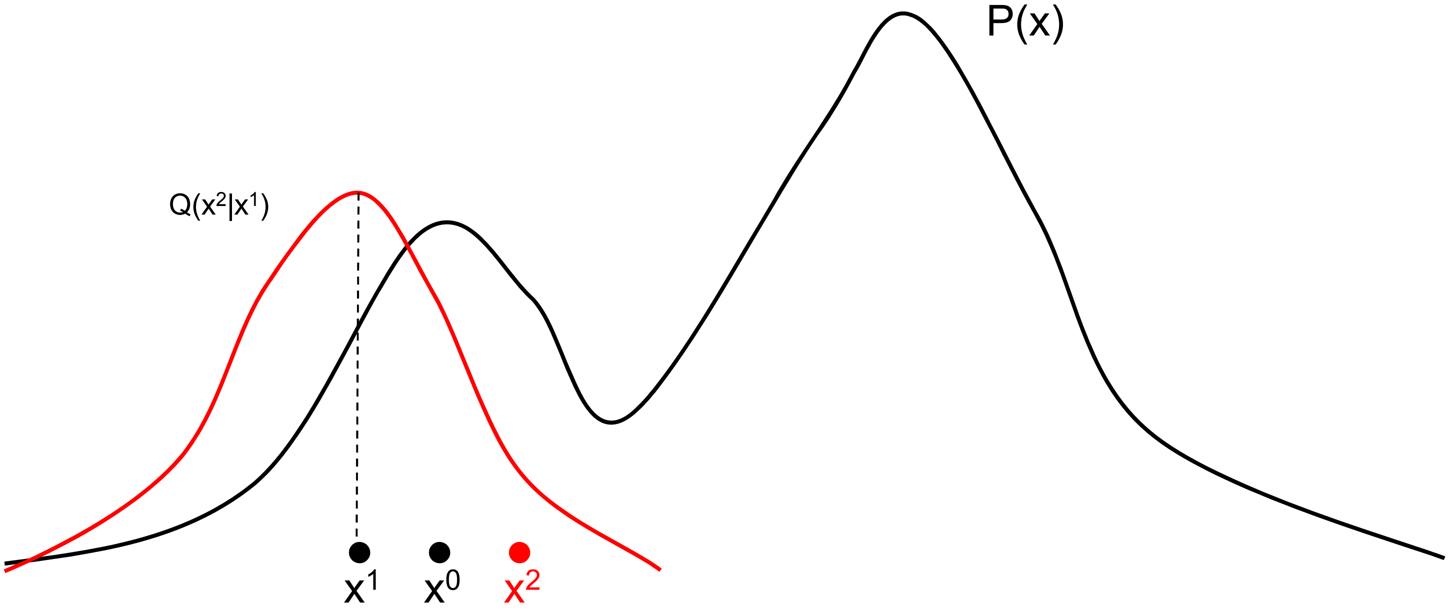


The MH Algorithm

$$A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$$

- Example:
  - Let Q(x'|x) be a Gaussian centered on x
  - We're trying to sample from a bimodal distribution P(x)

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

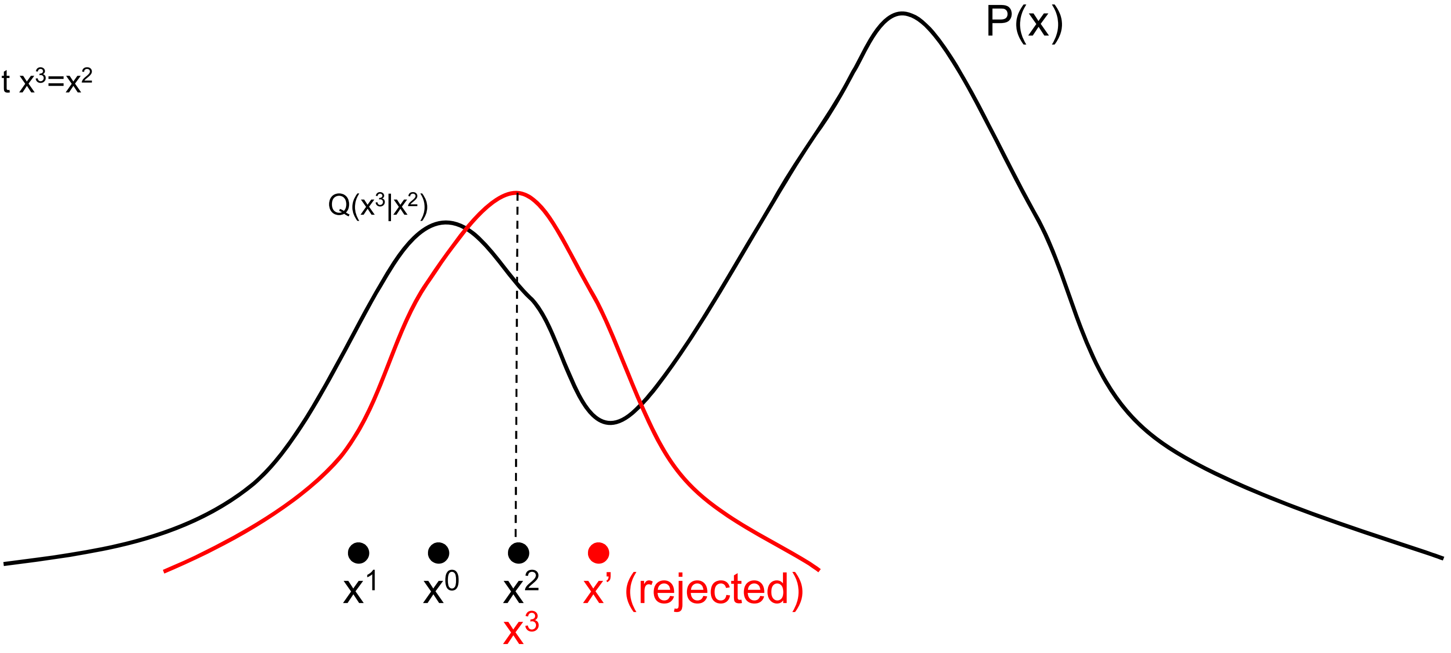


The MH Algorithm

$$A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$$

- Example:
  - Let Q(x'|x) be a Gaussian centered on x
  - We're trying to sample from a bimodal distribution P(x)

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



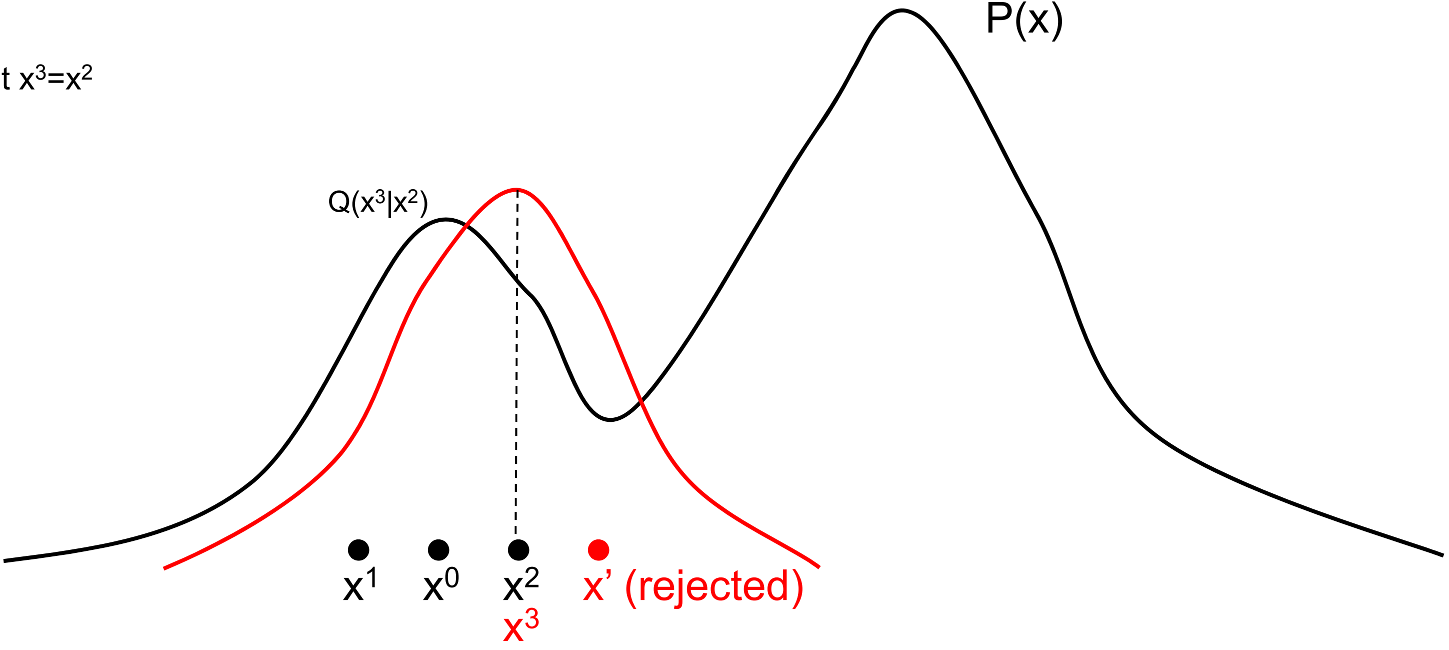
The MH Algorithm

$$A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$$

- Example:
  - Let Q(x’|x) be a Gaussian centered on x
  - We’re trying to sample from a bimodal distribution P(x)

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

We reject because $P(x')/Q(x'|x^2) < 1$ and $P(x^2)/Q(x^2|x') > 1$, hence $A(x'|x^2)$ is close to zero!

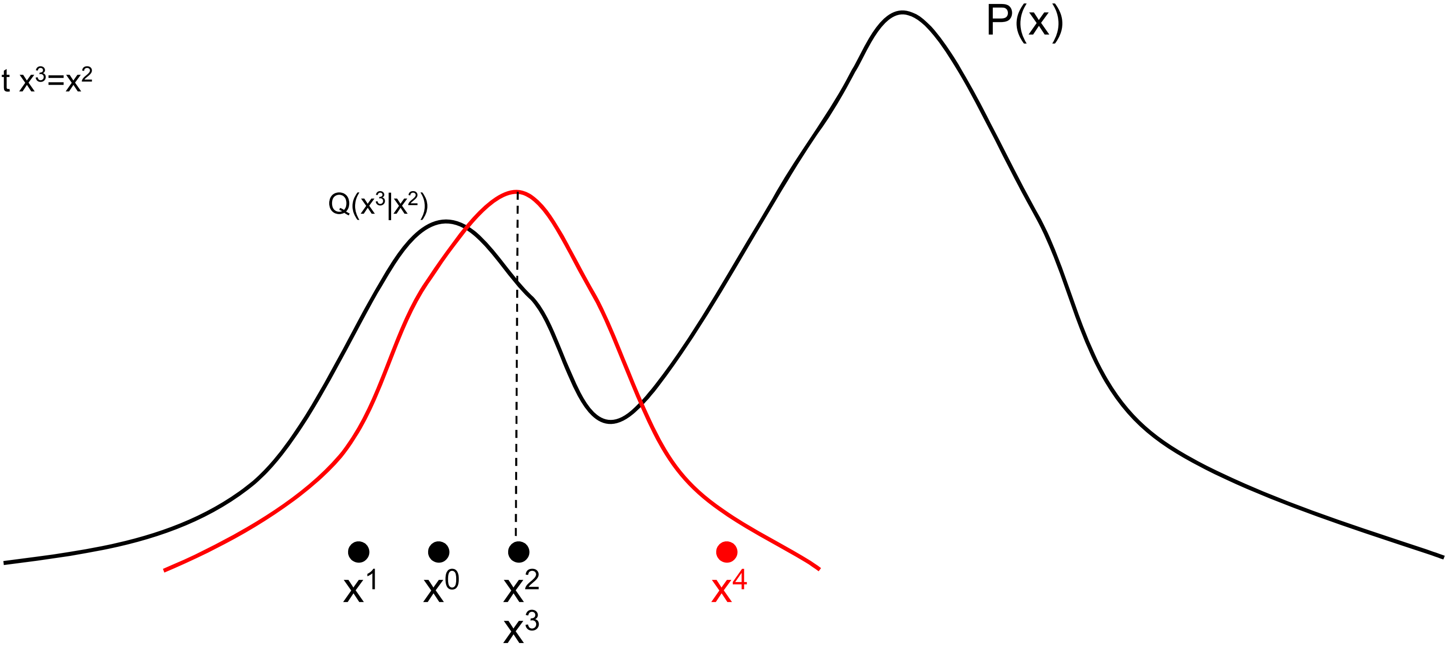


The MH Algorithm

$$A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$$

- Example:
  - Let Q(x'|x) be a Gaussian centered on x
  - We're trying to sample from a bimodal distribution P(x)

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

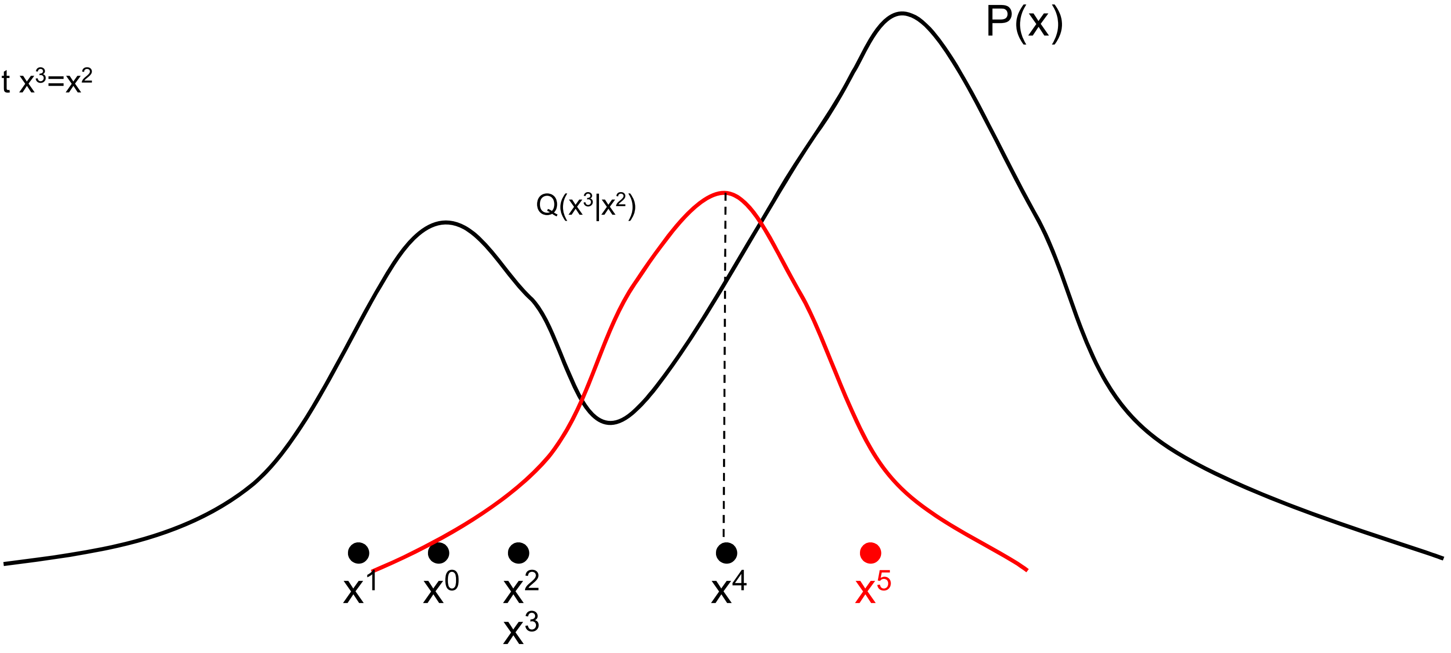


The MH Algorithm

$$A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$$

- Example:
  - Let Q(x’|x) be a Gaussian centered on x
  - We’re trying to sample from a bimodal distribution P(x)

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



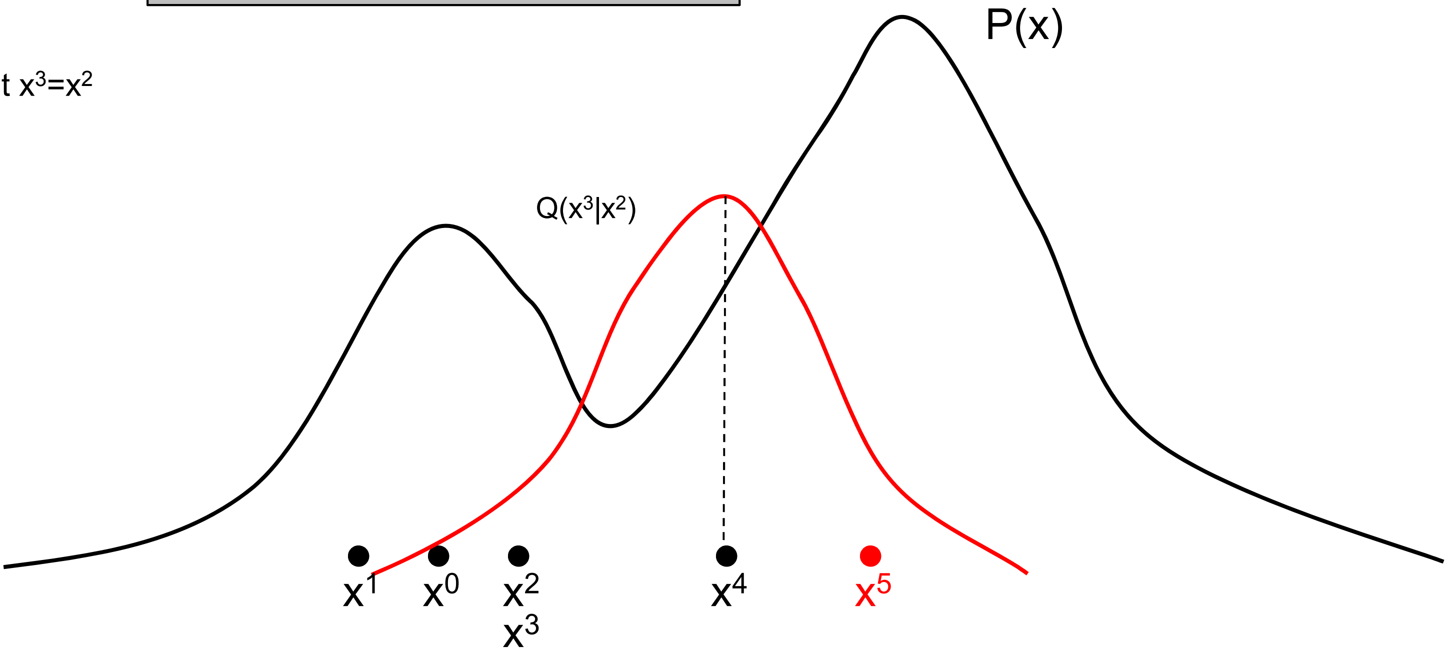
The MH Algorithm

$$A(x'|x) = \min\left(1, \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}\right)$$

- Example:
  - Let Q(x'|x) be a Gaussian centered on x
  - We're trying to sample from a bimodal distribution P(x)

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) allows us to sample both modes of P(x)!



Theoretical aspects of MCMC

- The MH algorithm has a “burn-in” period
  - Why do we throw away samples from burn-in?

- Why are the MH samples guaranteed to be from P(x)?
  - The proposal Q(x’|x) keeps changing with the value of x; how do we know the samples will eventually come from P(x)?

- What is the connection between Markov Chains and MCMC?

Markov Chains

- A Markov Chain is a sequence of random variables $x^{(1)},x^{(2)},\ldots,x^{(n)}$ with the Markov Property

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

  - $P(x^{(n)} = x \mid x^{(n-1)})$ is known as the transition kernel
  - The next state depends only on the preceding state – recall HMMs!
  - Note: the r.v.s $x^{(i)}$ can be vectors
    - We define $x^{(t)}$ to be the t-th sample of all variables in a graphical model
    - $X^{(t)}$ represents the entire state of the graphical model at time t

- We study homogeneous Markov Chains, in which the transition kernel $P(x^{(t)} = x \mid x^{(t-1)})$ is fixed with time
  - To emphasize this, we will call the kernel $T(x' \mid x)$, where x is the previous state and x' is the next state

MC Concepts

- To understand MCs, we need to define a few concepts:
  - Probability distributions over states: $\pi^{(t)}(x)$ is a distribution over the state of the system x, at time t
    - When dealing with MCs, we don't think of the system as being in one state, but as having a distribution over states
    - For graphical models, remember that x represents <u>all</u> variables
  - Transitions: recall that states transition from $x^{(t)}$ to $x^{(t+1)}$ according to the transition kernel $T(x'|x)$. We can also transition entire distributions:

$$\pi^{(t+1)}(x') = \sum_x \pi^{(t)}(x) T(x'|x)$$

    - At time t, state x has probability mass $\pi^{(t)}(x)$. The transition probability redistributes this mass to other states x'.
  - Stationary distributions: $\pi(x)$ is stationary if it does not change under the transition kernel:

$$\pi(x') = \sum_x \pi(x) T(x'|x) \qquad \text{for all } x'$$

MC Concepts

- Stationary distributions are of great importance in MCMC. To understand them, we need to define some notions:
  - Irreducible: an MC is irreducible if you can get from any state x to any other state x' with probability > 0 in a finite number of steps
    - i.e. there are no unreachable parts of the state space
  - Aperiodic: an MC is aperiodic if you can return to any state x at any time
    - Periodic MCs have states that need ≥2 time steps to return to (cycles)
  - Ergodic (or regular): an MC is ergodic if it is irreducible and aperiodic

- Ergodicity is important: it implies you can reach the stationary distribution $\pi_{st}(x)$, no matter the initial distribution $\pi^{(0)}(x)$
  - All good MCMC algorithms must satisfy ergodicity, so that you can't initialize in a way that will never converge

MC Concepts

- Reversible (detailed balance): an MC is reversible if there exists a distribution $\pi(x)$ such that the detailed balance condition is satisfied:

$$\pi(x')T(x \mid x') = \pi(x)T(x' \mid x)$$

  - Probability of x’→x and x→x’ can be different, but the joint of x amd x’ remain the same, no matter which direction to go

- Reversible MCs always have a stationary distribution! Proof:

$$\pi(x')T(x \mid x') = \pi(x)T(x' \mid x)$$

$$\sum_x \pi(x')T(x \mid x') = \sum_x \pi(x)T(x' \mid x)$$

$$\pi(x')\sum_x T(x \mid x') = \sum_x \pi(x)T(x' \mid x)$$

$$\pi(x') = \sum_x \pi(x)T(x' \mid x)$$

  - The last line is the definition of a stationary distribution!

Why does Metropolis-Hastings work?

- Recall that we draw a sample x' according to Q(x'|x), and then accept/reject according to A(x'|x).
  - In other words, the transition kernel is

$$T(x' \mid x) = Q(x' \mid x) A(x' \mid x)$$

- We can prove that MH satisfies detailed balance
  - Recall that

$$A(x' \mid x) = \min\left(1, \frac{P(x')Q(x \mid x')}{P(x)Q(x' \mid x)}\right)$$

  - Notice this implies the following:

$$\text{if } \; A(x' \mid x) \leq 1 \quad \text{then} \quad \frac{P(x)Q(x' \mid x)}{P(x')Q(x \mid x')} \geq 1 \quad \text{and thus} \quad A(x \mid x') = 1$$

Why does Metropolis-Hastings work?

if $A(x'|x) \leq 1$ then $\frac{P(x)Q(x'|x)}{P(x')Q(x|x')} \geq 1$ and thus $A(x|x') = 1$

- Now suppose A(x’|x) < 1 and A(x|x’) = 1. We have

$$A(x'|x) = \frac{P(x')Q(x|x')}{P(x)Q(x'|x)}$$

$$P(x)Q(x'|x)A(x'|x) = P(x')Q(x|x')$$

$$P(x)Q(x'|x)A(x'|x) = P(x')Q(x|x')A(x|x')$$

$$P(x)T(x'|x) = P(x')T(x|x')$$

- The last line is exactly the detailed balance condition
  - In other words, the MH algorithm leads to a stationary distribution P(x)
  - Recall we defined P(x) to be the true distribution of x
  - Thus, the MH algorithm eventually converges to the true distribution!

Caveats

- Although MH eventually converges to the true distribution P(x), we have no guarantees as to when this will occur
  - The burn-in period represents the un-converged part of the Markov Chain – that’s why we throw those samples away!
  - Knowing when to halt burn-in is an art. We will look at some techniques later in this lecture.

Gibbs Sampling

- Gibbs Sampling is an MCMC algorithm that samples each random variable of a graphical model, one at a time
  - GS is a special case of the MH algorithm

- GS algorithms…
  - Are fairly easy to derive for many graphical models (e.g. mixture models, Latent Dirichlet allocation)
  - Have reasonable computation and memory requirements, because they sample one r.v. at a time
  - Can be Rao-Blackwellized (integrate out some r.v.s) to decrease the sampling variance

Gibbs Sampling

- The GS algorithm:
  1. Suppose the graphical model contains variables $x_1,\ldots,x_n$
  2. Initialize starting values for $x_1,\ldots,x_n$
  3. Do until convergence:
     1. Pick an ordering of the n variables (can be fixed or random)
     2. For each variable x_i in order:
        1. Sample x from $P(x_i \mid x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$, i.e. the conditional distribution of x_i given the current values of all other variables
        2. Update $x_i \leftarrow x$

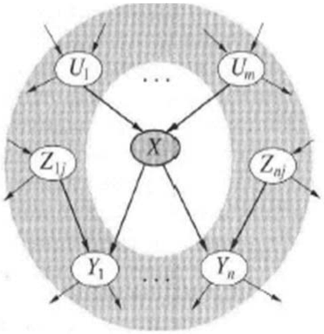
- When we update x_i, we <u>immediately</u> use its new value for sampling other variables x_j

Markov Blankets

- The conditional P(x_i | x_1, …, x_{i-1}, x_{i+1}, …, x_n) looks intimidating, but recall Markov Blankets:
  - Let MB(x_i) be the Markov Blanket of x_i, then

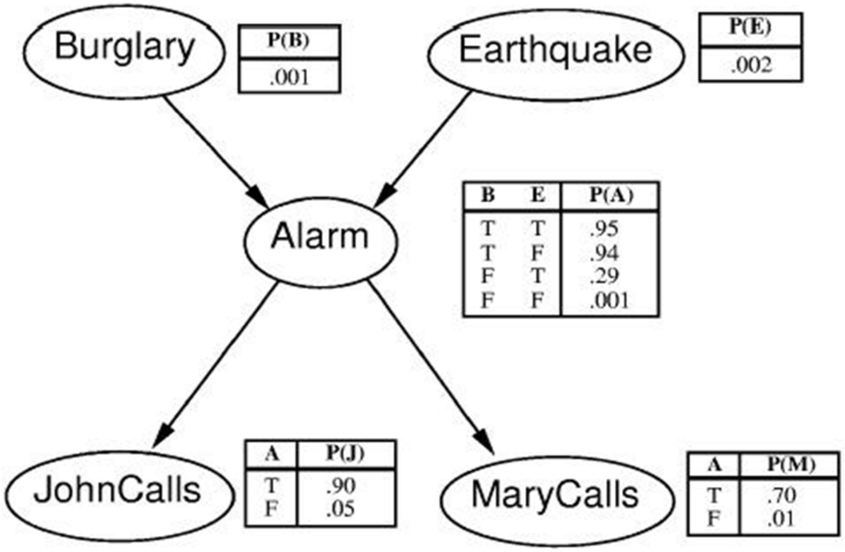
$$P(x_i \mid x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) = P(x_i \mid MB(x_i))$$

- For a BN, the Markov Blanket of x is the set containing its parents, children, and co-parents



- For an MRF, the Markov Blanket of x is its immediate neighbors

Gibbs Sampling: An Example



P(B)
.001

P(E)
.002

B	E	P(A)
T	T	.95
T	F	.94
F	T	.29
F	F	.001

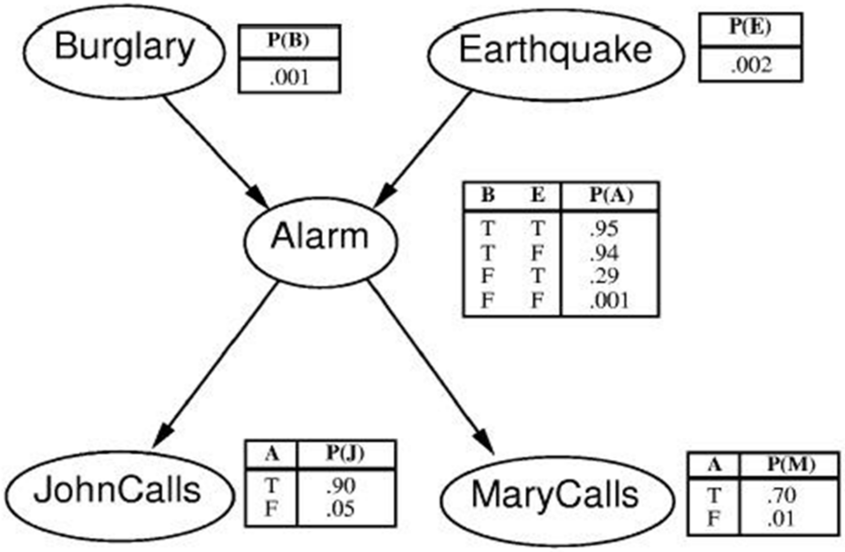
A	P(J)
T	.90
F	.05

A	P(M)
T	.70
F	.01

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

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

Gibbs Sampling: An Example



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

- Sampling P(B|A,E) at t = 1: Using Bayes Rule,

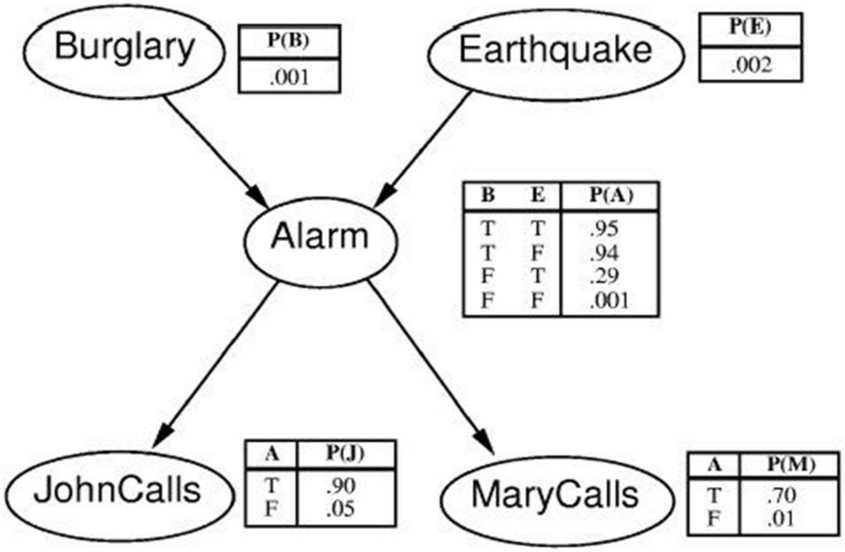
$$P(B \mid A, E) \propto P(A \mid B, E) P(B)$$

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

$$P(B = T \mid A = F, E = F) \propto (0.06)(0.01) = 0.0006$$

$$P(B = F \mid A = F, E = F) \propto (0.999)(0.999) = 0.9980$$

Gibbs Sampling: An Example



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2					
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- Sampling P(E|A,B): Using Bayes Rule,

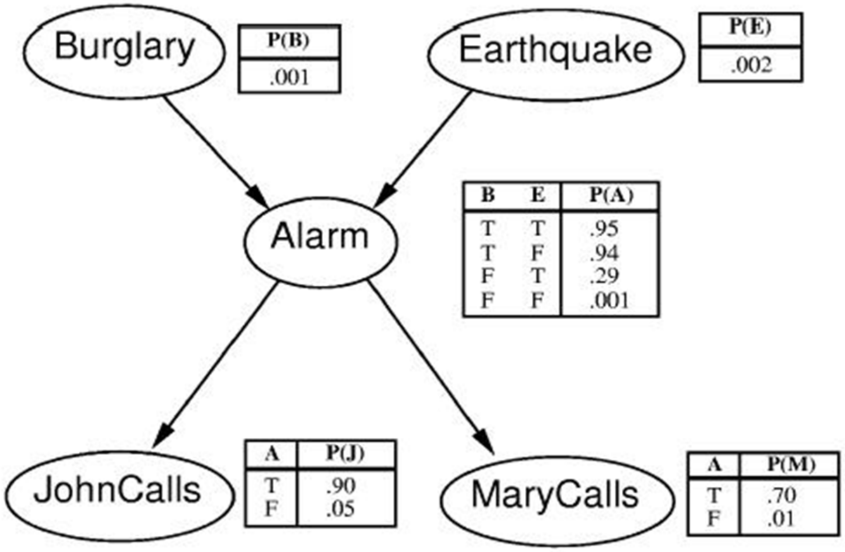
$$P(E \mid A, B) \propto P(A \mid B, E) P(E)$$

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

$$P(E = T \mid A = F, B = F) \propto (0.71)(0.02) = 0.0142$$

$$P(E = F \mid A = F, B = F) \propto (0.999)(0.998) = 0.9970$$

Gibbs Sampling: An Example



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0	F	F	F	F	F
1	F	T	F		
2					
3					
4					

- Sampling P(A|B,E,J,M): Using Bayes Rule,

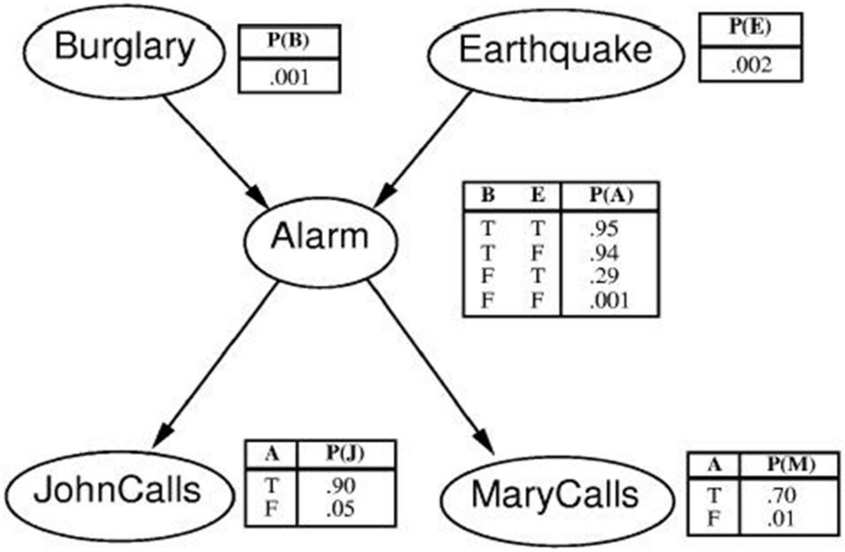
$$P(A \mid B,E,J,M) \propto P(J \mid A)P(M \mid A)P(A \mid B,E)$$

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

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

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

Gibbs Sampling: An Example



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1	F	T	F	T	
2					
3					
4					

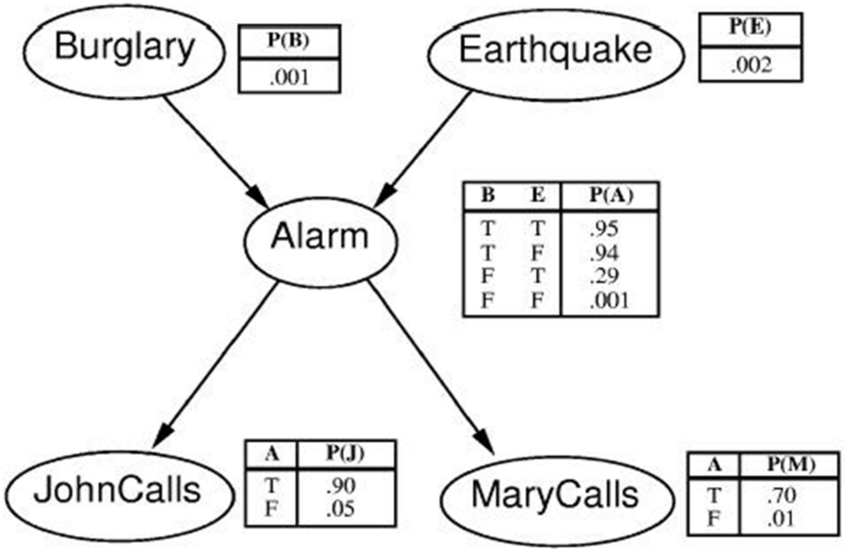
- Sampling P(J|A): No need to apply Bayes Rule

- A = F, so we compute the following, and sample J = T

$$P(J=T\mid A=F)\propto 0.05$$

$$P(J=F\mid A=F)\propto 0.95$$

Gibbs Sampling: An Example



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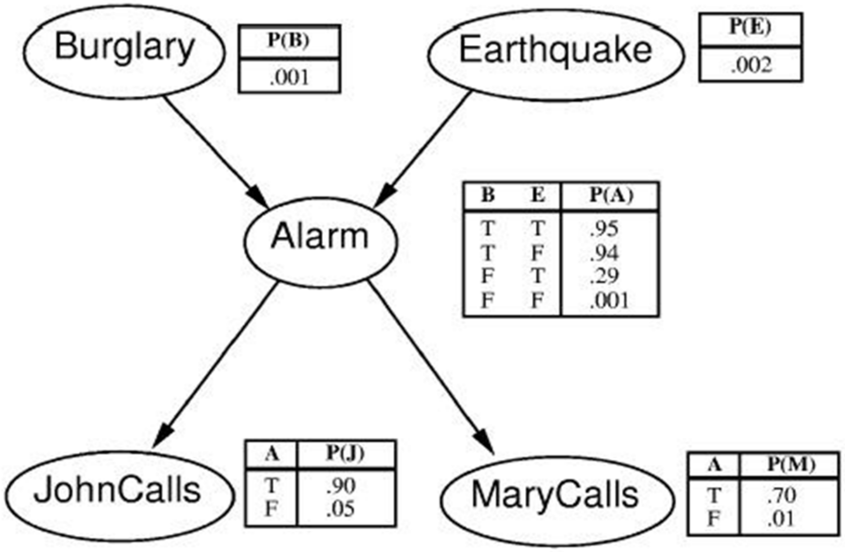
t	B	E	A	J	M
0	F	F	F	F	F
1	F	T	F	T	F
2					
3					
4					

- Sampling P(M|A): No need to apply Bayes Rule
- A = F, so we compute the following, and sample M = F

$$P(M = T \mid A = F) \propto 0.01$$

$$P(M = F \mid A = F) \propto 0.99$$

Gibbs Sampling: An Example



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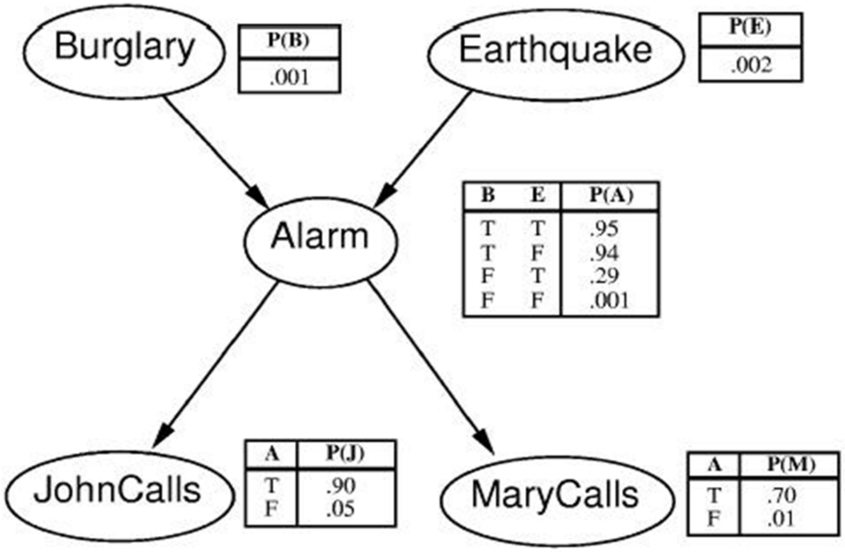
F	.01

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					
4					

- Now t = 2, and we repeat the procedure to sample new values of B,E,A,J,M …

Gibbs Sampling: An Example



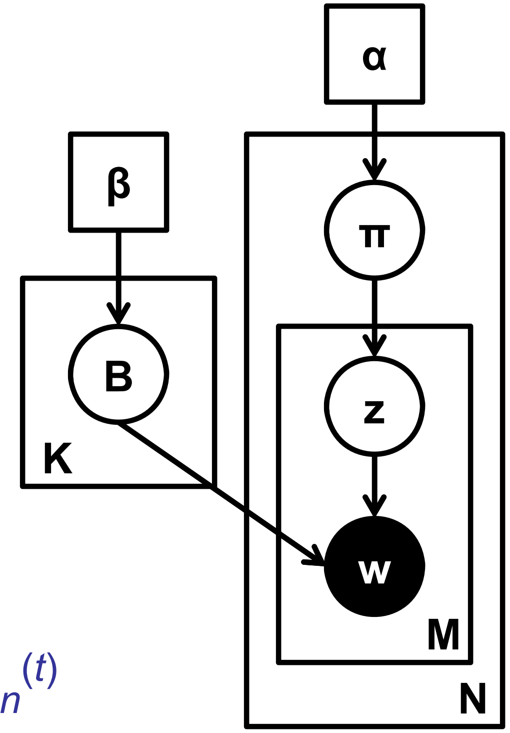
t	B	E	A	J	M
0	F	F	F	F	F
1	F	T	F	T	F
2	F	T	T	T	T
3	T	F	T	F	T
4	T	F	T	F	F

- 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.

Topic Models: Collapsed Gibbs

(Tom Griffiths & Mark Steyvers)

- Collapsed Gibbs sampling
  - Popular inference algorithm for topic models
  - Integrate out topic vectors π and topics B
  - Only need to sample word-topic assignments z



Algorithm:

For all variables $\mathbf{z} = z_1, z_2, \ldots, z_n$

Draw $z_i^{(t+1)}$ from $P(z_i|\mathbf{z}_{-i}, \boldsymbol{w})$

where $\mathbf{z}_{-i} = z_1^{(t+1)}, z_2^{(t+1)}, \ldots, z_{i-1}^{(t+1)}, z_{i+1}^{(t)}, \ldots, z_n^{(t)}$

Collapsed Gibbs sampling

- What is $P(z_i|\mathbf{z}_{-i}, \boldsymbol{w})$?
  - It is a product of two Dirichlet-Multinomial conditional distributions:

$$P(z_i = j|\mathbf{z}_{-i}, \mathbf{w}) \propto \underbrace{\frac{n^{(w_i)}_{-i,j} + \beta}{n^{(\cdot)}_{-i,j} + W\beta}}_{\text{“word-topic” term}} \underbrace{\frac{n^{(d_i)}_{-i,j} + \alpha}{n^{(d_i)}_{-i,\cdot} + T\alpha}}_{\text{“doc-topic” term}}$$

Collapsed Gibbs sampling

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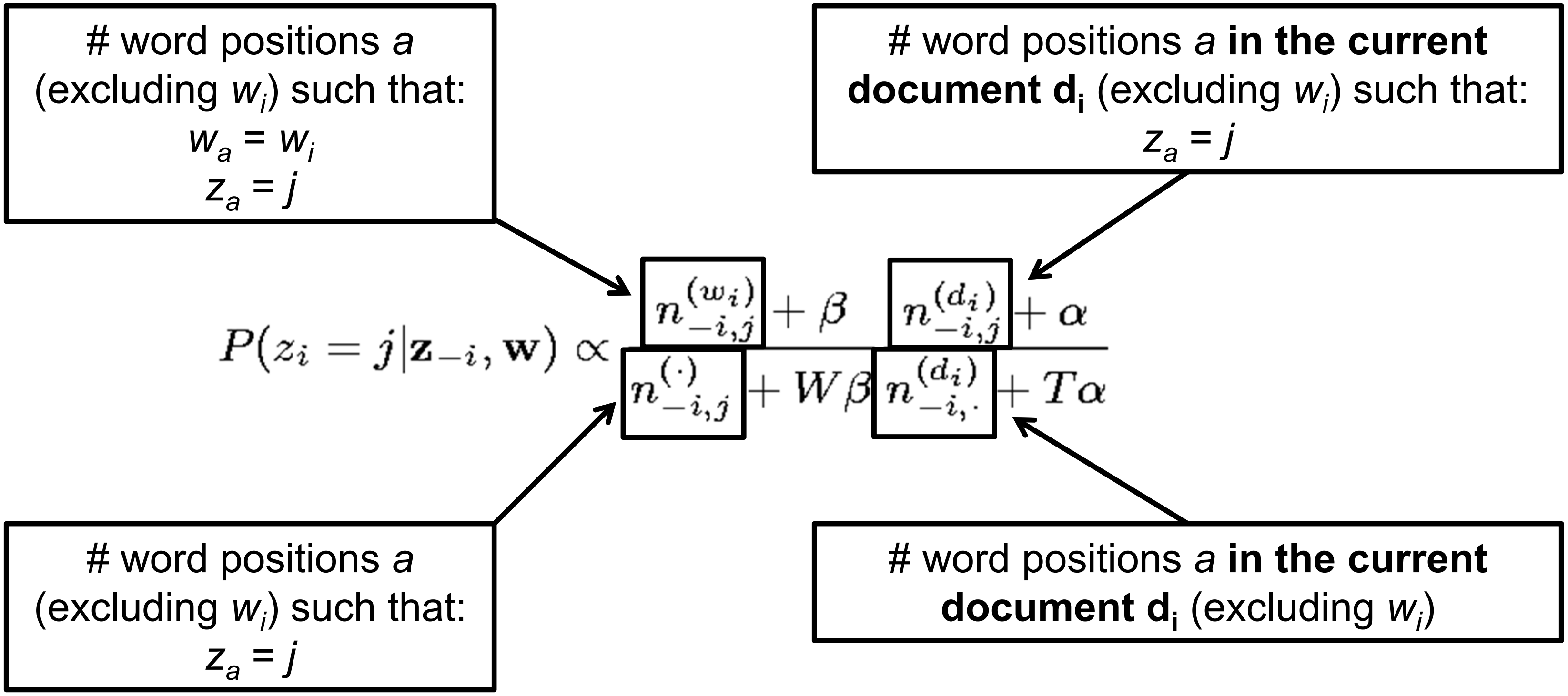

# word positions *a* (excluding w_i) such that:
$w_a = w_i$
$z_a = j$

# word positions *a* **in the current document d$_\mathbf{i}$** (excluding w_i) such that:
$z_a = j$

$$P(z_i = j|\mathbf{z}_{-i}, \mathbf{w}) \propto \frac{\boxed{n^{(w_i)}_{-i,j}} + \beta}{\boxed{n^{(\cdot)}_{-i,j}} + W\beta} \frac{\boxed{n^{(d_i)}_{-i,j}} + \alpha}{\boxed{n^{(d_i)}_{-i,\cdot}} + T\alpha}$$

# word positions *a* (excluding w_i) such that:
$z_a = j$

# word positions *a* **in the current document d$_\mathbf{i}$** (excluding w_i)

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Collapsed Gibbs illustration

			iteration 1
i	w_i	d_i	z_i
1	MATHEMATICS	1	2
2	KNOWLEDGE	1	2
3	RESEARCH	1	1
4	WORK	1	2
5	MATHEMATICS	1	1
6	RESEARCH	1	2
7	WORK	1	2
8	SCIENTIFIC	1	1
9	MATHEMATICS	1	2
10	WORK	1	1
11	SCIENTIFIC	2	1
12	KNOWLEDGE	2	1
.	.	.	.
.	.	.	.
.	.	.	.
50	JOY	5	2

Collapsed Gibbs illustration

			iteration	
			1	**2**
i	w_i	d_i	z_i	z_i
1	MATHEMATICS	1	2	?
2	KNOWLEDGE	1	2	
3	RESEARCH	1	1	
4	WORK	1	2	
5	MATHEMATICS	1	1	
6	RESEARCH	1	2	
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Collapsed Gibbs illustration

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.	.	.	.	
.	.	.	.	
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$$P(z_i = j | \mathbf{z}_{-i}, \mathbf{w}) \propto \frac{n_{-i,j}^{(w_i)} + \beta}{n_{-i,j}^{(\cdot)} + W\beta} \frac{n_{-i,j}^{(d_i)} + \alpha}{n_{-i,\cdot}^{(d_i)} + T\alpha}$$

Collapsed Gibbs illustration

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			1	2
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Collapsed Gibbs illustration

			iteration	
			1	**2**
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1	MATHEMATICS	1	2	2
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3	RESEARCH	1	1	?
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Collapsed Gibbs illustration

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			1	2
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3	RESEARCH	1	1	1
4	WORK	1	2	?
5	MATHEMATICS	1	1	
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.	.	.	.	
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Collapsed Gibbs illustration

			iteration	
			1	**2**
i	w_i	d_i	z_i	z_i
1	MATHEMATICS	1	2	2
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3	RESEARCH	1	1	1
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Collapsed Gibbs illustration

			iteration			
			1	**2**	**…**	**1000**
i	w_i	d_i	z_i	z_i		z_i
1	MATHEMATICS	1	2	2		2
2	KNOWLEDGE	1	2	1		2
3	RESEARCH	1	1	1		2
4	WORK	1	2	2		1
5	MATHEMATICS	1	1	2		2
6	RESEARCH	1	2	2		2
7	WORK	1	2	2		2
8	SCIENTIFIC	1	1	1	…	1
9	MATHEMATICS	1	2	2		2
10	WORK	1	1	2		2
11	SCIENTIFIC	2	1	1		2
12	KNOWLEDGE	2	1	2		2
.	.	.	.	.		.
.	.	.	.	.		.
.	.	.	.	.		.
50	JOY	5	2	1		1

$$P(z_i = j \mid \mathbf{z}_{-i}, \mathbf{w}) \propto \frac{n^{(w_i)}_{-i,j} + \beta}{n^{(\cdot)}_{-i,j} + W\beta} \frac{n^{(d_i)}_{-i,j} + \alpha}{n^{(d_i)}_{-i,\cdot} + T\alpha}$$

Gibbs Sampling is a special case of MH

- The GS proposal distribution is

$$Q(x_i', \mathbf{x}_{-i} \mid x_i, \mathbf{x}_{-i}) = P(x_i' \mid \mathbf{x}_{-i})$$

  - Where $\mathbf{x}_{-i}$ denotes all variables except x_i

- Applying MH to this proposal, we find that samples are always accepted (which is exactly what GS does):

$$A(x_i', \mathbf{x}_{-i} \mid x_i, \mathbf{x}_{-i}) = \min\left(1, \frac{P(x_i', \mathbf{x}_{-i}) Q(x_i, \mathbf{x}_{-i} \mid x_i', \mathbf{x}_{-i})}{P(x_i, \mathbf{x}_{-i}) Q(x_i', \mathbf{x}_{-i} \mid x_i, \mathbf{x}_{-i})}\right)$$

$$= \min\left(1, \frac{P(x_i', \mathbf{x}_{-i}) P(x_i \mid \mathbf{x}_{-i})}{P(x_i, \mathbf{x}_{-i}) P(x_i' \mid \mathbf{x}_{-i})}\right) = \min\left(1, \frac{P(x_i' \mid \mathbf{x}_{-i}) P(\mathbf{x}_{-i}) P(x_i \mid \mathbf{x}_{-i})}{P(x_i \mid \mathbf{x}_{-i}) P(\mathbf{x}_{-i}) P(x_i' \mid \mathbf{x}_{-i})}\right)$$

$$= \min(1,1) = 1$$

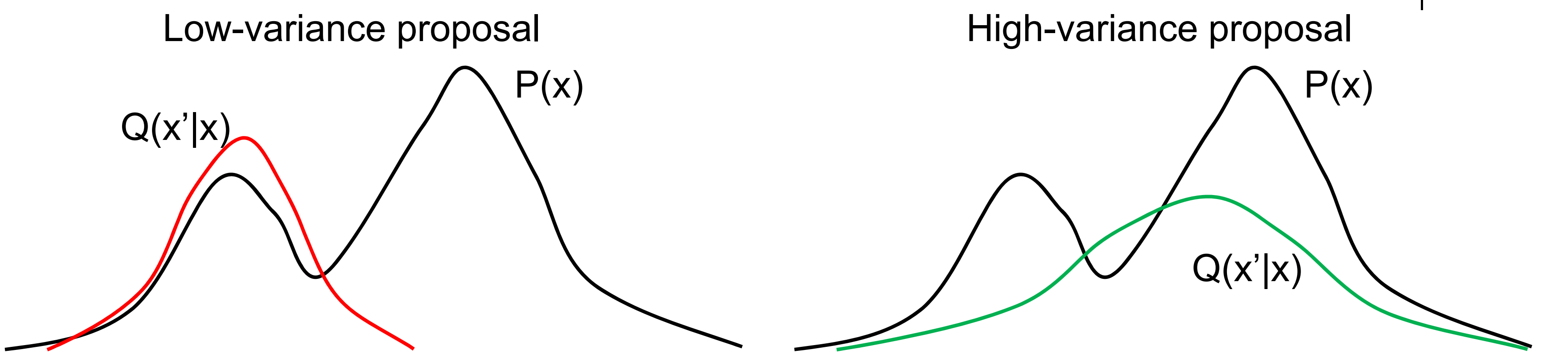
  - GS is simply MH with a proposal that is always accepted!

Practical Aspects of MCMC

- How do we know if our proposal Q(x'|x) is any good?
  - Monitor the acceptance rate
  - Plot the autocorrelation function

- How do we know when to stop burn-in?
  - Plot the sample values vs time
  - Plot the log-likelihood vs time

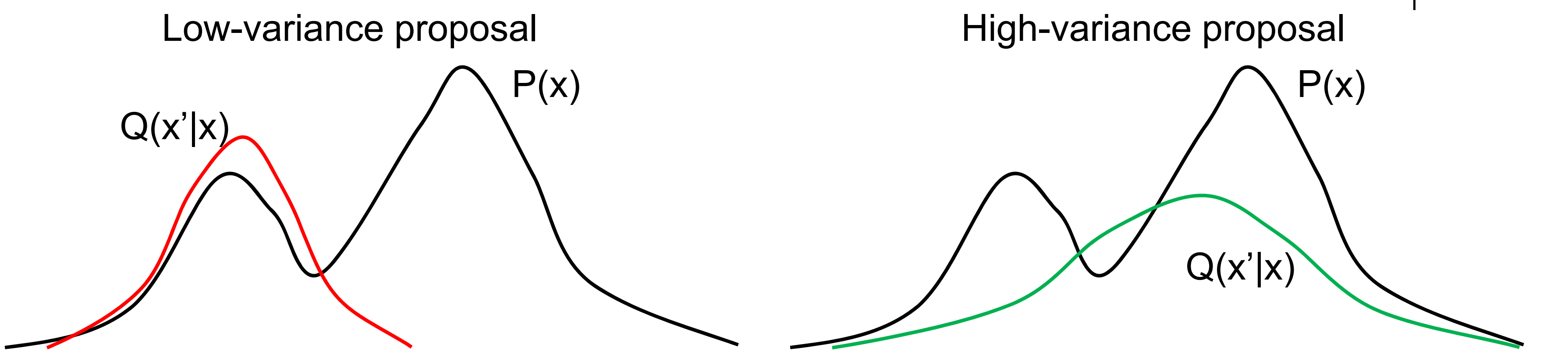
Acceptance Rate



- Choosing the proposal Q(x'|x) is a tradeoff:
  - "Narrow", low-variance proposals have high acceptance, but take many iterations to explore P(x) fully because the proposed x are too close
  - "Wide", high-variance proposals have the potential to explore much of P(x), but many proposals are rejected which slows down the sampler

- A good Q(x'|x) proposes distant samples x' with a sufficiently high acceptance rate

Acceptance Rate



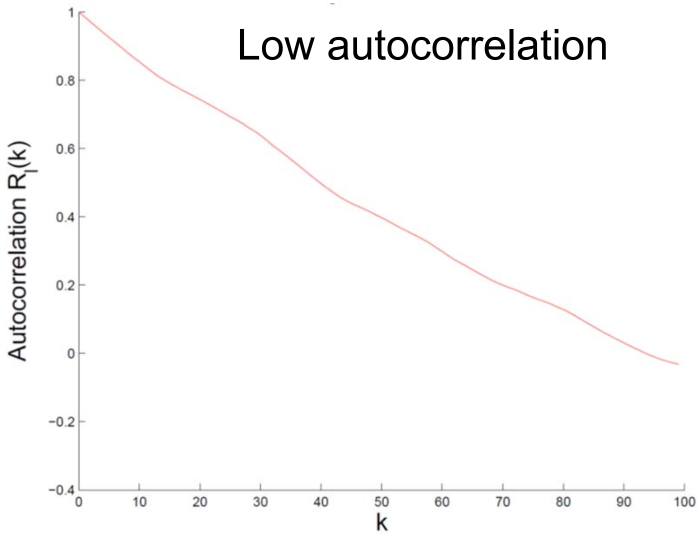
- Acceptance rate is the fraction of samples that MH accepts.
  - General guideline: proposals should have ~0.5 acceptance rate [1]

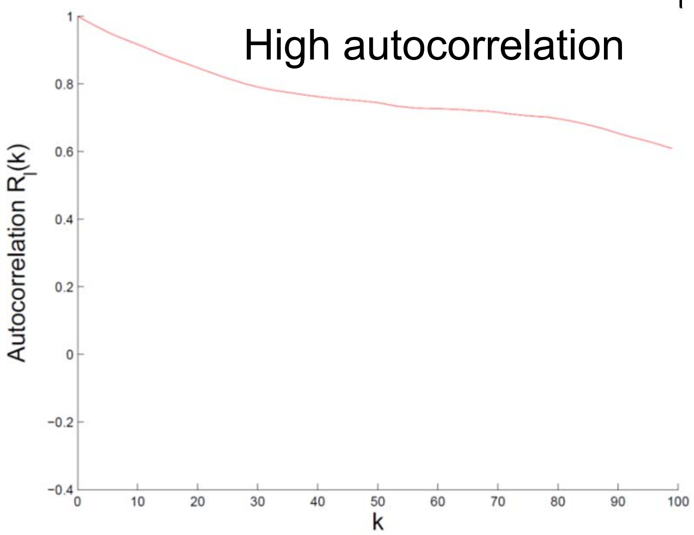
- Gaussian special case:
  - If both P(x) and Q(x'|x) are Gaussian, the optimal acceptance rate is ~0.45 for D=1 dimension and approaches ~0.23 as D tends to infinity [2]

[1] Muller, P. (1993). "A Generic Approach to Posterior Integration and Gibbs Sampling"

[2] Roberts, G.O., Gelman, A., and Gilks, W.R. (1994). "Weak Convergence and Optimal Scaling of Random Walk Metropolis Algorithms"

Autocorrelation function





- MCMC chains always show autocorrelation (AC)
  - AC means that adjacent samples in time are highly correlated
- We quantify AC with the autocorrelation function of an r.v. x:

$$R_x(k) = \frac{\sum_{t=1}^{n-k} (x_t - \bar{x})(x_{t+k} - \bar{x})}{\sum_{t=1}^{n-k} (x_t - \bar{x})^2}$$

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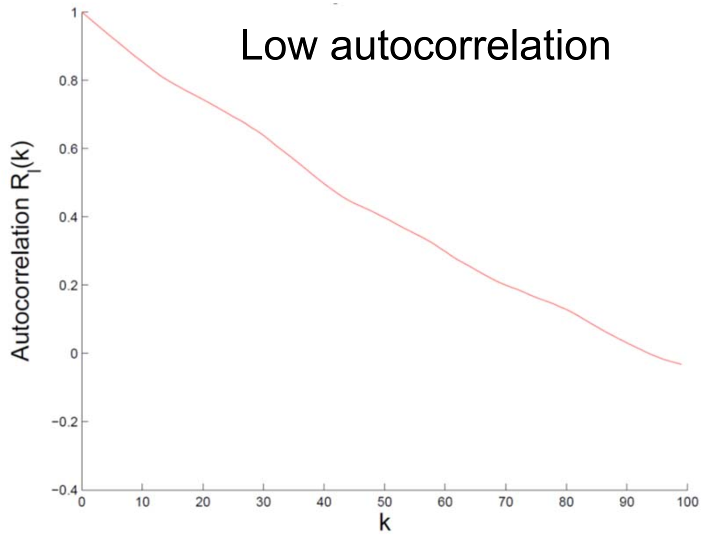
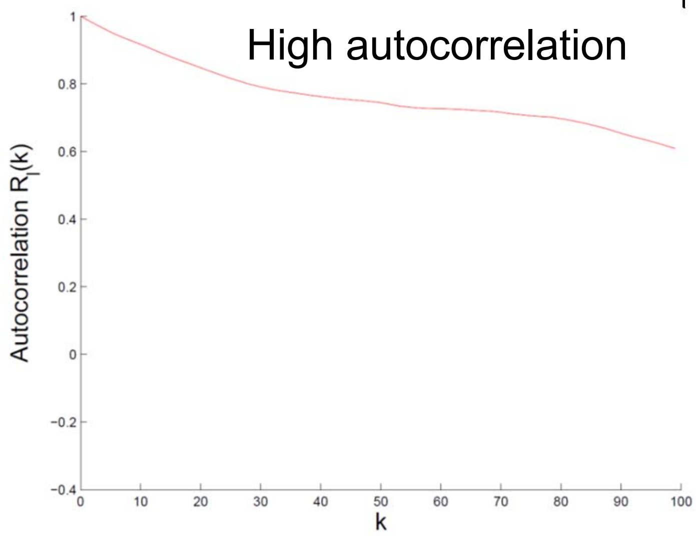
Autocorrelation function





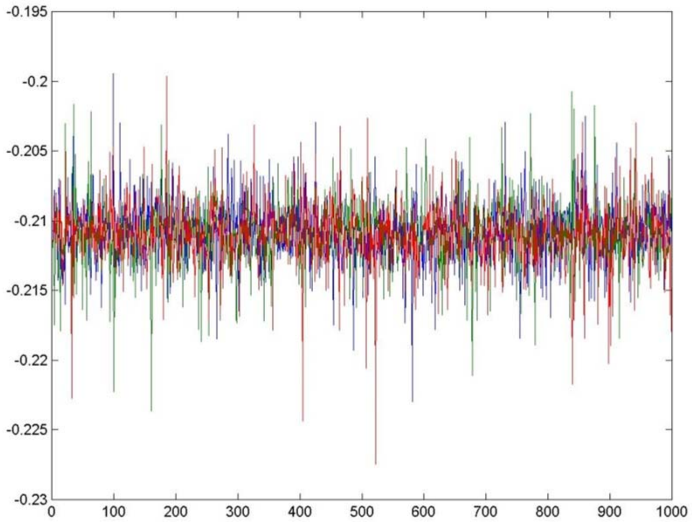
- The first-order AC $R_x(1)$ can be used to estimate the Sample Size Inflation Factor (SSIF):

$$s_x = \frac{1 + R_x(1)}{1 - R_x(1)}$$

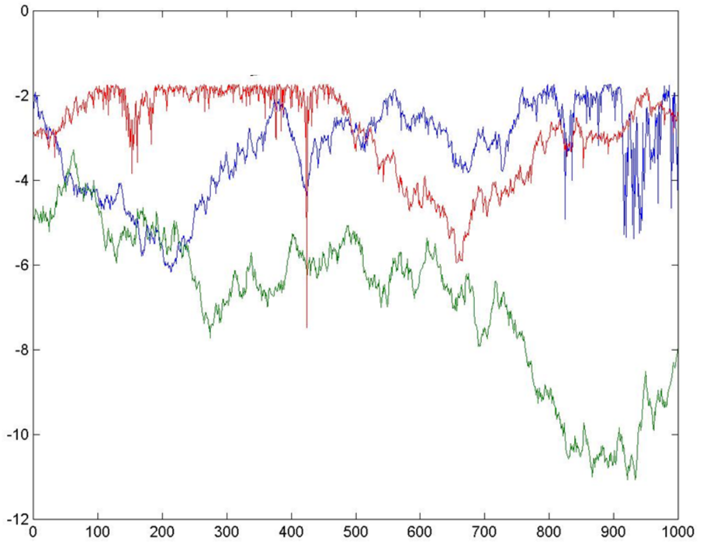
  - If we took n samples with SSIF s_x, then the effective sample size is n/s_x
  - High autocorrelation leads to smaller effective sample size!
  - We want proposals Q(x'|x) with low autocorrelation

Sample Values vs Time

Well-mixed chains

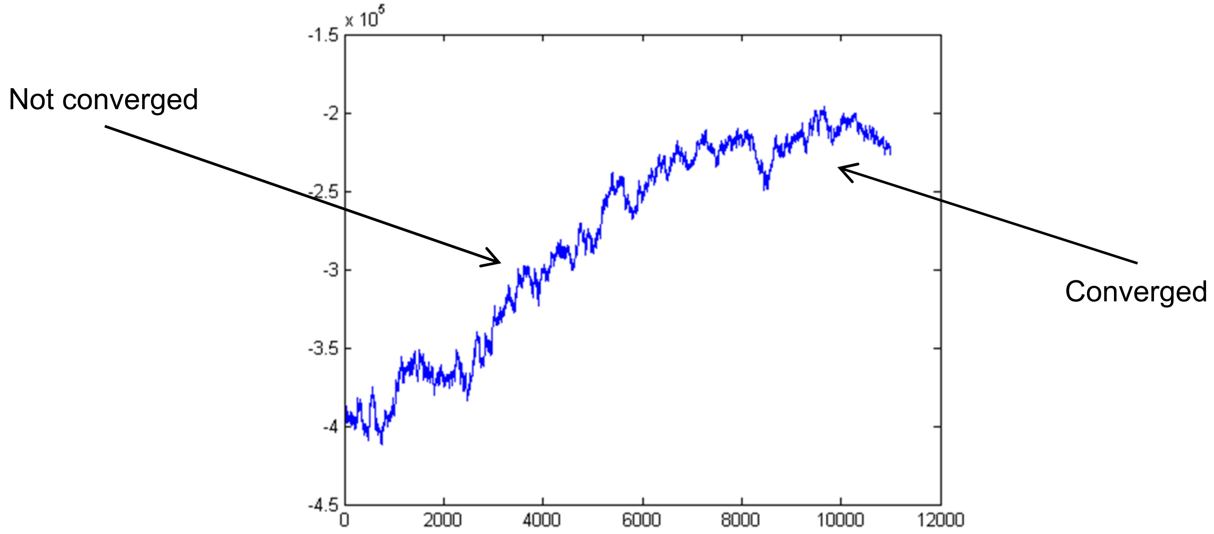


Poorly-mixed chains



- Monitor convergence by plotting samples (of r.v.s) from multiple MH runs (chains)
  - If the chains are well-mixed (left), they are probably converged
  - If the chains are poorly-mixed (right), we should continue burn-in

Log-likelihood vs Time



Not converged

Converged

- Many graphical models are high-dimensional
  - Hard to visualize all r.v. chains at once

- Instead, plot the complete log-likelihood vs. time
  - The complete log-likelihood is an r.v. that depends on all model r.v.s
  - Generally, the log-likelihood will climb, then eventually plateau

Summary

- Markov Chain Monte Carlo methods use adaptive proposals Q(x’|x) to sample from the true distribution P(x)

- Metropolis-Hastings allows you to specify any proposal Q(x’|x)
  - But choosing a good Q(x’|x) requires care

- Gibbs sampling sets the proposal Q(x’|x) to the conditional distribution P(x’|x)
  - Acceptance rate always 1!
  - But remember that high acceptance usually entails slow exploration
  - In fact, there are better MCMC algorithms for certain models

- Knowing when to halt burn-in is an art