10-418 / 10-618 Machine Learning for Structured Data

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Approximate Inference:
Markov Chain Monte Carlo (MCMC)

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Lecture 18
Oct. 28, 2019

Reminders

- Homework 3: Structured SVM
  - Out: Fri, Oct. 24
  - Due: Wed, Nov. 6 at 11:59pm
- Midterm Exam Viewing
- Project Milestones

Outline

- **Monte Carlo Methods**
- **MCMC (Basic Methods)**
  - Metropolis algorithm
  - Metropolis-Hastings (M-H) algorithm
  - Gibbs Sampling
- **Markov Chains**
  - Transition probabilities
  - Invariant distribution
  - Equilibrium distribution
  - Markov chain as a WFSM
  - Constructing Markov chains
  - Why does M-H work?
- **MCMC (Auxiliary Variable Methods)**
  - Slice Sampling
  - Hamiltonian Monte Carlo

Metropolis, Metropolis-Hastings, Gibbs Sampling

MCMC (BASIC METHODS)

A Few Problems for a Factor Graph

Suppose we already have the parameters of a Factor Graph…

1. How do we compute the probability of a specific assignment to the variables?
   $P(T=t, H=h, A=a, C=c)$

2. How do we draw a sample from the joint distribution?
   $t,h,a,c \sim P(T, H, A, C)$

3. How do we compute marginal probabilities?
   $P(A) = \ldots$

4. How do we draw samples from a conditional distribution?
   $t,h,a \sim P(T, H, A \mid C = c)$

5. How do we compute conditional marginal probabilities?
   $P(H \mid C = c) = \ldots$

Can we use samples ?

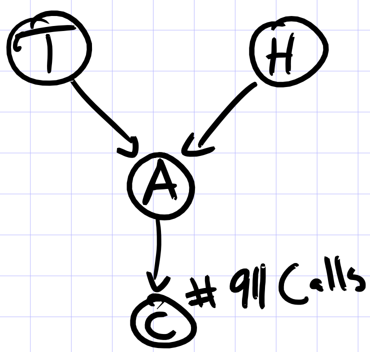
Inference for Bayes Nets

Whiteboard

- Background: Marginal Probability
- Sampling from a joint distribution
- Gibbs Sampling

Sampling from a Joint Distribution

Ex: Tornado



$T \sim \text{Bernoulli}(\tau)$ $\quad \tau = 1/2$

$H \sim \text{Bernoulli}(\eta)$ $\quad \eta = 1/3$

$A \sim \text{Bernoulli}(\alpha_{H,T})$ $\quad \alpha =$

	T=0	T=1
H=0	0	1/2
H=1	1/2	1

$C \sim \text{Unif}(\{1, \ldots, 63\}) + A * \text{Unif}(\{1, \ldots, 63\})$

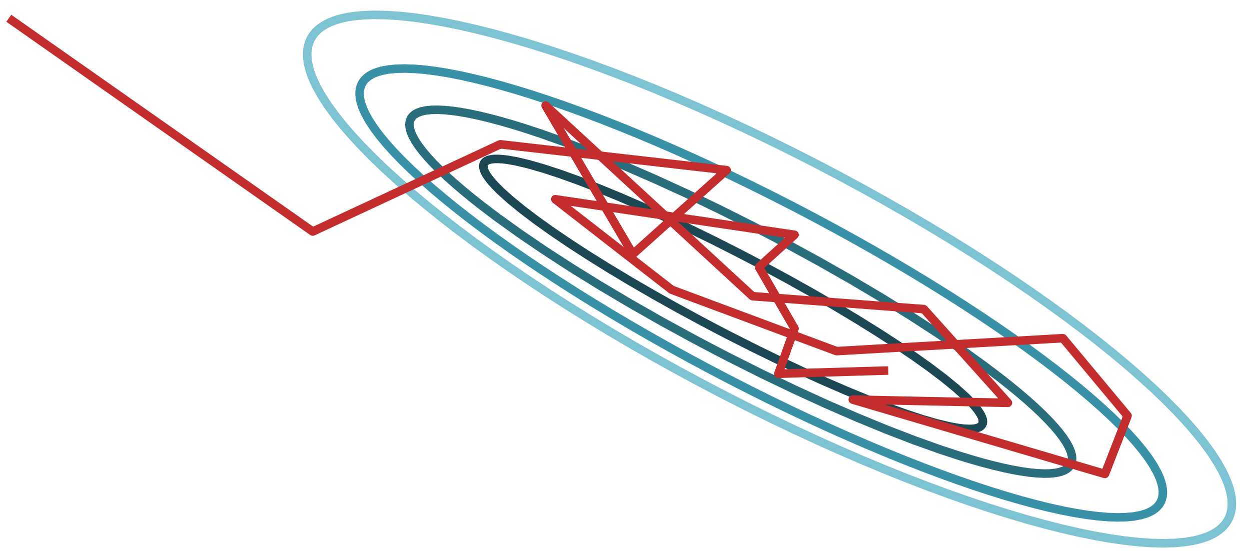
← integer

T	H	A	C

We can use these samples to estimate many different probabilities!

MCMC

- **Goal:** Draw approximate, correlated samples from a target distribution p(x)
- **MCMC:** Performs a biased random walk to explore the distribution



Simulations of MCMC

Visualization of Metroplis-Hastings, Gibbs Sampling, and Hamiltonian MCMC:

https://chi-feng.github.io/mcmc-demo/

http://twiecki.github.io/blog/2014/01/02/visualizing-mcmc/

GIBBS SAMPLING

Gibbs Sampling

Whiteboard

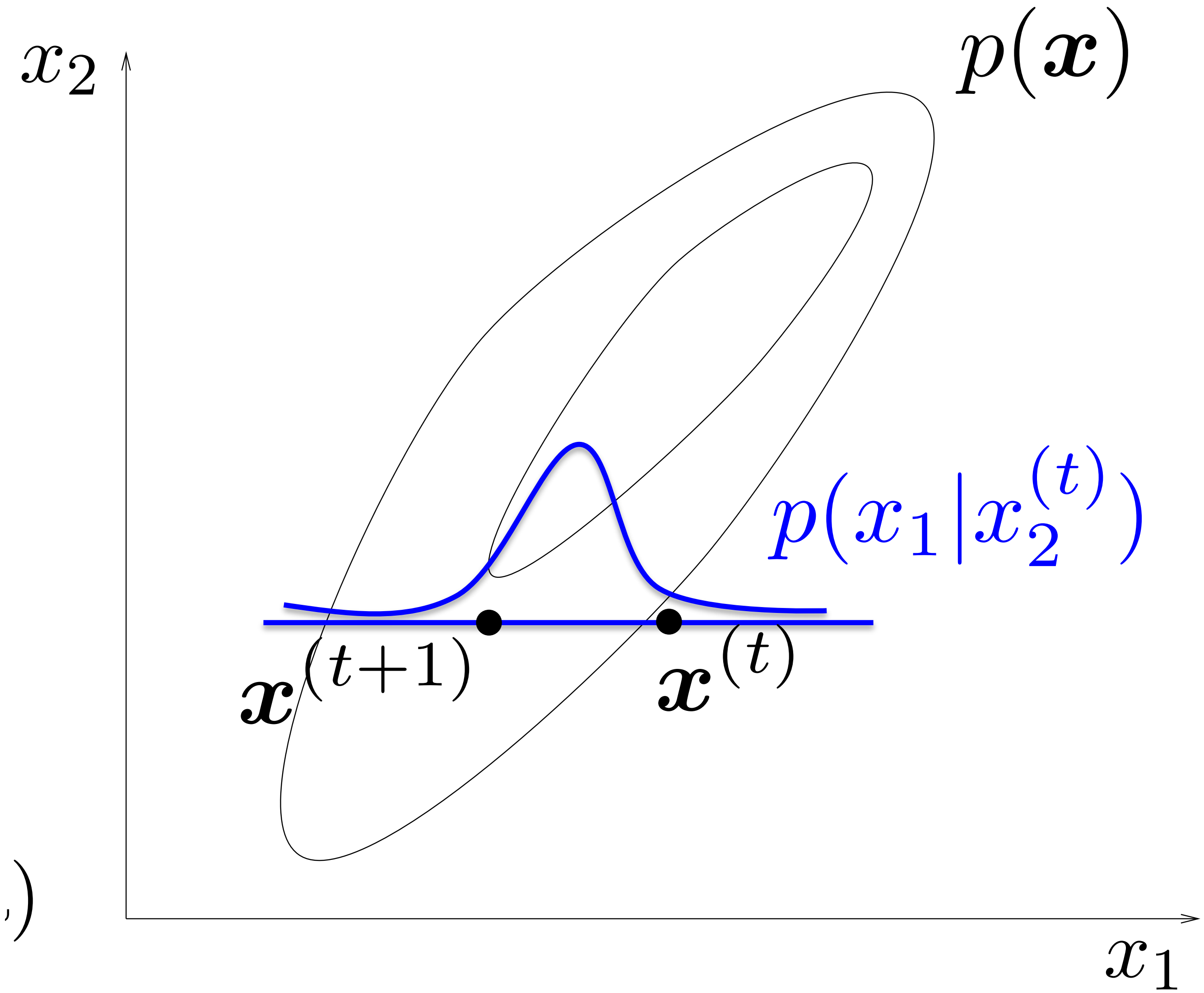
- Gibbs Sampling
- Example: 3-node Factor Graph

Gibbs Sampling

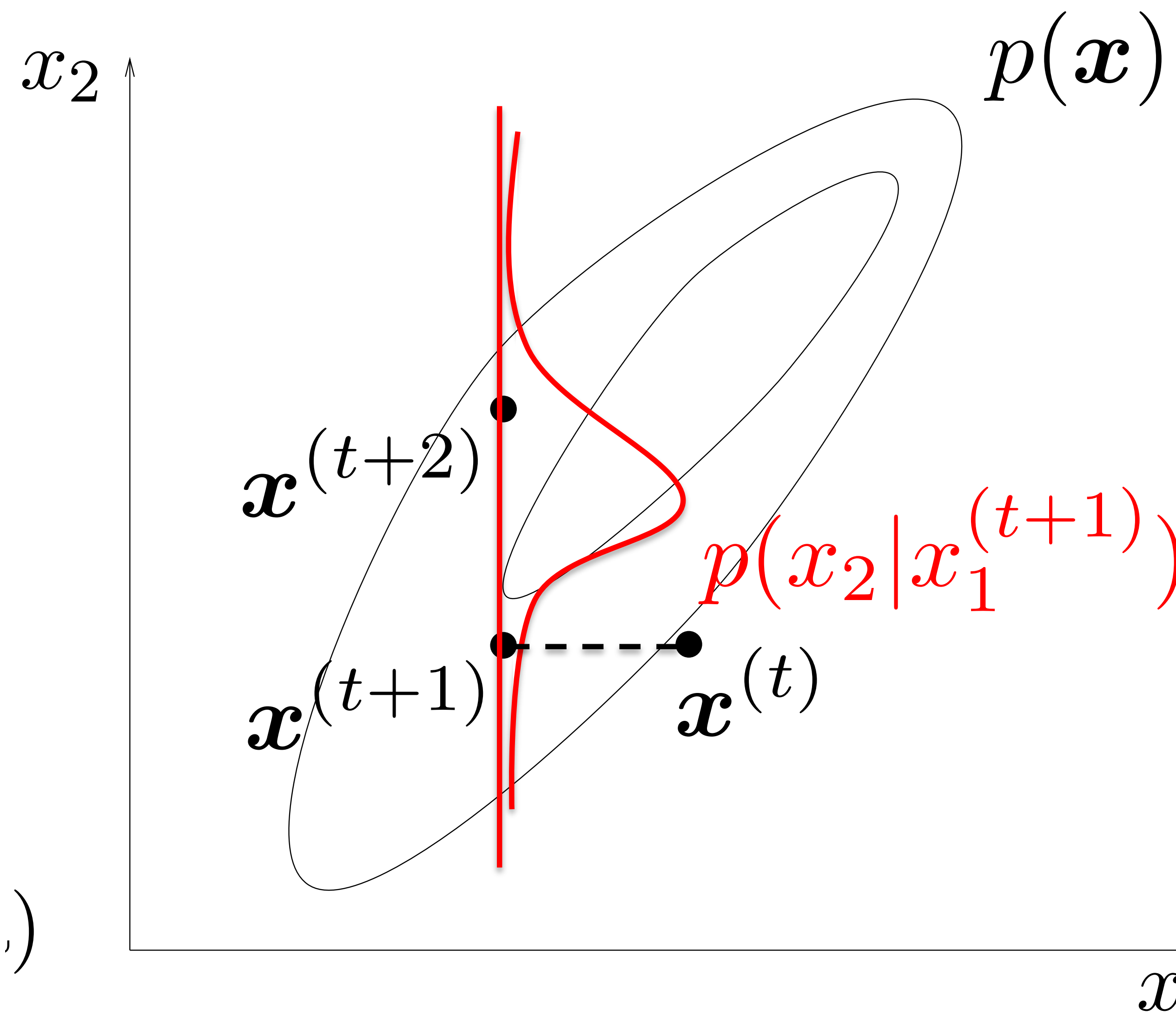
Example: 3-node Factor Graph

```python
import numpy as np
import random

def sample01(g0, g1):
    u = random.uniform(0, g0 + g1)
    if u < g0:
        return 0
    else:
        return 1

def gibbs_sampling():
    # Define factor graph
    psi_ab = np.array([[1, 2], [1, 1]])
    psi_ac = np.array([[2, 2], [2, 1]])
    psi_bc = np.array([[1, 1], [2, 1]])

    # Initialize variable values
    a = random.choice([0,1])
    b = random.choice([0,1])
    c = random.choice([0,1])

    counts = np.array([[0, 0], [0, 0], [0, 0]])
    # Gibbs sampling
    for i in range(10):
        a = sample01(psi_ab[0,b] * psi_ac[0,c],
                     psi_ab[1,b] * psi_ac[1,c])
        b = sample01(psi_ab[a,0] * psi_bc[0,c],
                     psi_ab[a,1] * psi_bc[1,c])
        c = sample01(psi_ac[a,0] * psi_bc[b,0],
                     psi_ac[a,1] * psi_bc[b,1])
        print(a, b, c)
        counts[0, a] += 1
        counts[1, b] += 1
        counts[2, c] += 1

    print('p(a = 0) ~= %.2f' % (counts[0,0] / (counts[0,0] + counts[0,1])))
    print('p(b = 0) ~= %.2f' % (counts[1,0] / (counts[1,0] + counts[1,1])))
    print('p(c = 0) ~= %.2f' % (counts[2,0] / (counts[2,0] + counts[2,1])))

if __name__ == '__main__':
    gibbs_sampling()
```

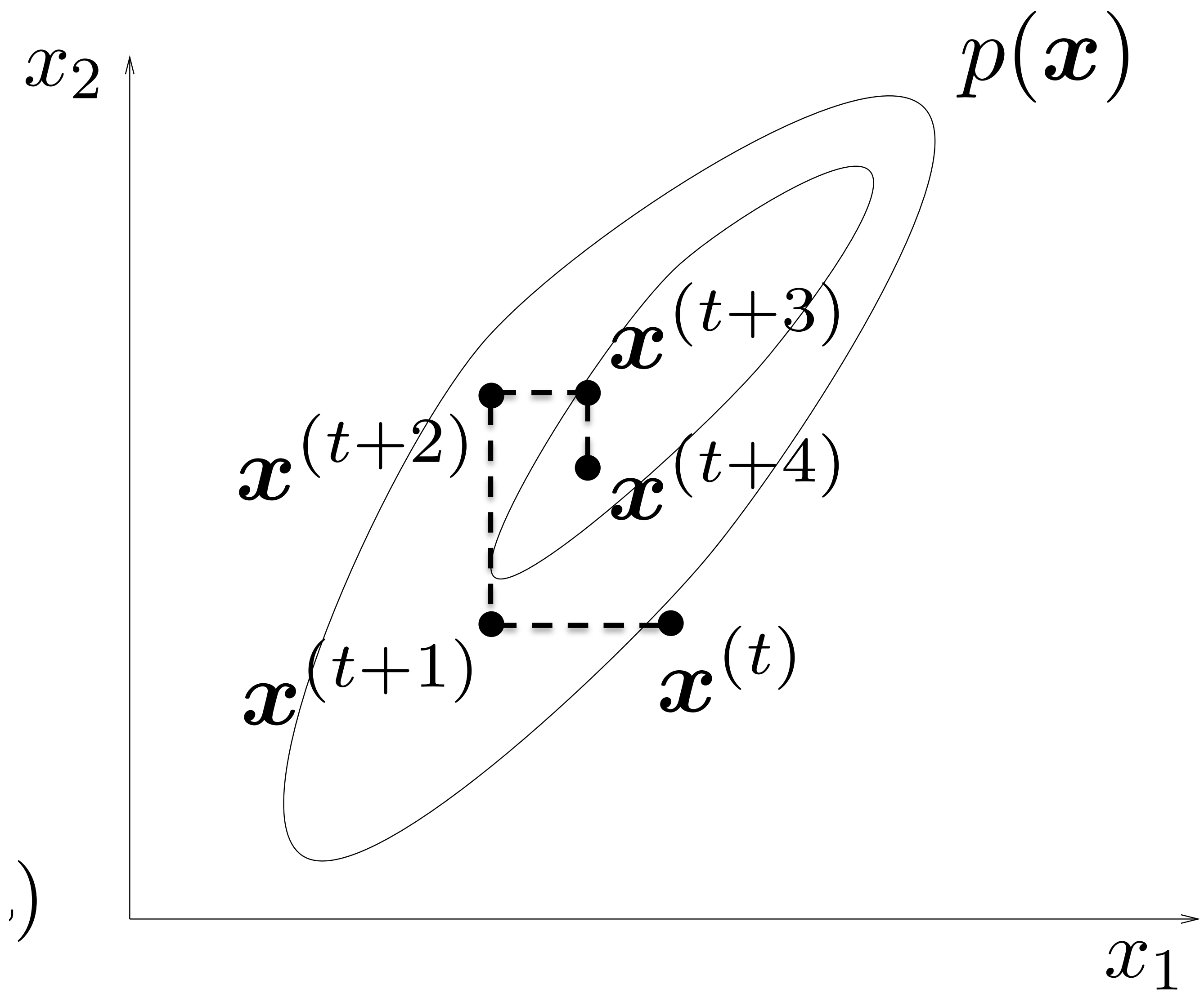
Gibbs Sampling



Gibbs Sampling



Gibbs Sampling



Gibbs Sampling

Question:

How do we draw samples from a conditional distribution?

$y_1, y_2, \ldots, y_J \sim p(y_1, y_2, \ldots, y_J \mid x_1, x_2, \ldots, x_J)$

(Approximate) Solution:

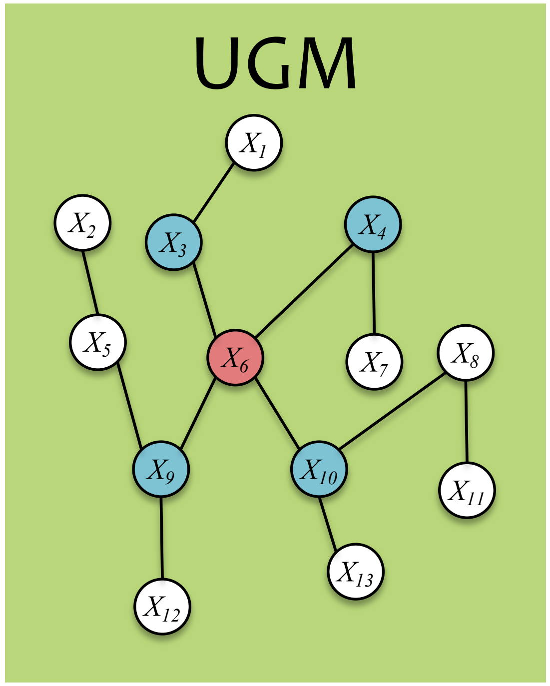
- Initialize $y_1^{(0)}, y_2^{(0)}, \ldots, y_J^{(0)}$ to arbitrary values
- For t = 1, 2, … :
  - $y_1^{(t+1)} \sim p(y_1 \mid y_2^{(t)}, \ldots, y_J^{(t)}, x_1, x_2, \ldots, x_J)$
  - $y_2^{(t+1)} \sim p(y_2 \mid y_1^{(t+1)}, y_3^{(t)}, \ldots, y_J^{(t)}, x_1, x_2, \ldots, x_J)$
  - $y_3^{(t+1)} \sim p(y_3 \mid y_1^{(t+1)}, y_2^{(t+1)}, y_4^{(t)}, \ldots, y_J^{(t)}, x_1, x_2, \ldots, x_J)$
  - …
  - $y_J^{(t+1)} \sim p(y_J \mid y_1^{(t+1)}, y_2^{(t+1)}, \ldots, y_{J-1}^{(t+1)}, x_1, x_2, \ldots, x_J)$

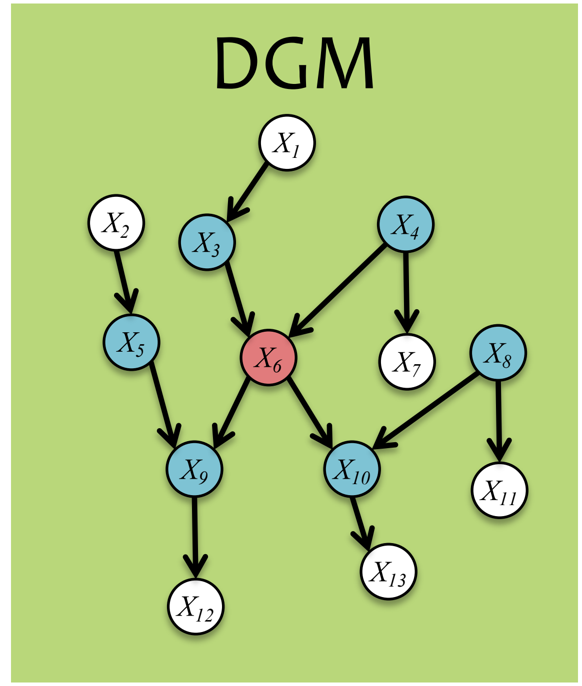
Properties:

- This will eventually yield samples from $p(y_1, y_2, \ldots, y_J \mid x_1, x_2, \ldots, x_J)$
- But it might take a long time -- just like other Markov Chain Monte Carlo methods

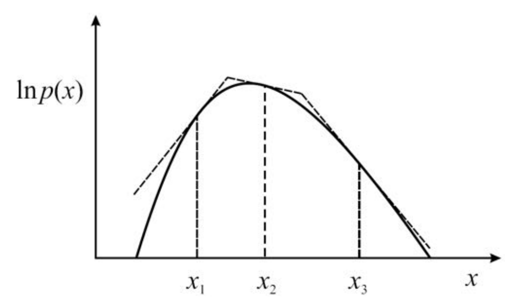
Gibbs Sampling

Full conditionals only need to condition on the **Markov Blanket**





- Must be "easy" to sample from conditionals
- Many conditionals are log-concave and are amenable to adaptive rejection sampling



METROPOLIS-HASTINGS

Metropolis-Hastings

Whiteboard

- Metropolis Algorithm
- Metropolis-Hastings Algorithm

Random Walk Behavior of M-H

- For Metropolis-Hastings, a generic proposal distribution is: $$q(x|x^{(t)}) = \mathcal{N}(0, \epsilon^2)$$

- If ϵ is large, many rejections
- If ϵ is small, slow mixing

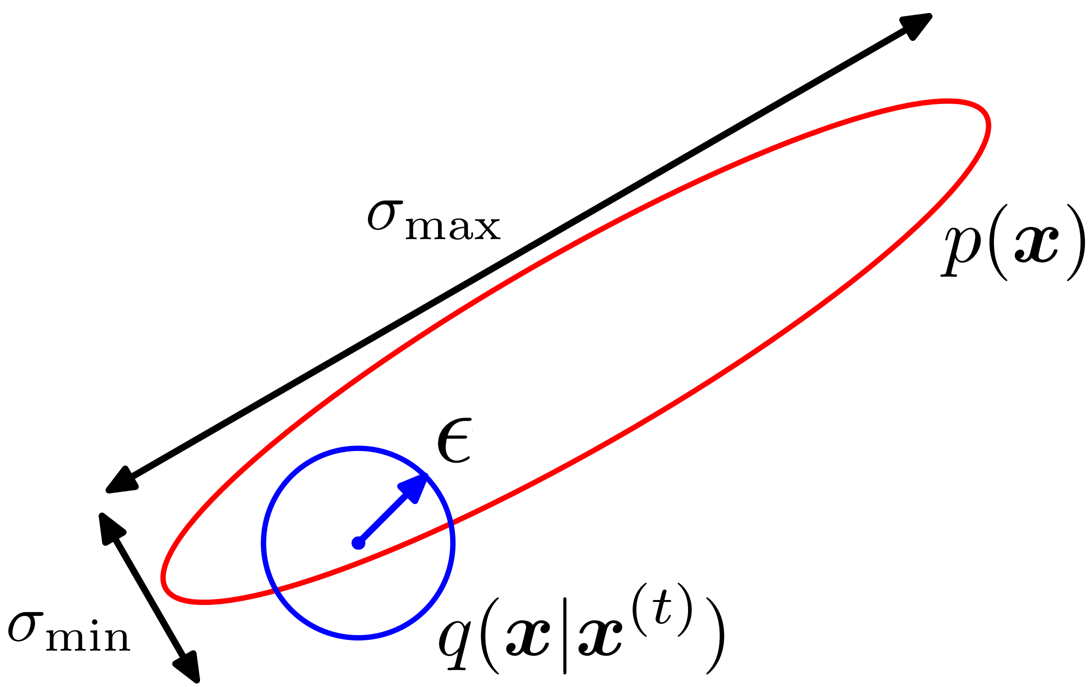
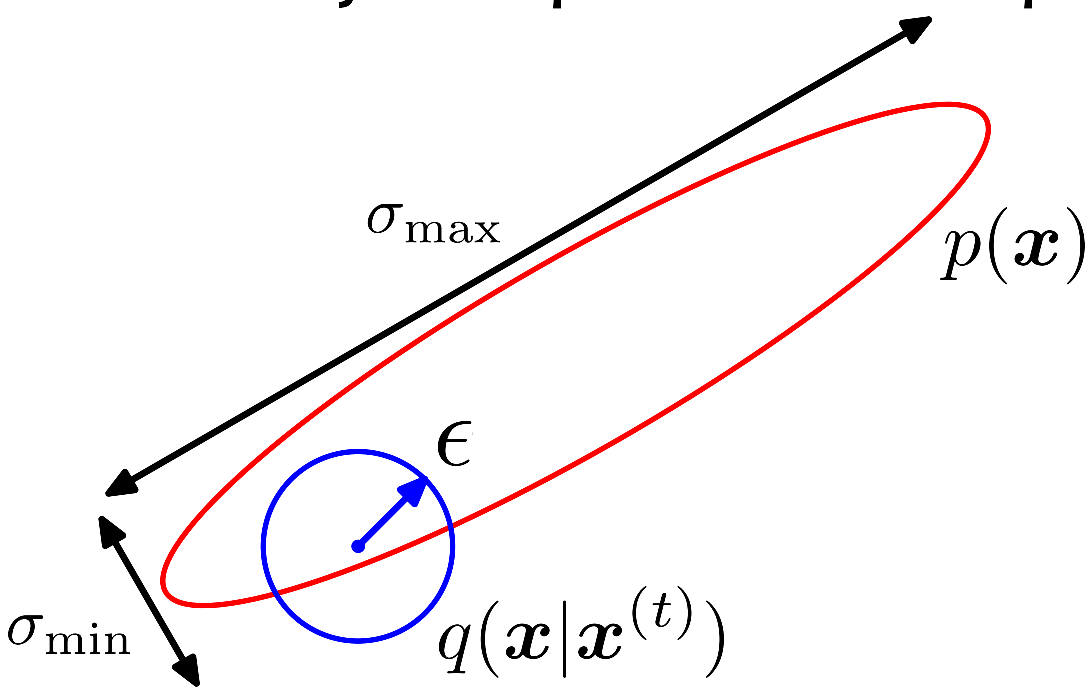


Figure from Bishop (2006)

Random Walk Behavior of M-H

- For Rejection Sampling, the accepted samples are are **independent**
- But for Metropolis-Hastings, the samples are **correlated**
- **Question:** How long must we wait to get effectively independent samples?



A: independent states in the M-H random walk are separated by roughly $(\sigma_{\max}/\sigma_{\min})^2$ steps

Whiteboard

- Gibbs Sampling as M-H