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

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Exam 1 Review

+

MCMC

Matt Gormley
Lecture 12
Oct. 10, 2022

Reminders

- Homework 2: Learning to Search for RNNs
  - Programming + Empirical Questions
    - Due: Mon, Oct 24 at 9:00am
  - Policy: 65 points or more on the autograder gives 100% autograder credit
- Homework 3: General Graph CRF Module
  - Out: Thu, Sep 29
  - Due: Mon, Oct 10 at 11:59pm
- Practice Problems 1
- Exam 1: Fri, Oct 14, in-class

EXAM 1 LOGISTICS

Exam 1

- **Time / Location**
  - **Time:** In-Class Exam
    Fri, Oct. 14 at 1:25pm – 2:45pm
  - **Location**: The same room as lecture/recitation.
    Please arrive a few minutes early.
  - Please watch Piazza carefully for announcements.
- **Logistics**
  - Covered material: Lecture 1 – Lecture 10
  - Format of questions:
    - Multiple choice
    - True / False (with justification)
    - Derivations
    - Short answers
    - Interpreting figures
    - Implementing algorithms on paper
    - Drawing
  - No electronic devices
  - You are allowed to **bring** one 8½ x 11 sheet of notes (front and back)

Topics for Exam 1

- Search-Based Structured Prediction
  - Reductions to Binary Classification
  - Learning to Search
  - RNN-LMs
  - seq2seq models
- Graphical Model Representation
  - Directed GMs vs. Undirected GMs vs. Factor Graphs
  - Bayesian Networks vs. Markov Random Fields vs. Conditional Random Fields
- Graphical Model Learning
  - ~~Fully observed Bayesian Network learning~~
  - Fully observed MRF learning
  - Fully observed CRF learning
  - Parameterization of a GM
  - Neural potential functions
- Exact Inference
  - Three inference problems: (1) marginals (2) partition function (3) most probably assignment
  - Variable Elimination
  - Belief Propagation (sum-product and max-product)

SAMPLE QUESTIONS

Sample Questions

Learning to Search

Suppose you are training a seq2seq model for supervised POS Tagging.

- Let the inputs to the encoder be e_1, e_2, e_3, …
- Let the inputs to the decoder be d_1, d_2, d_3, …
- Let the outputs of the decoder be o_1, o_2, o_3, …

1. (1 point) **Short Answer**: Describe in words what the inputs to the encoder would be. Assume you are training with Teacher Forcing.

2. (1 point) **Short Answer**: Describe in words what the inputs of the decoder would be. Assume you are training with Teacher Forcing.

3. (1 point) **Short Answer**: Describe in words what the outputs of the decoder would be. Assume you are training with Teacher Forcing.

Sample Questions

Learning to Search

Suppose you are training a seq2seq model for supervised POS Tagging.

- Let the inputs to the encoder be e_1, e_2, e_3, …
- Let the inputs to the decoder be d_1, d_2, d_3, …
- Let the outputs of the decoder be o_1, o_2, o_3, …

4. (1 point) **Short Answer**: Describe in words what the inputs to the encoder would be. Assume you are training with Scheduled Sampling. *(If your answer is the same as for Teacher Forcing, simply write "same".)*

same

5. (1 point) **Short Answer**: Describe in words what the inputs of the decoder would be. Assume you are training with Scheduled Sampling. *(If your answer is the same as for Teacher Forcing, simply write "same".)*

diff

6. (1 point) **Short Answer**: Describe in words what the outputs of the decoder would be. Assume you are training with Scheduled Sampling. *(If your answer is the same as for Teacher Forcing, simply write "same".)*

Sample Questions

6 Factor Graphs

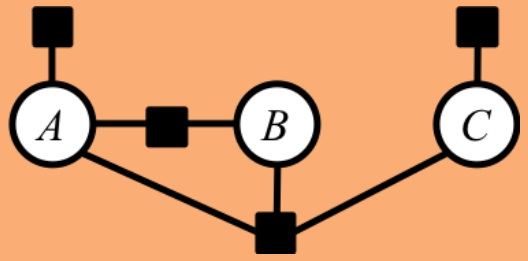

Figure 4: A factor graph over three binary random variables A, B, C, i.e. sampled values a, b, c from the random variables are in $\{0, 1\}$. Assume the factors are named $\psi_A(a)$, $\psi_{A,B}(a, b)$, $\psi_{A,B,C}(a, b, c)$, and $\psi_C(c)$.

1. (2 points) **Short answer:** Consider the factor graph in Figure 4. Using the given factor names, write the partition function Z that ensures the joint probability distribution $p(a, b, c)$ sums-to-one.

Sample Questions

6 Factor Graphs

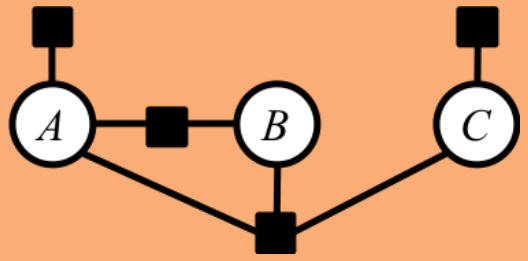

Figure 4: A factor graph over three binary random variables A, B, C, i.e. sampled values a, b, c from the random variables are in $\{0, 1\}$. Assume the factors are named $\psi_A(a)$, $\psi_{A,B}(a, b)$, $\psi_{A,B,C}(a, b, c)$, and $\psi_C(c)$.

2. (2 points) **Short answer:** Using the given factor names, write the joint probability mass function $p(a, b, c)$ defined by the factor graph shown in Figure 4. *You may include the term Z directly in your answer—no need to copy it from above.*

Sample Questions

6 Factor Graphs

3. (2 points) **Drawing:** Suppose we have a joint probability distribution that factorizes as below:

$$p(w, x, y, z) \propto \psi_X(x)\psi_{X,Y}(x, y)\psi_{X,Y,Z}(x, y, z)\psi_{W,Z}(w, z)\psi_{Y,Z}(y, z)$$

where $\propto$ denotes *proportional to*. Draw the factor graph corresponding to this factorization of the joint distribution.

Sample Questions

7 Inference in Graphical Models

Consider yet another factor graph consisting of two random variables $Q \in \{\text{red,green,blue}\}$, $R \in \{\text{pencil, crayon}\}$. Suppose we have the following factors:

Q	$\psi_Q(q)$
red	3
green	1
blue	2

Q	R	$\psi_{Q,R}(q,r)$
red	pencil	2
red	crayon	2
green	pencil	1
green	crayon	3
blue	pencil	4
blue	crayon	1

1. (2 points) **Short answer:** Draw a table containing all values of the function $s(q,r) = \psi_Q(q)\psi_{Q,R}(q,r)$. *You may use the integer abbreviations: red=1, green=2, blue=3, pencil=1, crayon=2.*

Sample Questions

Q1

Question:

Answer:

7 Inference in Graphical Models

Consider yet another factor graph consisting of two random variables $Q \in \{\text{red,green,blue}\}$, $R \in \{\text{pencil, crayon}\}$. Suppose we have the following factors:

Q	$\psi_Q(q)$
red	3
green	1
blue	2

Q	R	$\psi_{Q,R}(q,r)$
red	pencil	2
red	crayon	2
green	pencil	1
green	crayon	3
blue	pencil	4
blue	crayon	1

2. (2 points) **Numerical answer:** What is the value of the partition function Z for the joint distribution $p(q, r)$?

Sample Questions

7 Inference in Graphical Models

Consider yet another factor graph consisting of two random variables $Q \in \{\text{red,green,blue}\}$, $R \in \{\text{pencil, crayon}\}$. Suppose we have the following factors:

Q	$\psi_Q(q)$
red	3
green	1
blue	2

Q	R	$\psi_{Q,R}(q,r)$
red	pencil	2
red	crayon	2
green	pencil	1
green	crayon	3
blue	pencil	4
blue	crayon	1

$\psi_Q(q)$ $s(q,r)$

3 6
3 6
1 1
1 3
2 8
2 2

\+

$\Rightarrow Z = 26$

3. (2 points) **Numerical answer:** What is the value of the joint probability $P(Q = \textit{green}, R = \textit{crayon})$? *You may leave your answer in the form of an unsimplified fraction—no calculator necessary.*

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Sample Questions

7 Inference in Graphical Models

Consider yet another factor graph consisting of two random variables $Q \in \{\text{red,green,blue}\}$, $R \in \{\text{pencil, crayon}\}$. Suppose we have the following factors:

Q	$\psi_Q(q)$
red	3
green	1
blue	2

Q	R	$\psi_{Q,R}(q,r)$
red	pencil	2
red	crayon	2
green	pencil	1
green	crayon	3
blue	pencil	4
blue	crayon	1

4. (2 points) **Numerical answer:** What is the value of the marginal probability $P(Q = \textit{green})$? *You may leave your answer in the form of an unsimplified fraction—no calculator necessary.*

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Sample Questions

7 Inference in Graphical Models

Consider yet another factor graph consisting of two random variables $Q \in \{\text{red,green,blue}\}$, $R \in \{\text{pencil, crayon}\}$. Suppose we have the following factors:

Q	$\psi_Q(q)$
red	3
green	1
blue	2

Q	R	$\psi_{Q,R}(q,r)$
red	pencil	2
red	crayon	2
green	pencil	1
green	crayon	3
blue	pencil	4
blue	crayon	1

5. (2 points) **Short answer:** Suppose you run the Variable Elimination algorithm to eliminate the variable Q, resulting in a new factor graph with just one factor $m(r)$. Draw a table containing the values of this new factor.

Sample Questions

7 Inference in Graphical Models

Consider yet another factor graph consisting of two random variables $Q \in \{\text{red,green,blue}\}$, $R \in \{\text{pencil, crayon}\}$. Suppose we have the following factors:

Q	$\psi_Q(q)$
red	3
green	1
blue	2

Q	R	$\psi_{Q,R}(q,r)$
red	pencil	2
red	crayon	2
green	pencil	1
green	crayon	3
blue	pencil	4
blue	crayon	1

6. (2 points) **Numerical answer:** What is the value of the marginal probability $P(R = \textit{crayon})$? *You may leave your answer in the form of an unsimplified fraction—no calculator necessary.*

Sample Questions

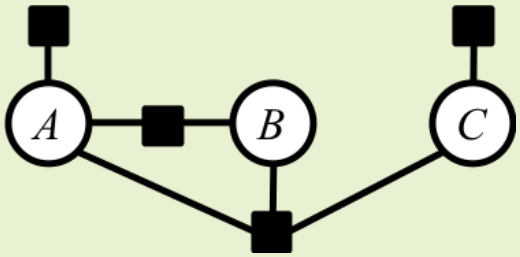
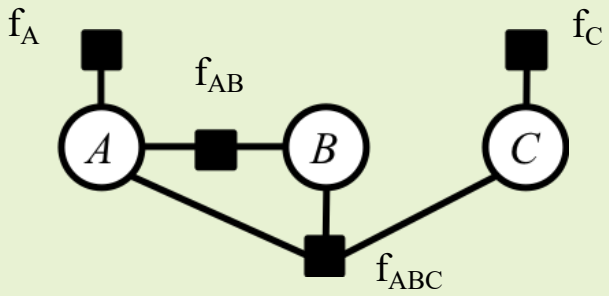


Figure 4: A factor graph over three binary random variables A, B, C, i.e. sampled values a, b, c from the random variables are in $\{0, 1\}$. Assume the factors are named $\psi_A(a)$, $\psi_{A,B}(a, b)$, $\psi_{A,B,C}(a, b, c)$, and $\psi_C(c)$.

1. (1 point) **Drawing**: Suppose you are running the Variable Elimination algorithm. The first variable you eliminate is B. Draw the factor graph that results after you have eliminated variable B.

Sample Questions



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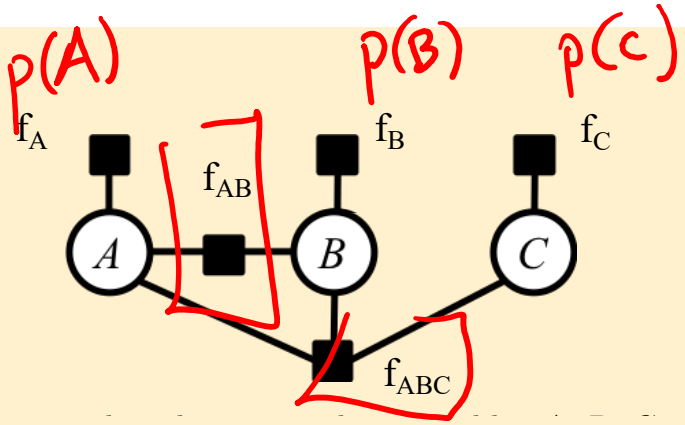
2. (1 point) **Numerical Answer**: Suppose you are running the Belief Propagation algorithm? How many messages are required to send a message from f_{ABC} to C?

Sample Questions

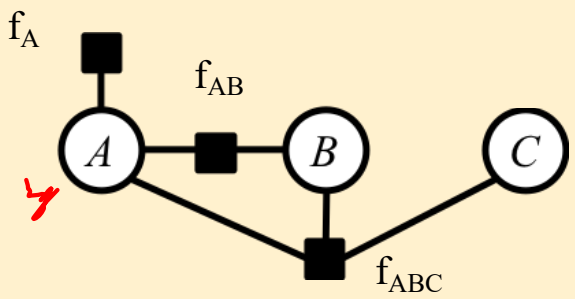
Question:

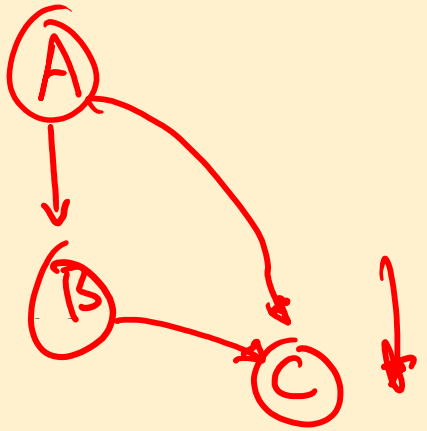
Answer:
A = Yes B = No
C = toxic



Q2 1. (1 point) Is there a Bayesian Network that would convert to the factor graph shown above? Is yes, draw an example of such a Bayesian Network. If not, explain why not.

No 62%





Q3 2. (1 point) Is there a Bayesian Network that would convert to the factor graph shown above? Is yes, draw an example of such a Bayesian Network. If not, explain why not.

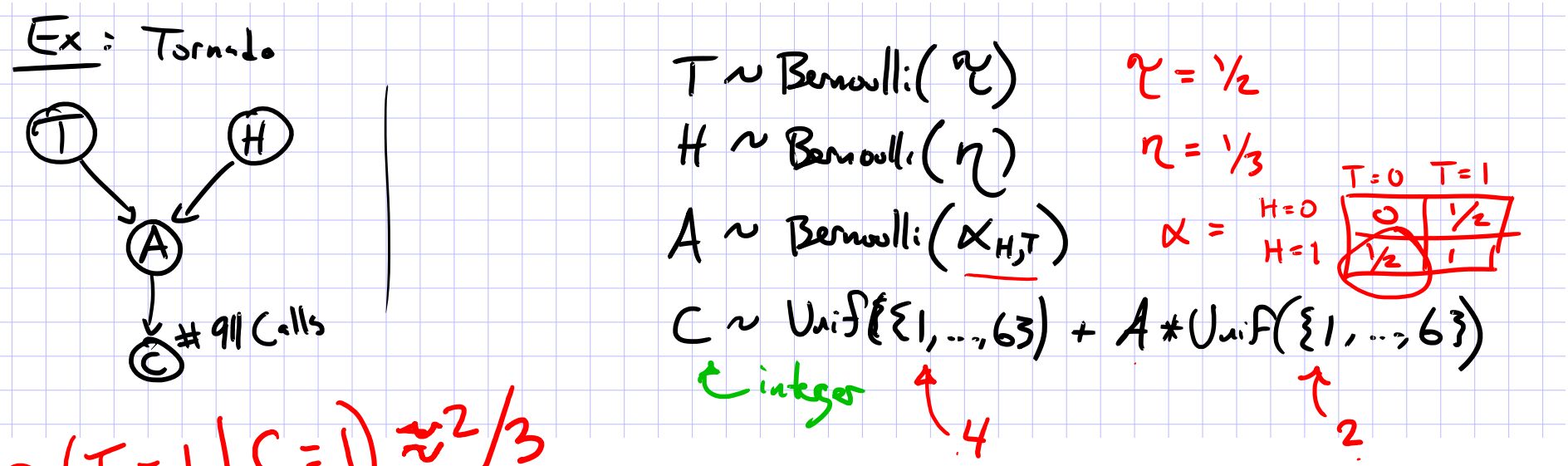
Yes 65%

Q&A

Metropolis, Metropolis-Hastings, Gibbs Sampling

MCMC (BASIC METHODS)

Sampling from a Joint Distribution



$P(T=1 \mid C=1) \approx 2/3$

T	H	A	C
1	0	1	6
1	1	0	1
0	0	1	7
1	0	1	4
0	0	0	1
1	0	1	1

We can use these samples to estimate many different probabilities!

$P(T=1 \mid C=12)$

Ancestral Sampling

sample in topological order (ie. roots to leaves)

(e.g. RNN-LM)

A Few Problems for a Factor Graph

Suppose we already have the parameters of a Factor Graph…

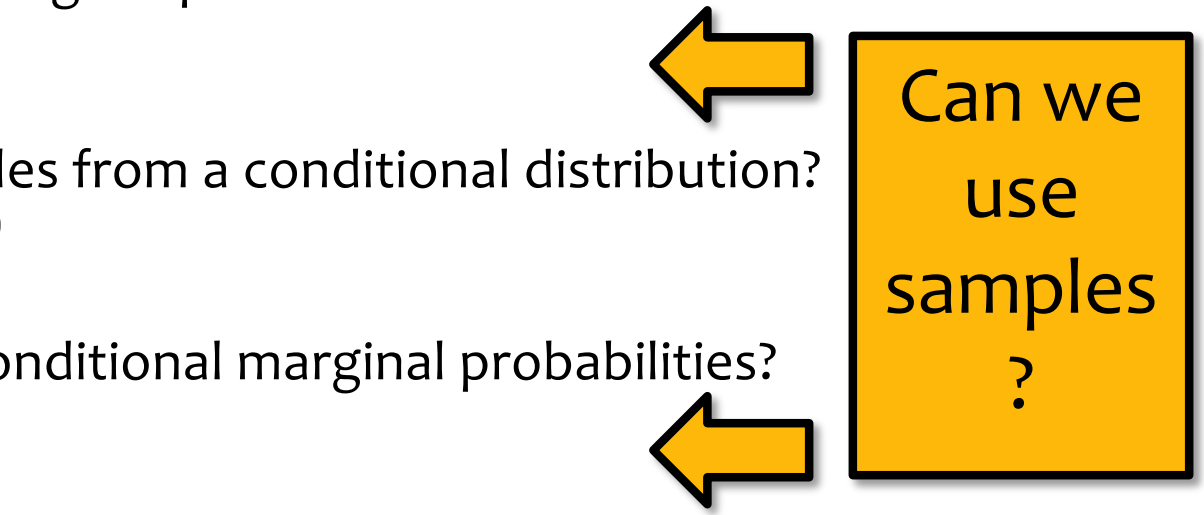
1. How do we compute the probability of a specific assignment to the variables?
   $P(T=t, H=h, A=a, C=c)$

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?
   $P(A) = \ldots$

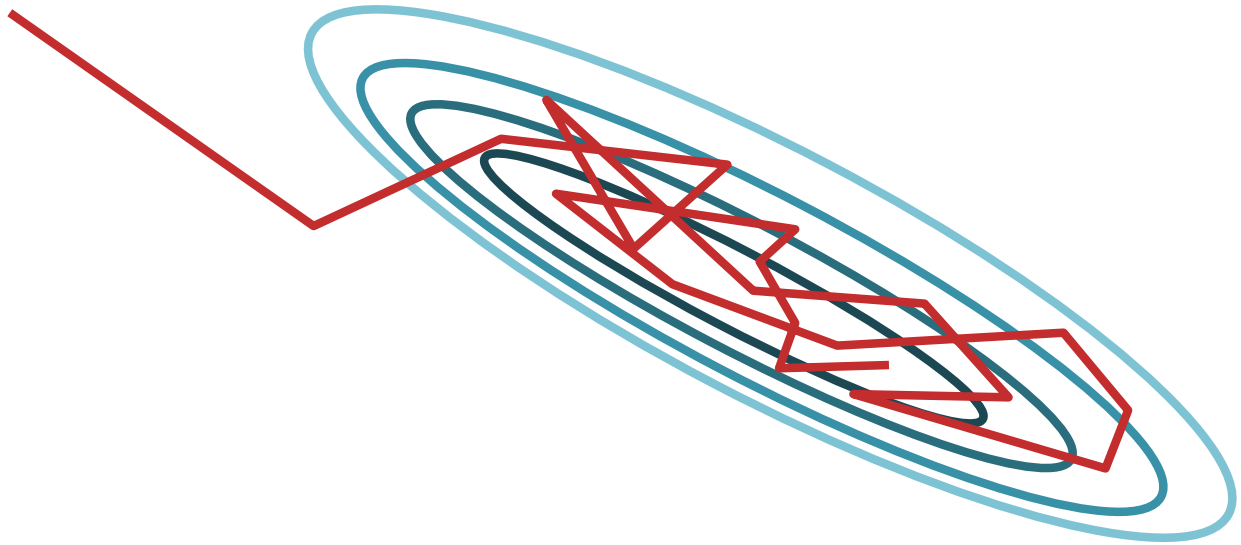
4. How do we draw samples from a conditional distribution?
   $t,h,a \sim P(T, H, A \mid C = c)$

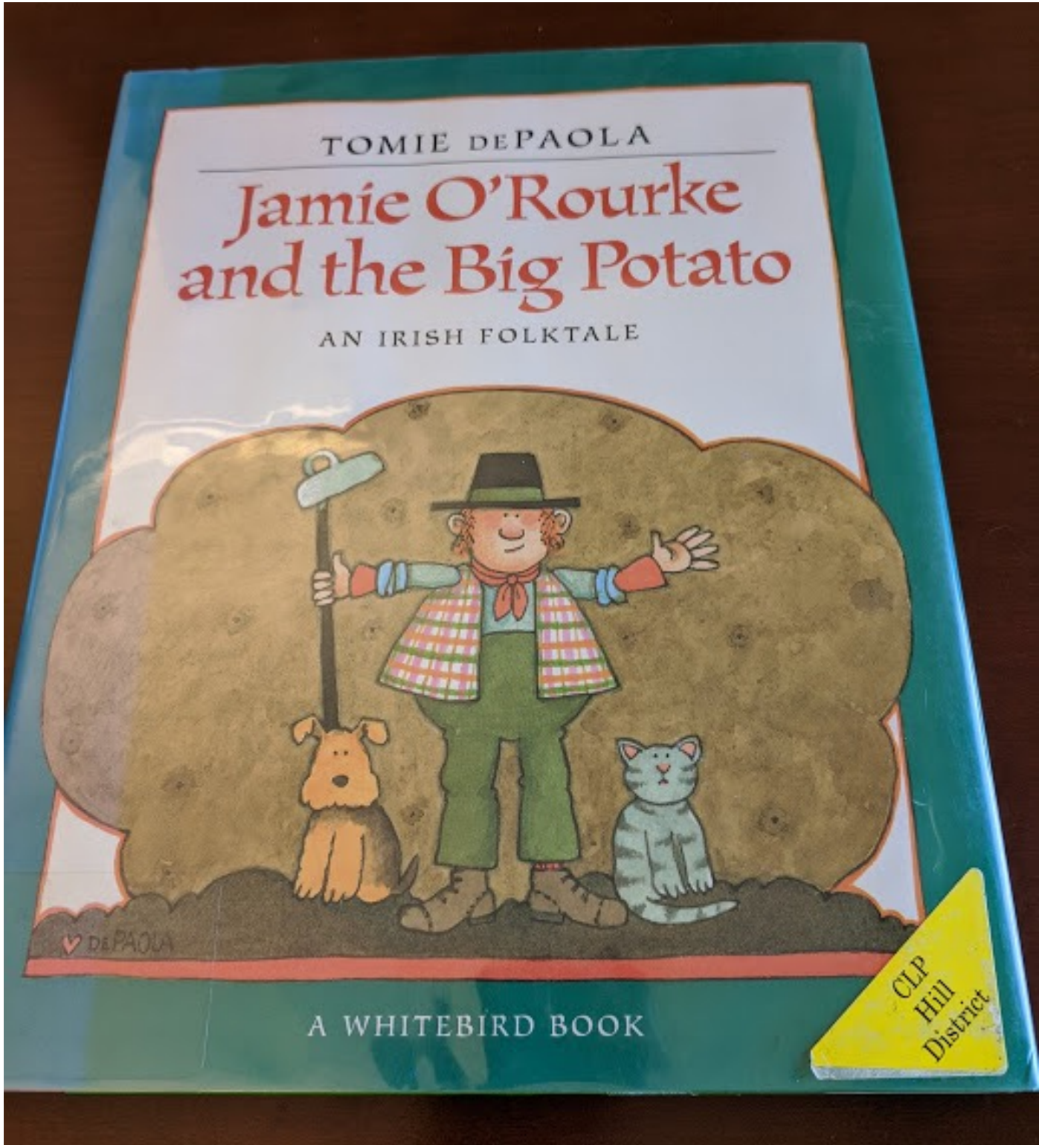
5. How do we compute conditional marginal probabilities?
   $P(H \mid C = c) = \ldots$



MCMC

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




TOMIE DEPAOLA
Jamie O'Rourke and the Big Potato
AN IRISH FOLKTALE
DEPAOLA
A WHITEBIRD BOOK
CLP
Hill
District

https://commons.wikimedia.org/wiki/File:Map_of_ireland.jpg

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

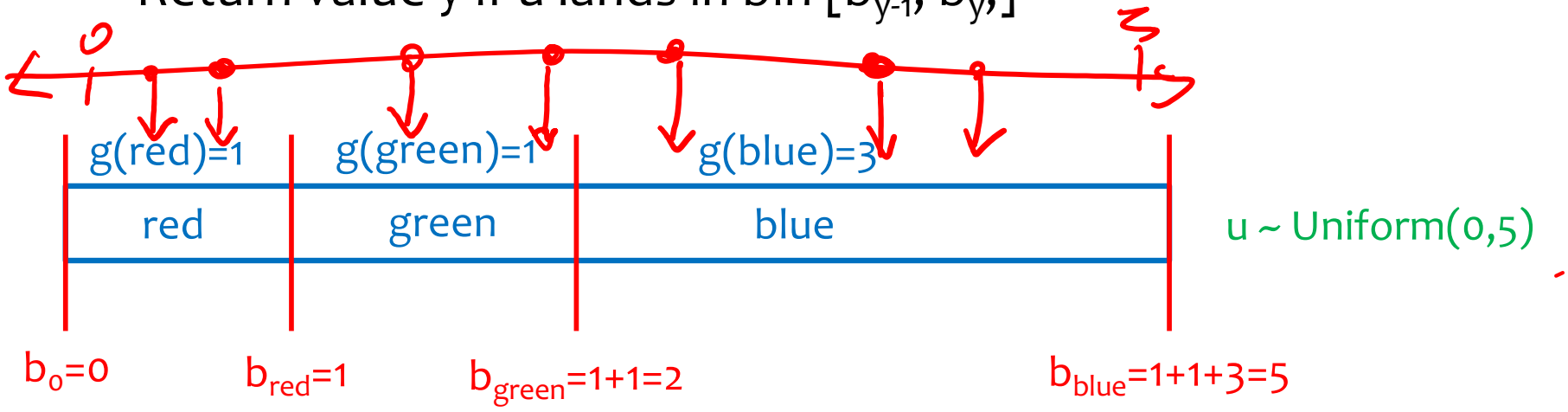
– Gibbs Sampling

Sampling from a Discrete Distribution

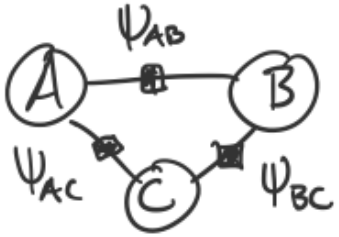
- To sample from a discrete distribution p(y) we only need a function proportional to it
  e.g., g(·) s.t. $p(y) \propto g(y)$
- **Recipe:**
  - Define a bin cutoff b_y for each value $y \in \{1, \ldots, V\}$

$$b_y = \sum_{t=1}^{y} g(t), \forall y \in \{1, \ldots, V\} \qquad b_0 = 0$$

  - Sample $u \sim \text{Uniform}(0, b_V)$
  - Return value y if u lands in bin $[b_{y-1}, b_y,]$



Example: Gibbs Sampling



$A, B, C \in \{+, -\}$

a	b	$\psi_{AB}(a,b)$
+	+	1
+	−	2
−	+	1
−	−	1

a	c	ψ_{AC}
+	+	2
+	−	2
−	+	2
−	−	1

b	c	ψ_{BC}
+	+	1
+	−	1
−	+	2
−	−	1

might change at each iteration.

full conditionals:

① $p(a \mid b,c) \propto \psi(a,b)\psi(a,c)$ → $g(a)$ = 

② $p(b \mid a,c) \propto \psi(a,b)\psi(b,c)$ → $g(b)$ = 

③ $p(c \mid a,b) \propto \psi(a,c)\psi(b,c)$ → $g(c)$ = 

fixed while sampling

Algo: Initialize a, b, c randomly $\in \{+, -\}$

For $i = 1, 2, 3, \ldots$

$a \sim p(a \mid b,c)$

$b \sim p(b \mid a,c)$

$c \sim p(c \mid a,b)$

table entries: 2 or 8

$$p(a \mid b,c) = \frac{p(a,b,c)}{p(b,c)} \propto p(a,b,c)$$

table entries: 8

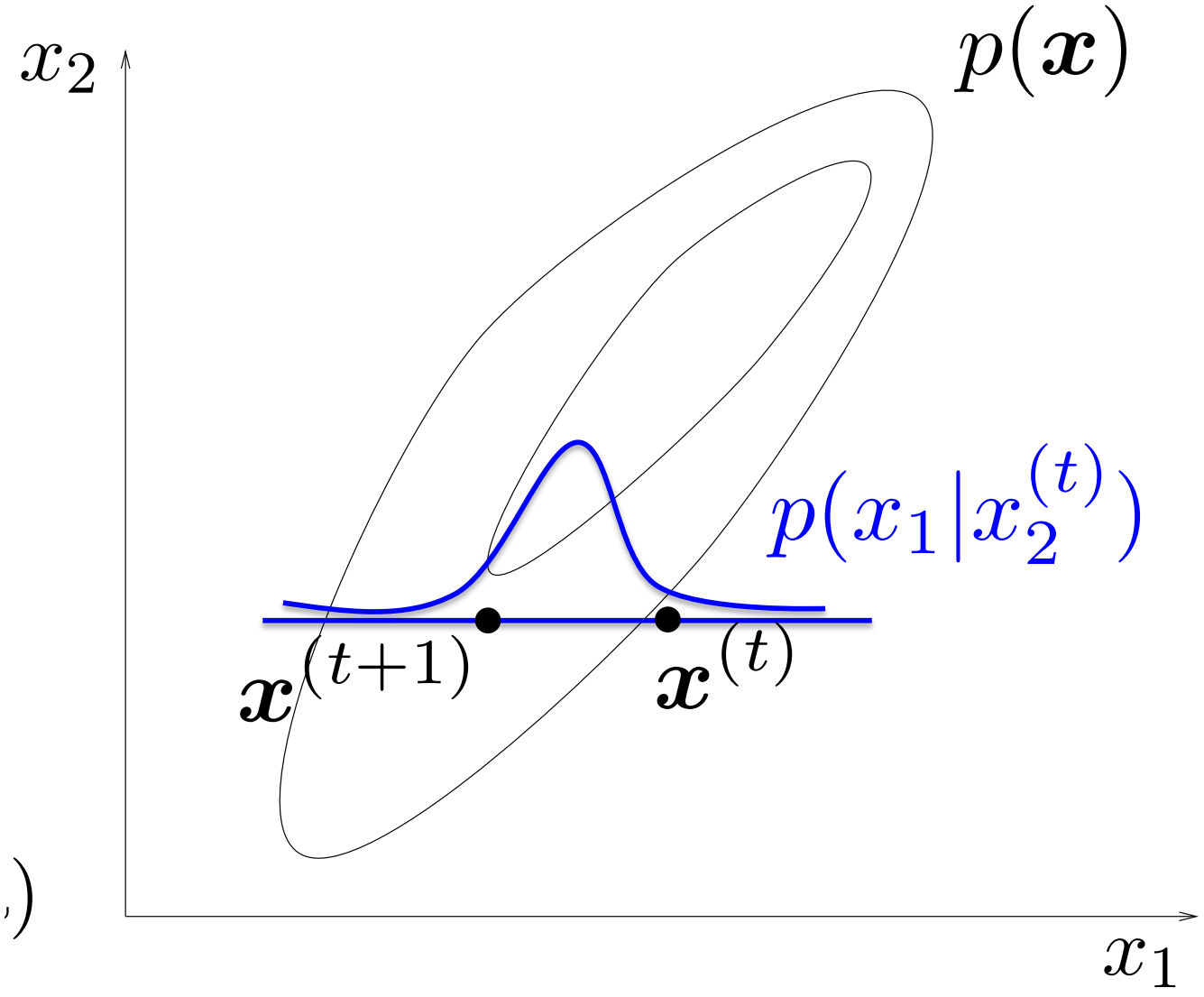
$$p(a,b,c) \triangleq \frac{1}{Z}\psi(a,b)\psi(a,c)\psi(b,c)$$

Example: Gibbs Sampling

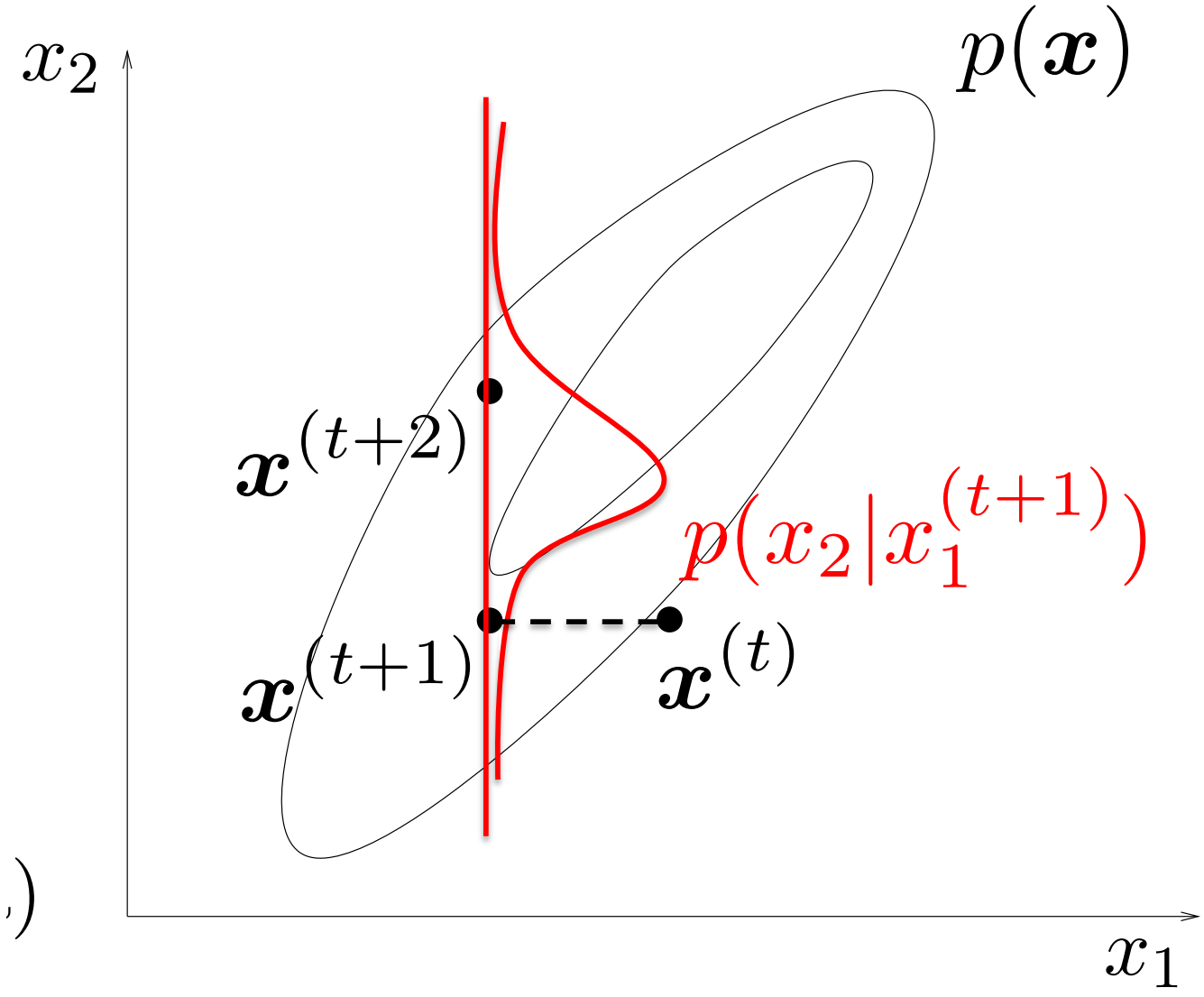
Example: 3-node Factor Graph

```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()
```

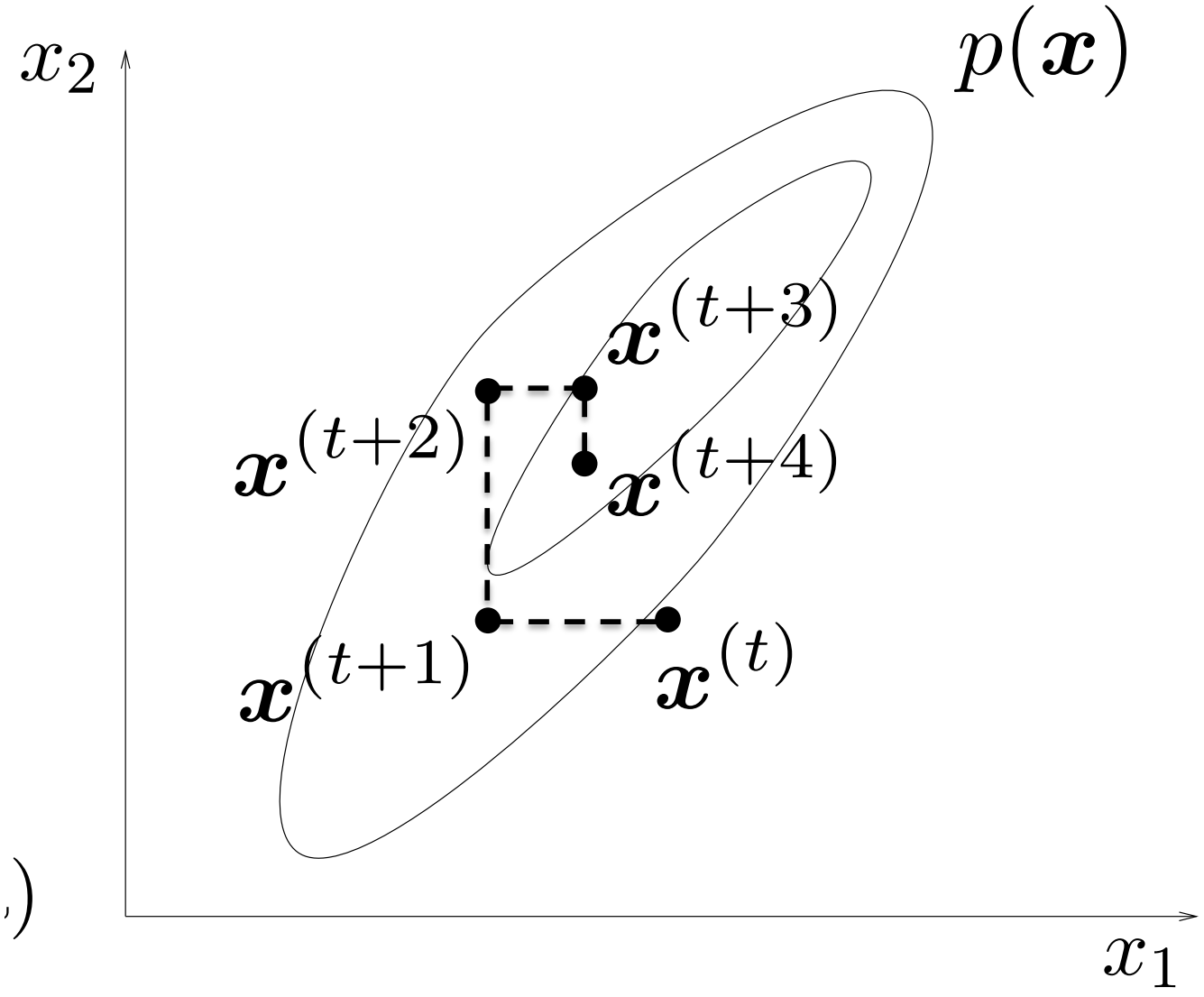
Gibbs Sampling



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:

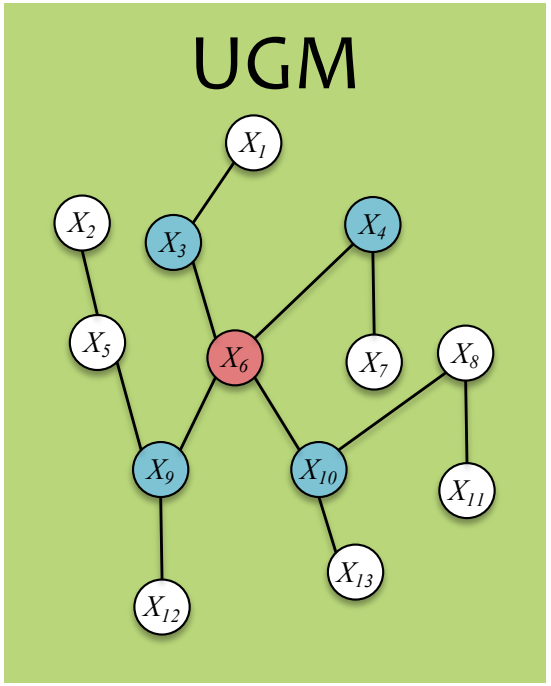
- Initialize $y_1^{(0)}, y_2^{(0)}, \ldots, y_J^{(0)}$ to arbitrary values
- For t = 1, 2, … :
  - $y_1^{(t+1)} \sim p(y_1 \mid y_2^{(t)}, \ldots, y_J^{(t)}, x_1, x_2, \ldots, x_J)$
  - $y_2^{(t+1)} \sim p(y_2 \mid y_1^{(t+1)}, y_3^{(t)}, \ldots, y_J^{(t)}, x_1, x_2, \ldots, x_J)$
  - $y_3^{(t+1)} \sim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

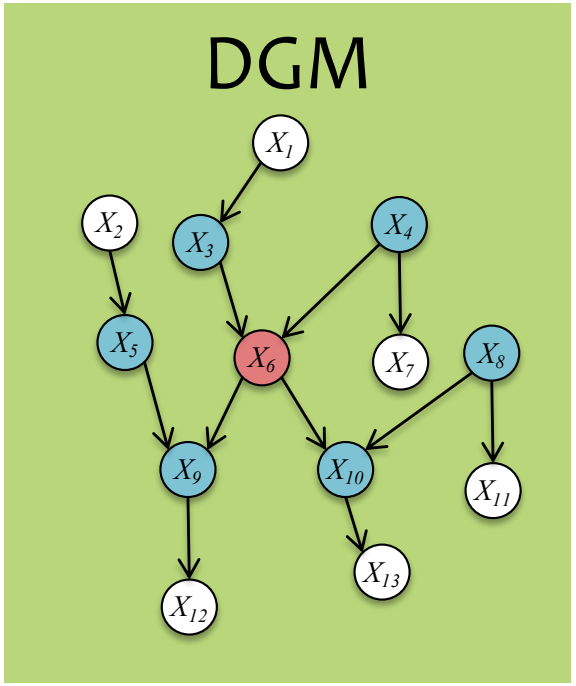
Properties:

- 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

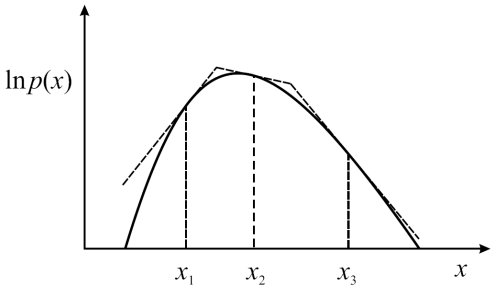
Gibbs Sampling

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

Figure from Bishop (2006)

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

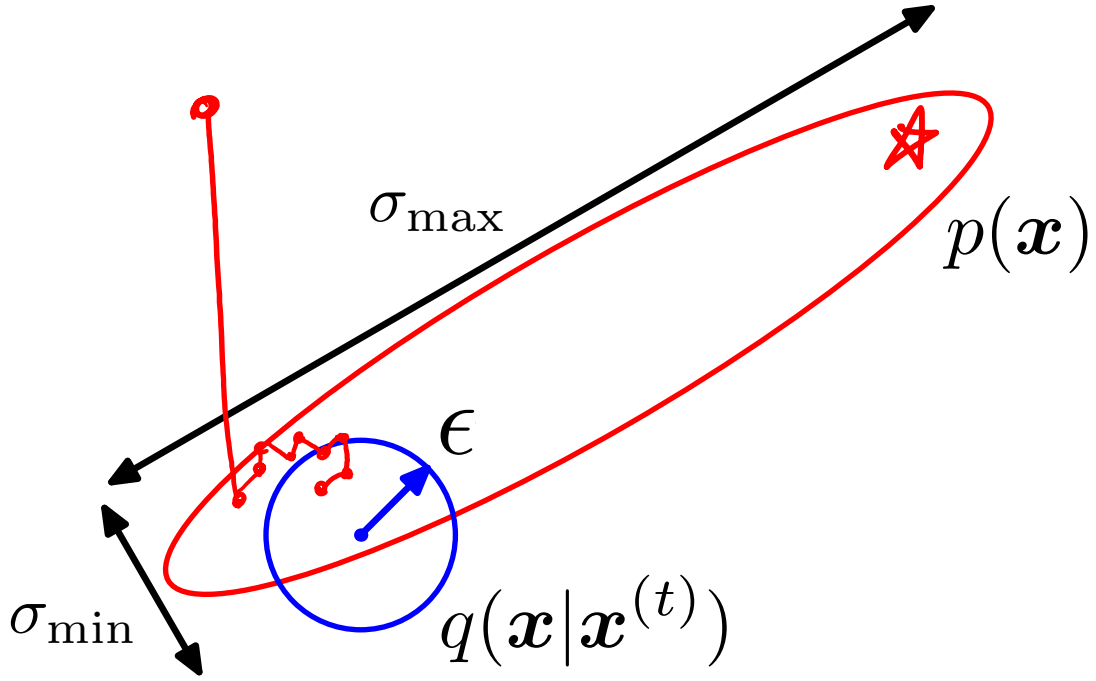
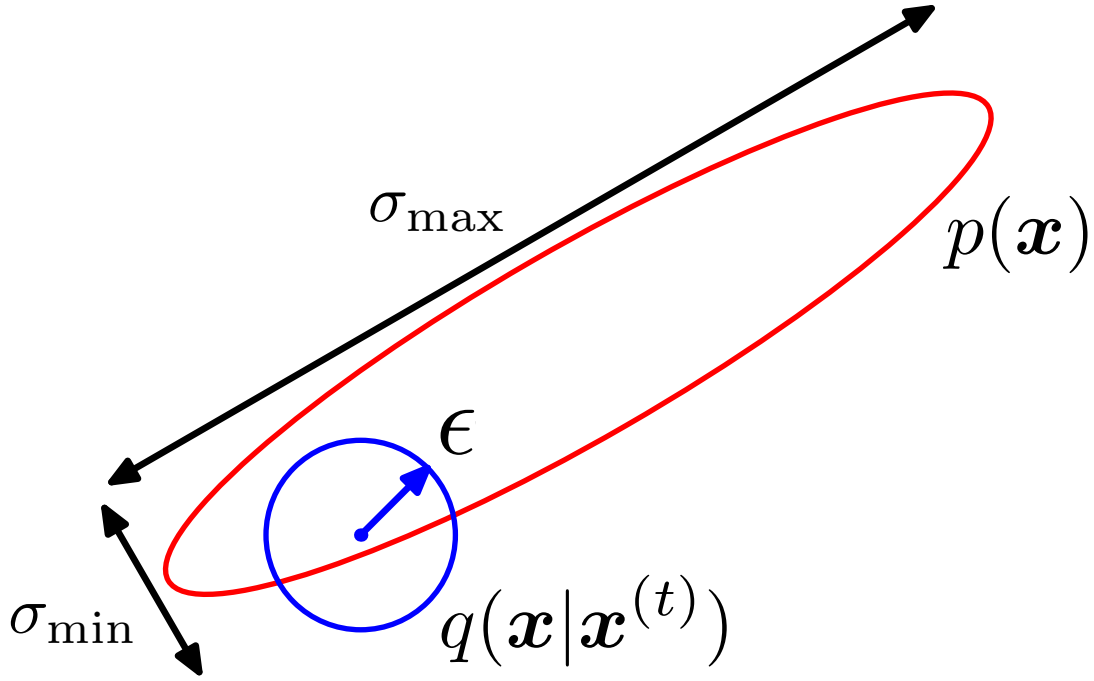


Figure from Bishop (2006)

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