Graphical Model & Gibbs Sampling Hung-yi Lee

Structured Learning

We also know how to involve hidden information.

Problem 1: Evaluation

• What does F(x,y) look like? $F(x,y) = w \cdot \phi(x,y)$

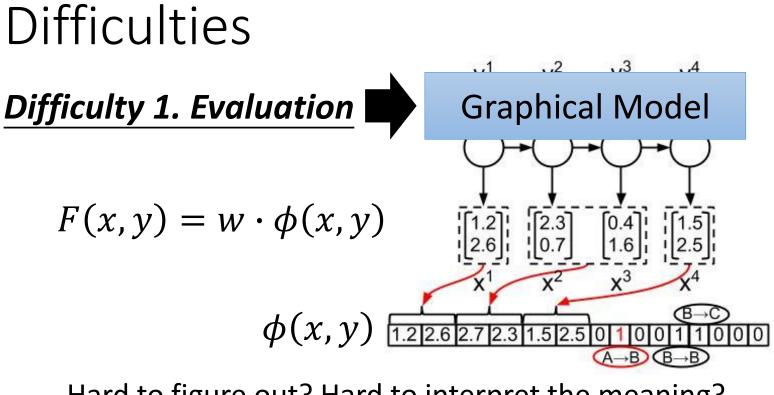
Problem 2: Inference

• How to solve the "arg max" problem

$$y = \arg\max_{y \in Y} F(x, y)$$

Problem 3: Training

• Given training data, how to find F(x,y) Structured SVM, etc.



Hard to figure out? Hard to interpret the meaning?

Difficulty 2. Inference



Gibbs Sampling

We can use Viterbi algorithm to deal with sequence labeling. How about other cases?

Graphical Model A language which describes the evaluation function

Graphical Model

$$F(x,y)$$
 Graph

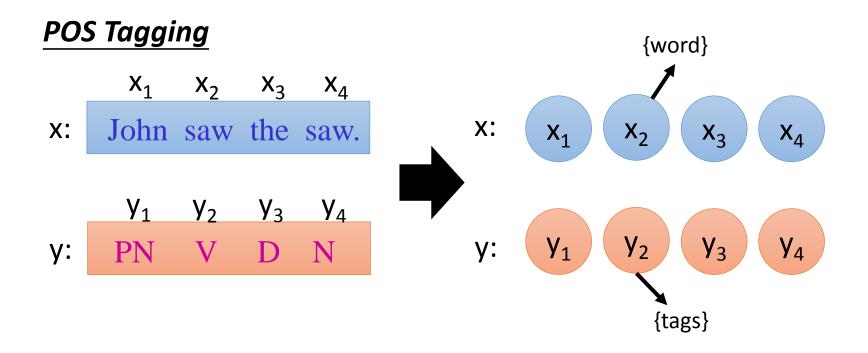
- Define and describe your evaluation function F(x,y) by a graph
- There are three kinds of graphical model.
 - Factor graph, Markov Random Field (MRF) and Bayesian Network (BN)
 - Only *factor graph* and *MRF* will be briefly mentioned today.

Decompose F(x,y)

- *F*(*x*, *y*) is originally a *global* function
 - Define over the whole x and y
- Based on graphical model, F(x, y) is the composition of some <u>local</u> functions
 - x and y are decomposed into smaller components
 - Each local function defines on only a few related components in x and y
 - Which components are related → defined by Graphical model

Decomposable x and y

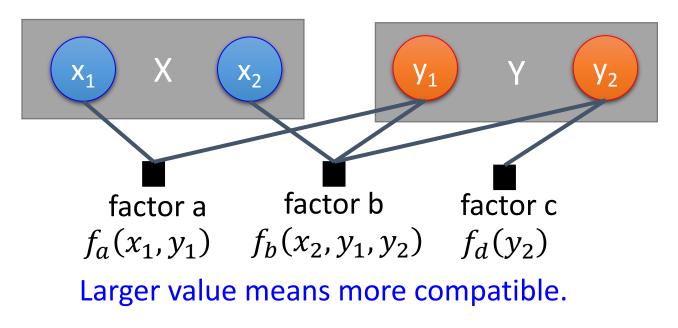
• x and y are decomposed into smaller components



Factor Graph

Each factor influences some components.

Each factor corresponds to a local function.

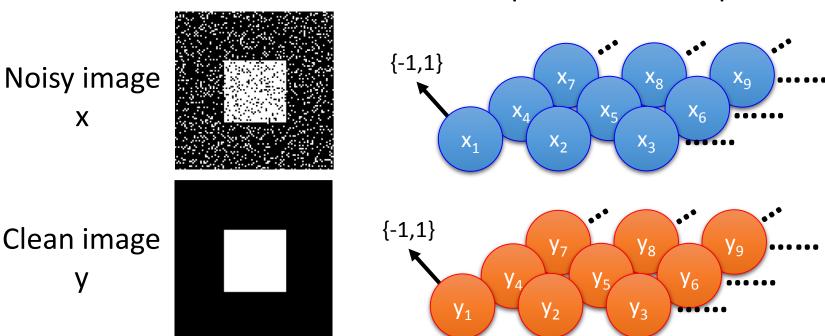


$$F(x, y) = f_a(x_1, y_1) + f_b(x_2, y_1, y_2) + f_c(y_2)$$

You only have to define the factors.

The local functions of the factors are learned from data.

Image De-noising

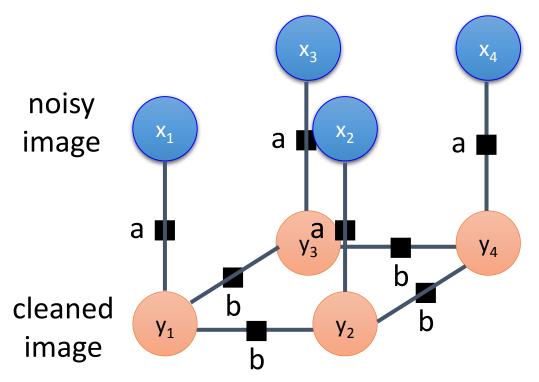


Each pixel is one component

http://cs.stanford.edu/people/karpathy/visml/ising_example.html

Noisy and clean images are related
 ➤ a: the values of x_i and y_i
 The colors in the clean image is smooth.

b: the values of the neighboring y_i



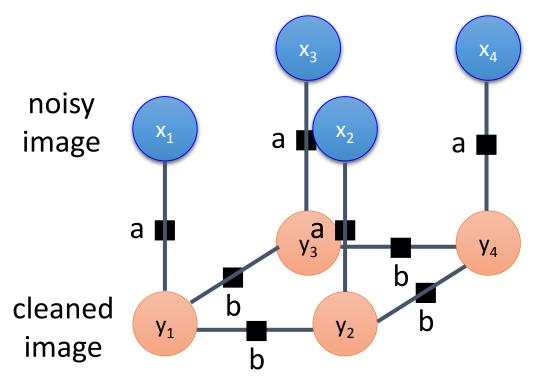
Factor:

$$f_a(x_i, y_i) = \begin{cases} 1 & x_i = y_i \\ -1 & x_i \neq y_i \end{cases}$$
$$f_b(y_i, y_j) = \begin{cases} 2 & y_i = y_j \\ -2 & y_i \neq y_j \end{cases}$$

The weights can be learned from data.

Noisy and clean images are related
 ➤ a: the values of x_i and y_i
 The colors in the clean image is smooth.

b: the values of the neighboring y_i



Factor:

Realize F(x, y) easily from the factor graph

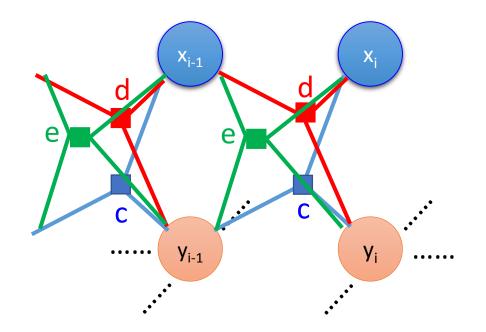
$$F(x, y) = \sum_{i=1}^{4} f_a(x_i, y_i)$$

 $+f_b(y_1, y_2) + f_b(y_1, y_3)$ $+f_b(y_2, y_4) + f_b(y_3, y_4)$

Factor:

c: the values of x_i and the values of the neighboring y_i

d: the values of the neighboring x_i and the values of y_i



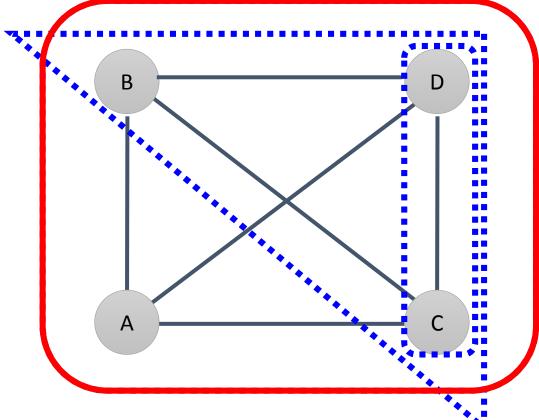
 $f_c(x_i, y_i, y_{i-1})$

 $f_d(x_i, x_{i-1}, y_i)$

 $f_e(x_i, x_{i-1}, y_i, y_{i-1})$

Markov Random Field (MRF)

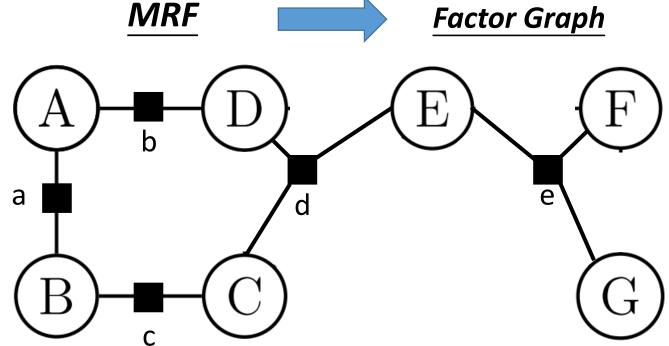
Clique: a set of components connecting to each other Maximum Clique: a clique that is not included by other cliques



MRF Each maximum clique on the graph corresponds to a factor

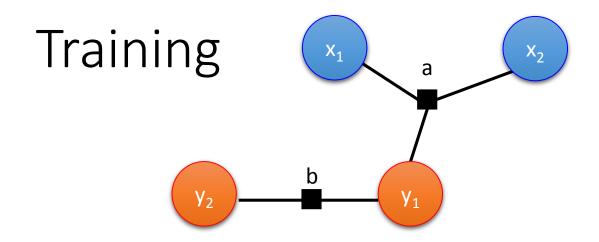
Factor Graph MRF А В Α В f(A,B)В В С Α Α С f(A, B, C)В D В С Α D A С f(A, B, C, D)

MRF



Evaluation Function

 $f_a(A,B) + f_b(A,D) + f_c(B,C) + f_d(C,D,E) + f_e(E,F,G)$



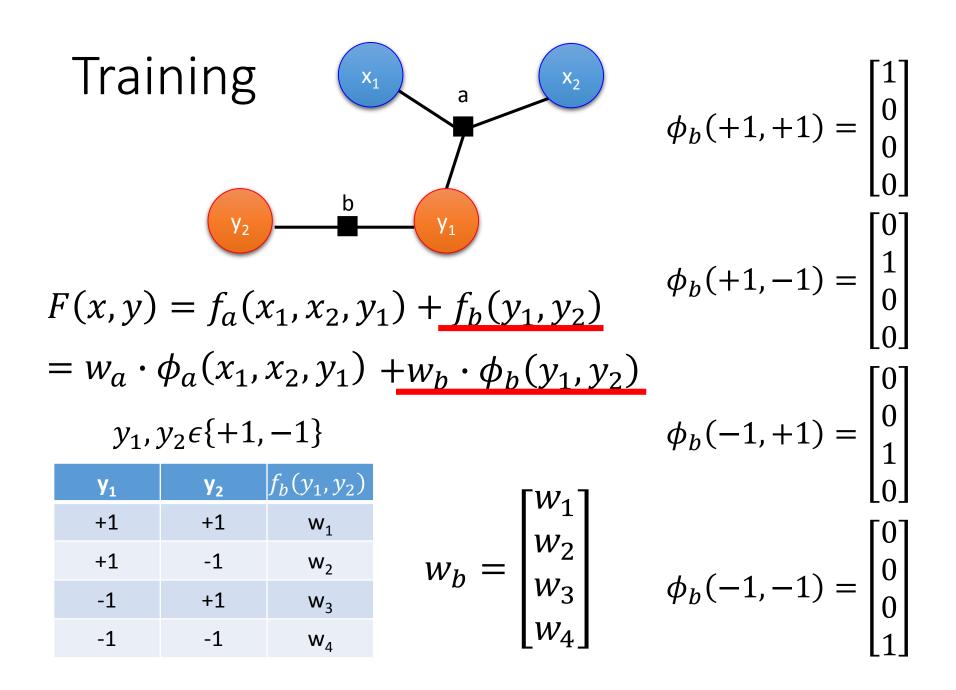
 $F(x, y) = f_a(x_1, x_2, y_1) + f_b(y_1, y_2)$ = $w_a \cdot \phi_a(x_1, x_2, y_1) + w_b \cdot \phi_b(y_1, y_2)$

 $= \begin{bmatrix} w_a \\ w_b \end{bmatrix} \begin{bmatrix} \phi_a(x_1, x_2, y_1) \\ \phi_b(y_1, y_2) \end{bmatrix}$

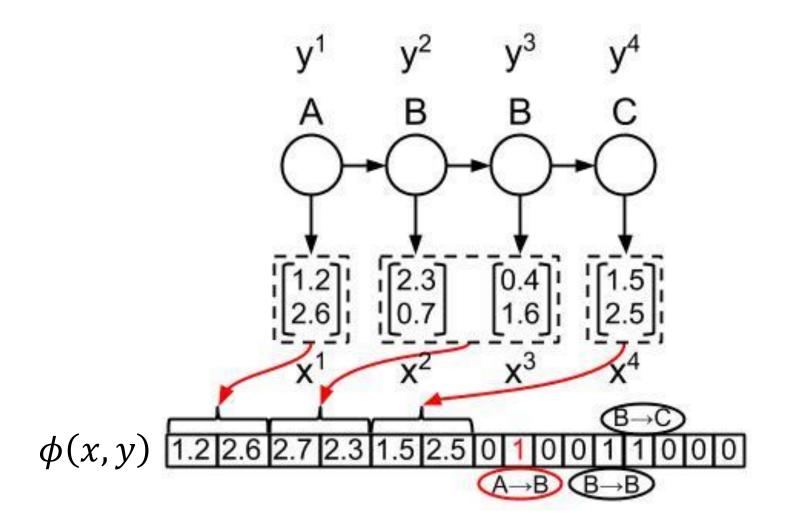
 $= w \cdot \phi(x, y)$

Simply training by structured perceptron or structured SVM

Max-Margin Markov Networks (M3N)

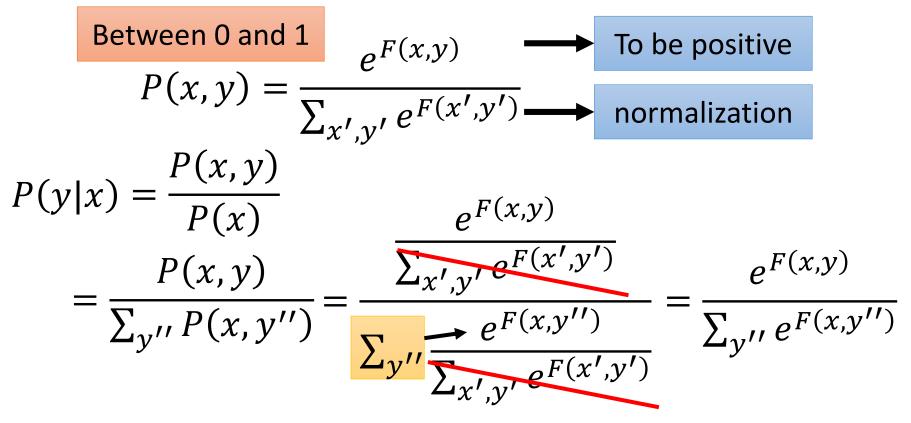


Now can you interpret this?



Probability Point of View

- F(x, y) can be any real number
- If you like probability

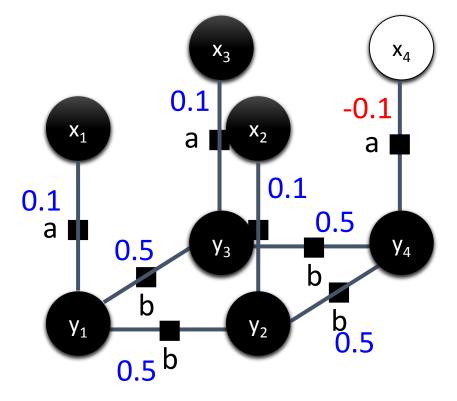


Gibbs Sampling Inference for the dumb

$$f_{a}(x_{i}, y_{i}) = \begin{cases} 0.1 & x_{i} = y_{i} \\ -0.1 & x_{i} \neq y_{i} \end{cases}$$
$$f_{b}(y_{i}, y_{j}) = \begin{cases} 0.5 & y_{i} = y_{j} \\ -0.5 & y_{i} \neq y_{j} \end{cases}$$

Given input noisy image x

 $x_1, x_2, x_3, x_4 = -1, -1, -1, 1$



Inference:

$$\tilde{y} = \arg \max_{y} F(x,y)$$

$$y_1, y_2, y_3, y_4 = -1, -1, -1, -1$$

 $F(x, y) = 2.2$ max

$$y_1, y_2, y_3, y_4 = 1,1,1,1$$

$$F(x, y) = 1.8$$

y₁, y₂, y₃, y₄ = -1,1,1, -1

$$F(x, y) = -2.2$$

Enumerate all possible y

Design an efficient algorithm to do that is not always easy.

Sampling?

Probability point of view:

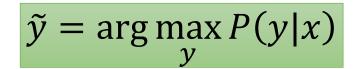
$$P(x, y) = \frac{e^{F(x, y)}}{\sum_{x', y'} e^{F(x', y')}}$$

$$P(y|x) = \frac{e^{F(x,y)}}{\sum_{y''} e^{F(x,y'')}} \quad \begin{array}{c} \text{Independent} \\ \text{of } y \end{array} \propto F(x, y)$$

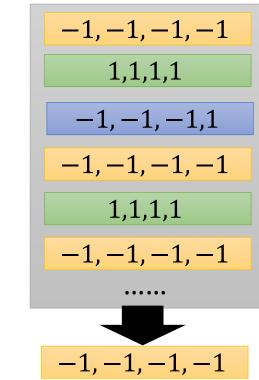
y)

$$\tilde{y} = \arg \max_{y} F(x,y) = \tilde{y} = \arg \max_{y} P(y|x)$$

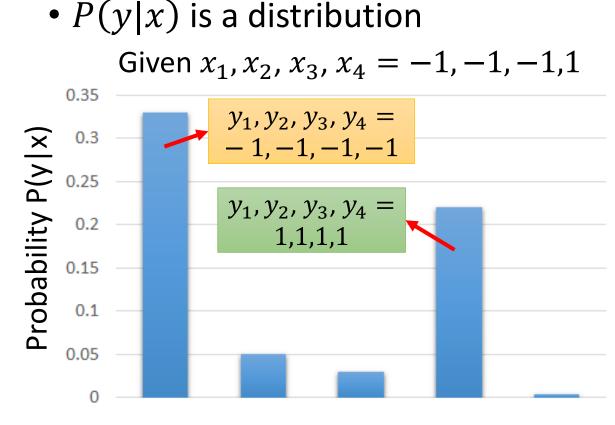
Sampling?



Sample from the distribution



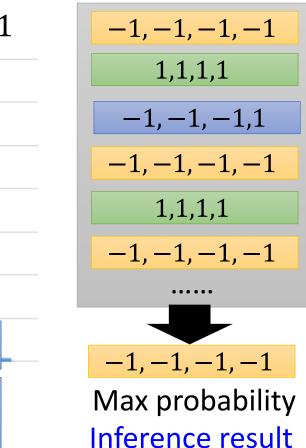
Max probability Inference result

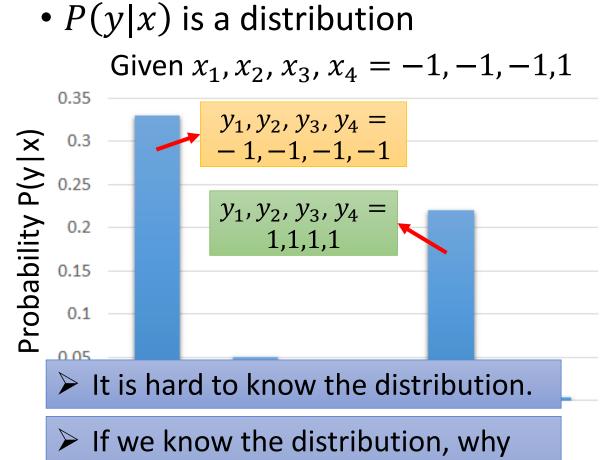


Sampling?

$$P(y|x) = \frac{e^{F(x,y)}}{\sum_{y''} e^{F(x,y'')}}$$

Sample from the distribution





bother with the sampling?

Gibbs Sampling

• There is a probability distribution P(y|x)

• $\mathbf{y} = \{y_1, y_2, ..., y_N\}$

- We want to sample from P(y|x), but it is too complex to do that
- However, P(y_i | y₁, y₂, ..., y_{i-1}, y_{i+1}, ..., y_N, x) can be computed
- We can sample from P(y|x) by Gibbs sampling

Gibbs Sampling

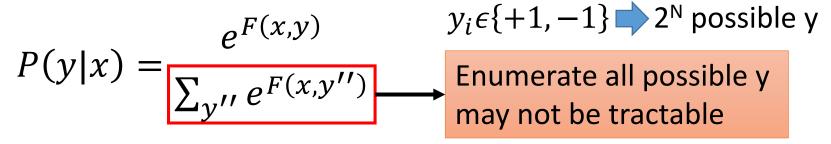
 $y^1, y^2, y^3, ..., y^T$

 $y^0 = \{y_1^0, y_2^0, \dots, y_N^0\}$ Initialization For t = 1 to T: T samples $y_1^t \sim P(y_1 | y_2 = y_2^{t-1}, y_3 = y_3^{t-1}, y_4 = y_4^{t-1}, \dots, y_N = y_N^{t-1}, x)$ $v_2^t \sim P(v_2 | v_1 = v_1^t, v_3 = v_3^{t-1}, v_4 = v_4^{t-1}, \dots, v_N = v_N^{t-1}, x)$ $y_{3}^{t} \sim P(y_{3}|y_{1} = y_{1}^{t}, y_{2} = y_{2}^{t}, y_{4} = y_{4}^{t-1}, \cdots, y_{N} = y_{N}^{t-1}, x)$ $y_N^t \sim P(y_N | y_1 = y_1^t, y_2 = y_2^t, y_3 = y_3^t, \dots, y_{N-1} = y_{N-1}^t, x)$ Get a sample: $y^t = \{y_1^t, y_2^t, \cdots, y_N^t\}$

As sampling from P(y|x)

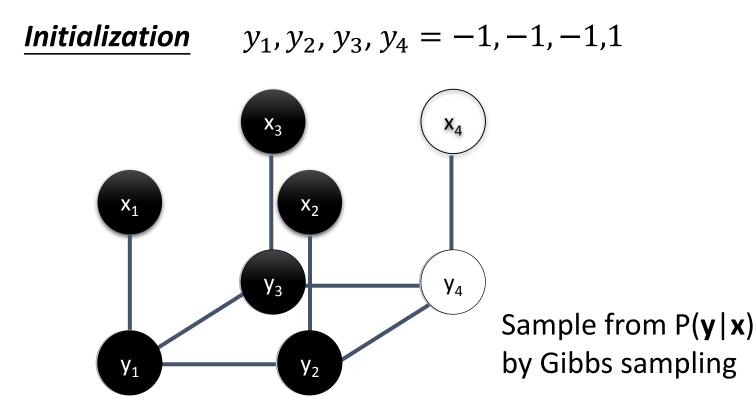
Gibbs Sampling

Is P(y_i|y₁, y₂, ..., y_{i-1}, y_{i+1}, ..., y_N,x) easy to be computed?



$$P(y_i|y_1, y_2, \cdots, y_{i-1}, y_{i+1}, \cdots, y_N, x)$$

$$= \underbrace{e^{F(x,y_{-i},y_i)}}_{\sum_{y_i'} e^{F(x,y_{-i},y_i')}} \underbrace{y_i \epsilon\{+1,-1\}}_{i} 2 \text{ possible } y_i}_{y_i \text{ may be tractable}}$$



Sample y₁ given all the other variables

$$y_{1} \sim P(y_{1}|y_{-1}, x) \quad y_{-1} = \{y_{2}, y_{3}, y_{4}\}$$

$$\xrightarrow{x_{1}} 0.1 \quad x_{2} \quad 0.1 \quad x_{4} \quad 0.1 \quad y_{4} \quad = \frac{P(x, y)}{\sum_{x', y'} e^{F(x', y')}}$$

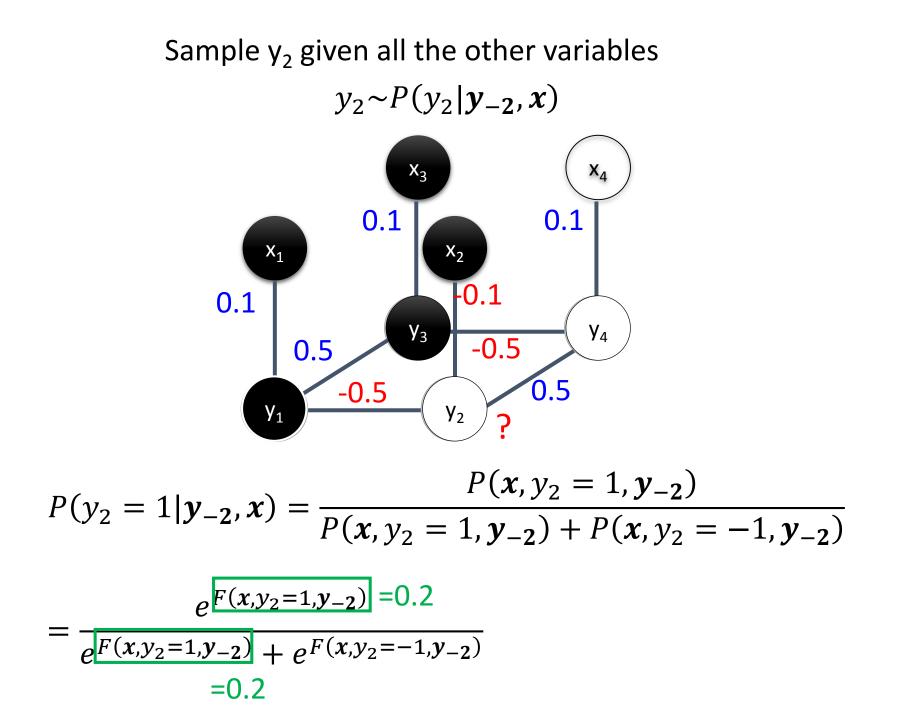
$$\xrightarrow{-0.1} 0.1 \quad y_{3} \quad 0.1 \quad y_{4} \quad = \frac{P(x, y)}{\sum_{x', y'} e^{F(x', y')}}$$
Compute $P(y_{1} = 1|y_{-1}, x)$ and $P(y_{1} = -1|y_{-1}, x)$

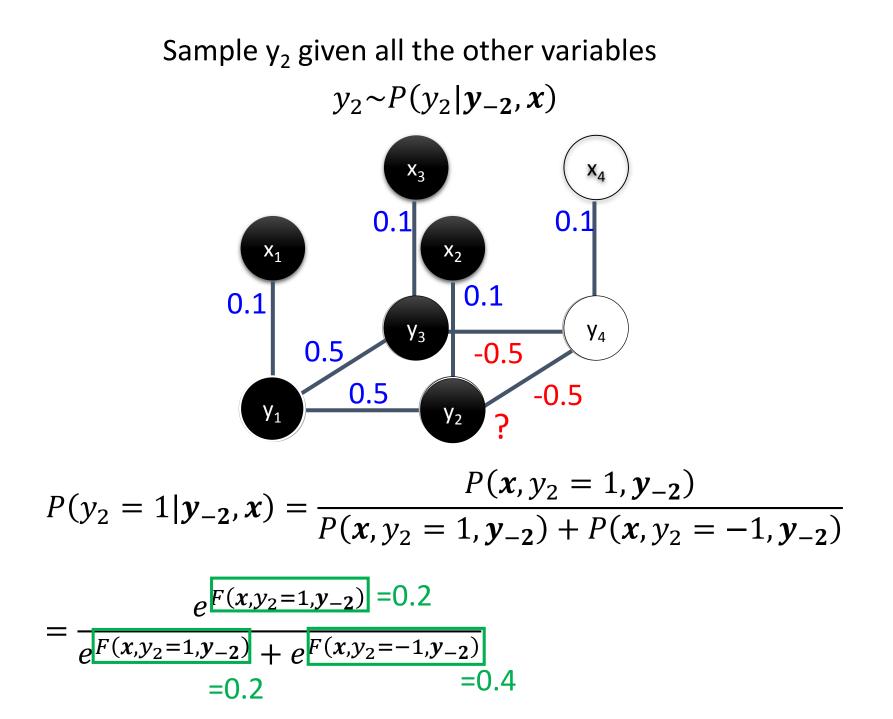
$$P(y_{1} = 1|y_{-1}, x) = \frac{P(x, y_{1} = 1, y_{-1})}{P(x, y_{1} = 1, y_{-1}) + P(x, y_{1} = -1, y_{-1})}$$

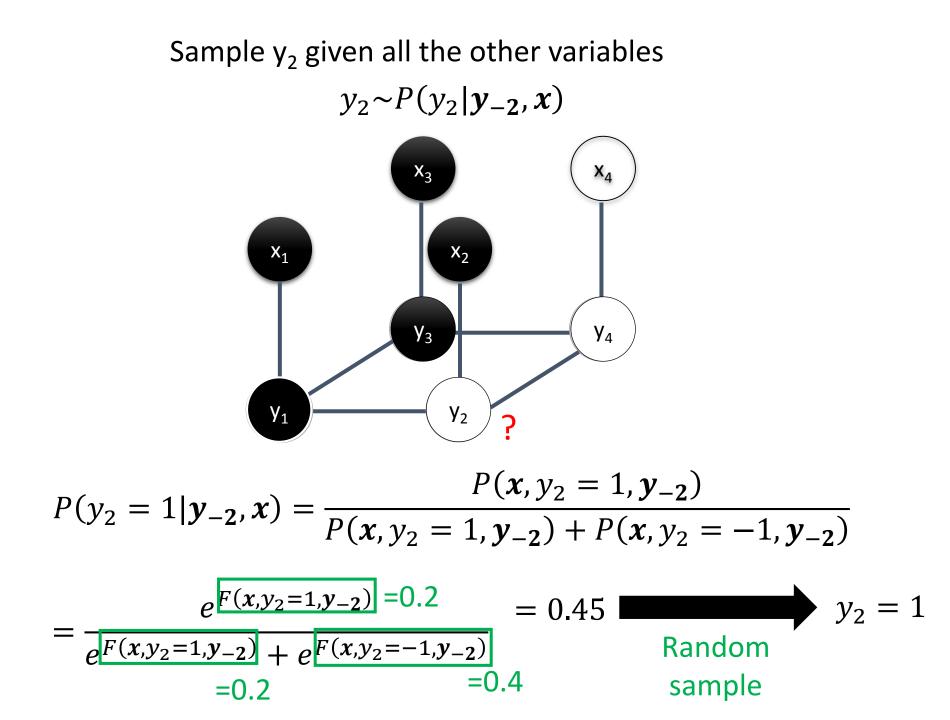
$$= \frac{e^{F(x, y_{1} = 1, y_{-1})} = -1.8}{e^{F(x, y_{1} = 1, y_{-1})} + e^{F(x, y_{1} = -1, y_{-1})}}$$

$$= -1.8$$

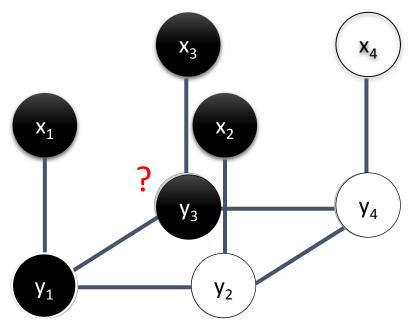
Sample y_1 given all the other variables $y_1 \sim P(y_1 | y_{-1}, x) \quad y_{-1} = \{y_2, y_3, y_4\}$ Х₃ X_4 0.1 0.1 X_2 X_1 0.1 0.1 **y**₃ **Y**₄ 0.5 -0.5 0.5 0.5 **y**₁ y_2 Compute $P(y_1 = 1 | y_{-1}, x)$ and $P(y_1 = -1 | y_{-1}, x)$ $P(y_1 = 1 | y_{-1}, x) = \frac{P(x, y_1 = 1, y_{-1})}{P(x, y_1 = 1, y_{-1}) + P(x, y_1 = -1, y_{-1})}$ $e^{F(x,y_1=1,y_{-1})} = -1.8 = 0.10$ $y_1 = -1$ $= \frac{1}{\rho} F(x, y_1 = 1, y_{-1}) + \rho F(x, y_1 = -1, y_{-1})$ Random sample =0.4= -1.8

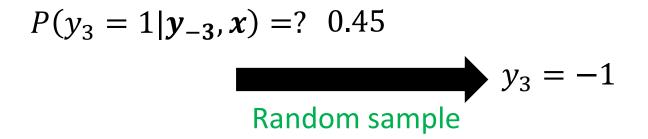


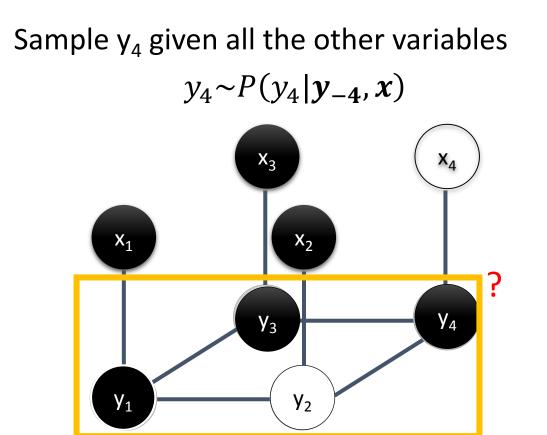




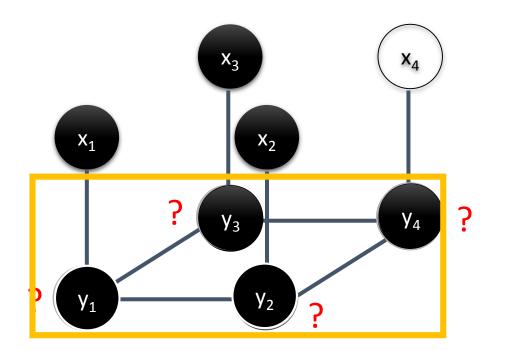
Sample y_3 given all the other variables $y_3 \sim P(y_3 | y_{-3}, x)$







Get **1**-st sample
$$y_1$$
=-1, y_2 =1, y_3 =-1, y_4 =-1



Get **1**-st sample
$$y_1$$
=-1, y_2 =1, y_3 =-1, y_4 =-1

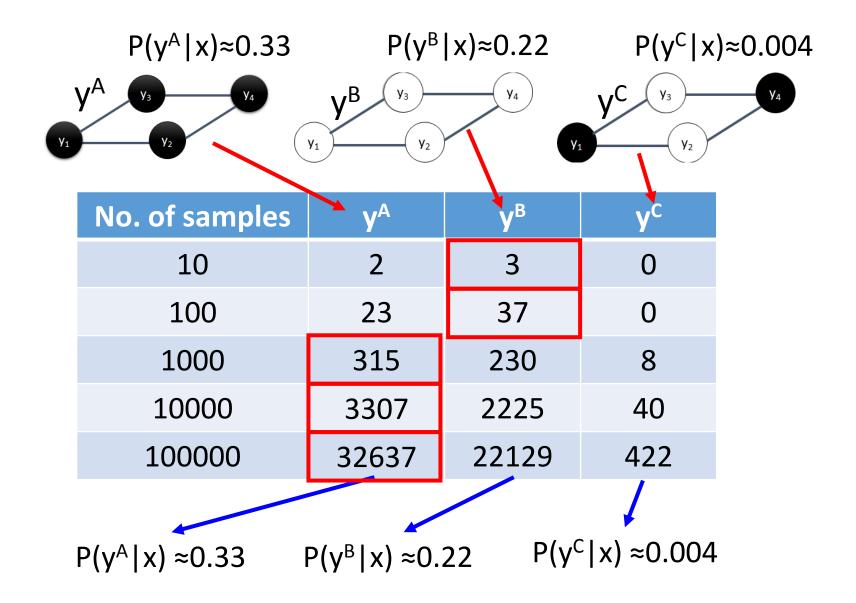
Get **<u>2-nd</u>** sample y₁=-1, y₂=-1, y₃=-1, y₄=-1

Get **2-nd** sample
$$y_1 = -1$$
, $y_2 = -1$, $y_3 = -1$, $y_4 = -1$

Get 4-th sample
$$y_1$$
=-1, y_2 =1, y_3 =-1, y_4 =1

Get 5-th sample
$$y_1=1$$
, $y_2=1$, $y_3=1$, $y_4=1$

Until you want to stop



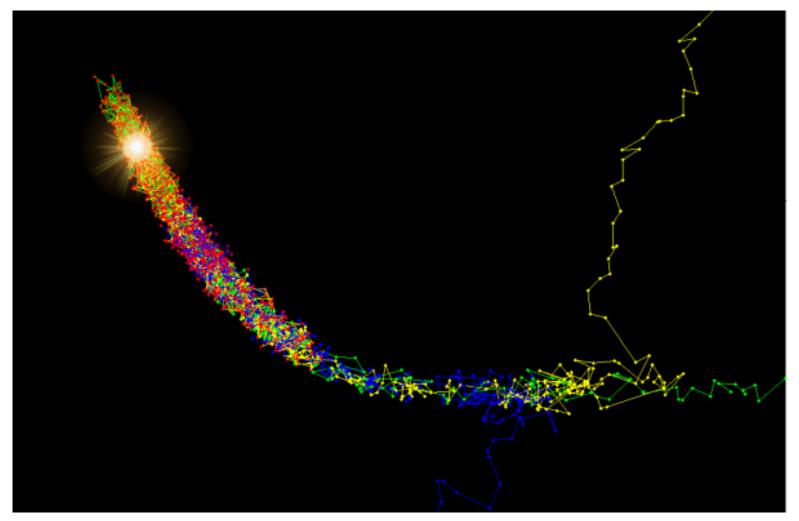
From sampling: y^A would be the results of inference.

How about starting from different initialization?

Not really change the final results.

| | No. of samples | Α | В | С |
|--|----------------|-----------|-----------|--------|
| Starting from | 10 | 3 | 1 | 0 |
| Y ₃ Y ₄ Y ₁ Y ₂ | 100 | 40 | 11 | 1 |
| | 1000 | 331 | 237 | 2 |
| | 10000 | 3251 | 2176 | 31 |
| | 100000 | 32911 | 21845 | 385 |
| | No. of samples | Α | В | С |
| Starting from | 10 | 0 | 3 | 0 |
| \frown \frown | | | | |
| (\mathbf{y}_3) (\mathbf{y}_4) | 100 | 28 | 31 | 0 |
| | 100 1000 | 28 318 | 31 226 | 0 2 |
| Y ₃ Y ₄ Y ₁ Y ₂ | | - | | |

All rivers run into the sea.



http://www.juergenwiki.de/work/wiki/doku.php?id=public:mcmc

Practical Suggestion

- "burn-in"
 - "burn-in" period: The first few of samples would be influenced by the initialization

c > 1

- Discard the samples in the "burn-in" period
- Modify the sampling distribution

$$P(y_i|y_1, y_2, \cdots, y_{i-1}, y_{i+1}, \cdots, y_N, \mathbf{x}) = \frac{e^{F(x, y_{-i}, y_i) \mathbf{X} \mathbf{c}}}{\sum_{y'_i} e^{F(x, y_{-i}, y'_i) \mathbf{X} \mathbf{c}}}$$
Increase c after each interaction

Gibbs Sampling A little bit of theory

Gibbs Sampling

 $z^1, z^2, z^3, ..., z^T$

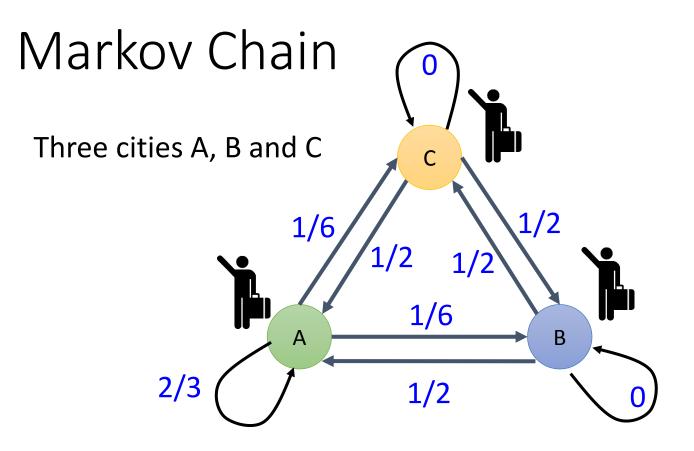
Gibbs sampling from a distribution P(z) ($z = \{z_1, ..., z_N\}$)

$$z^{0} = \{z_{1}^{0}, z_{2}^{0}, \dots, z_{N}^{0}\}$$

For t = 1 to T:
$$z_{1}^{t} \sim P(z_{1} | z_{2} = z_{2}^{t-1}, z_{3} = z_{3}^{t-1}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$z_{2}^{t} \sim P(z_{2} | z_{1} = z_{1}^{t}, z_{3} = z_{3}^{t-1}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$z_{3}^{t} \sim P(z_{3} | z_{1} = z_{1}^{t}, z_{2} = z_{2}^{t}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$\vdots$$
$$z_{N}^{t} \sim P(z_{N} | z_{1} = z_{1}^{t}, z_{2} = z_{2}^{t}, z_{3} = z_{3}^{t}, \dots, z_{N-1} = z_{N-1}^{t})$$
Output: $z^{t} = \{z_{1}^{t}, z_{2}^{t}, \dots, z_{N}^{t}\}$

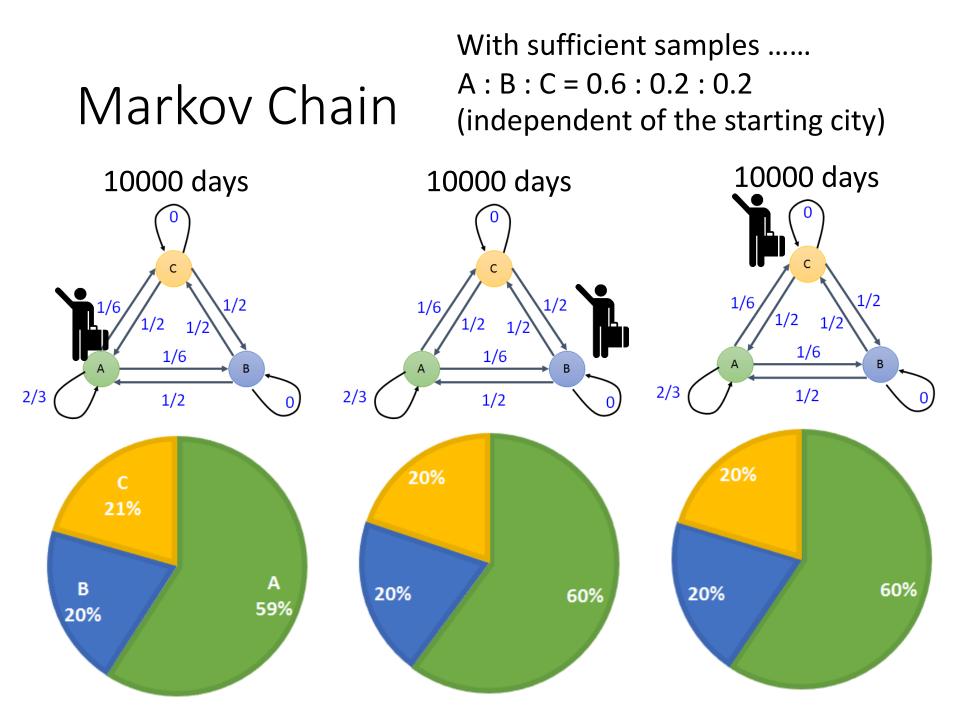
As sampling from P(z)

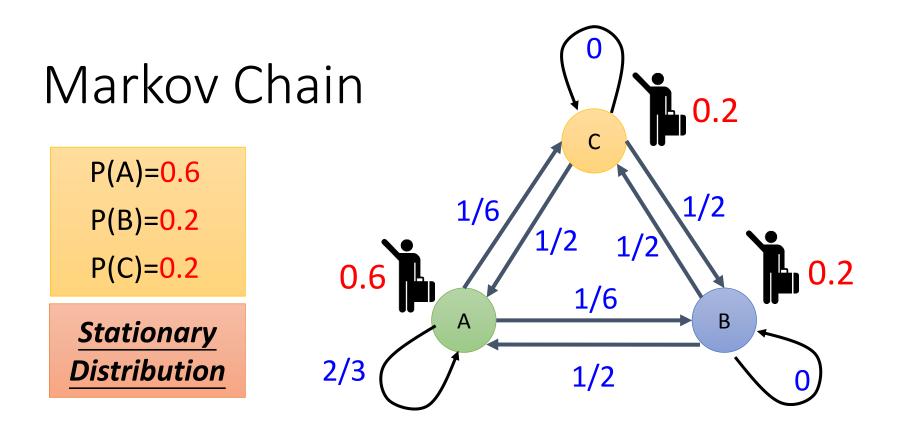
Why?



The traveler recorded the cities he visited each day.





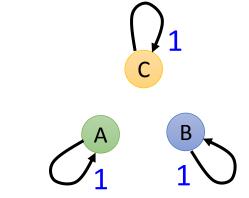


2/3 0.6 1/2 0.2 1/2 0.2 0.6 $P_T(A|A)P(A) + P_T(A|B)P(B) + P_T(A|C)P(C) = P(A)$ $P_T(B|A)P(A) + P_T(B|B)P(B) + P_T(B|C)P(C) = P(B)$ $P_T(C|A)P(A) + P_T(C|B)P(B) + P_T(C|C)P(C) = P(C)$ The distribution will not change.

Markov Chain

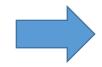
A Markov Chain can have multiple stationary distributions.

Reaching which stationary distribution depends on starting state



The Markov Chain fulfill some conditions will have unique stationary distribution.

P_T(s'|s) for any states s and s' is not zero (*sufficient* but not *necessary* condition)



Unique stationary distribution

 $z^1, z^2, z^3, ..., z^T$

Gibbs sampling from a distribution P(z) ($z = \{z_1, ..., z_N\}$)

$$z^{0} = \{z_{1}^{0}, z_{2}^{0}, \dots, z_{N}^{0}\}$$

For t = 1 to T:
$$z_{1}^{t} \sim P(z_{1} | z_{2} = z_{2}^{t-1}, z_{3} = z_{3}^{t-1}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$z_{2}^{t} \sim P(z_{2} | z_{1} = z_{1}^{t}, z_{3} = z_{3}^{t-1}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$z_{3}^{t} \sim P(z_{3} | z_{1} = z_{1}^{t}, z_{2} = z_{2}^{t}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$\vdots$$
$$z_{N}^{t} \sim P(z_{N} | z_{1} = z_{1}^{t}, z_{2} = z_{2}^{t}, z_{3} = z_{3}^{t}, \dots, z_{N-1} = z_{N-1}^{t})$$
Output: $z^{t} = \{z_{1}^{t}, z_{2}^{t}, \dots, z_{N}^{t}\}$

state

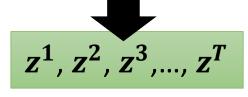
This is a Markov Chain
 z^t only depend on z^{t-1}

Gibbs sampling from a distribution P(z) ($z = \{z_1,...,z_N\}$)

$$z^{0} = \{z_{1}^{0}, z_{2}^{0}, \dots, z_{N}^{0}\}$$

For t = 1 to T:
$$z_{1}^{t} \sim P(z_{1} | z_{2} = z_{2}^{t-1}, z_{3} = z_{3}^{t-1}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$z_{2}^{t} \sim P(z_{2} | z_{1} = z_{1}^{t}, z_{3} = z_{3}^{t-1}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$z_{3}^{t} \sim P(z_{3} | z_{1} = z_{1}^{t}, z_{2} = z_{2}^{t}, z_{4} = z_{4}^{t-1}, \dots, z_{N} = z_{N}^{t-1})$$
$$\vdots$$
$$z_{N}^{t} \sim P(z_{N} | z_{1} = z_{1}^{t}, z_{2} = z_{2}^{t}, z_{3} = z_{3}^{t}, \dots, z_{N-1} = z_{N-1}^{t})$$

Output: $z^{t} = \{z_{1}^{t}, z_{2}^{t}, \dots, z_{N}^{t}\}$



Proof that the Markov chain has unique stationary distribution which is P(z).

- Markov chain from Gibbs sampling has unique stationary distribution? Yes
 - $P_T(z'|z) > 0$, for any z and z'

$$z_{1}^{t} \sim P(z_{1}|z_{2} = z_{2}^{t-1}, z_{3} = z_{3}^{t-1}, \cdots, z_{N} = z_{N}^{t-1})$$

$$z_{2}^{t} \sim P(z_{2}|z_{1} = z_{1}^{t}, z_{3} = z_{3}^{t-1}, \cdots, z_{N} = z_{N}^{t-1})$$

$$z_{3}^{t} \sim P(z_{3}|z_{1} = z_{1}^{t}, z_{2} = z_{2}^{t}, \cdots, z_{N} = z_{N}^{t-1})$$

$$\vdots$$

$$z_{N}^{t} \sim P(z_{N}|z_{1} = z_{1}^{t}, z_{2} = z_{2}^{t}, \cdots, z_{N-1} = z_{N-1}^{t})$$

$$can be any z^{t}$$

None of the conditional probability is zero

• Show that P(z) is a stationary distribution

$$\sum_{z} P_{T}(z'|z) P(z) = P(z')$$

$$P_{T}(z'|z) = P(z'_{1}|z_{2}, z_{3}, z_{4}, \dots, z_{N})$$

$$\times P(z'_{2}|z'_{1}, z_{3}, z_{4}, \dots, z_{N})$$

$$\times P(z'_{3}|z'_{1}, z'_{2}, z_{4}, \dots, z_{N})$$

$$\vdots$$

$$\times P(z'_{N}|z'_{1}, z'_{2}, z'_{3}, \dots, z'_{N-1})$$

There is only one stationary distribution for Gibbs sampling, so we are done.

Thank you for your attention!

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