Sampling Based Inference

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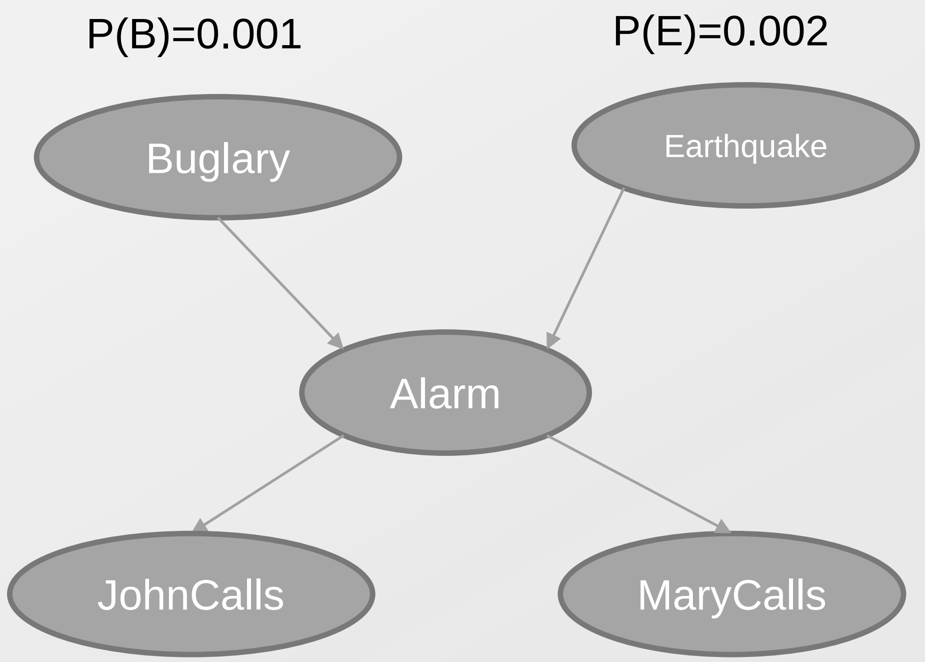
SAMPLING BASED INFERENCE

Forward Sampling

- Generate a sample from the Bayesian network
  - Follow topological order
    - Buglary → false
    - Earthquake → false
    - Alarm|B=F,E=F → true
    - JC|A=T → true
    - MC|A=T → false
  - Create such sample many, many, many times
- Then, count the samples match the case
  - P(E=T|MC=T)=?
    - Count the cases of E=T and MC=T
    - Count the cases of MC=T
- Any problem?



B	E	P(A|B,E)
T	T	0.95
T	F	0.94
F	T	0.29
F	F	0.001

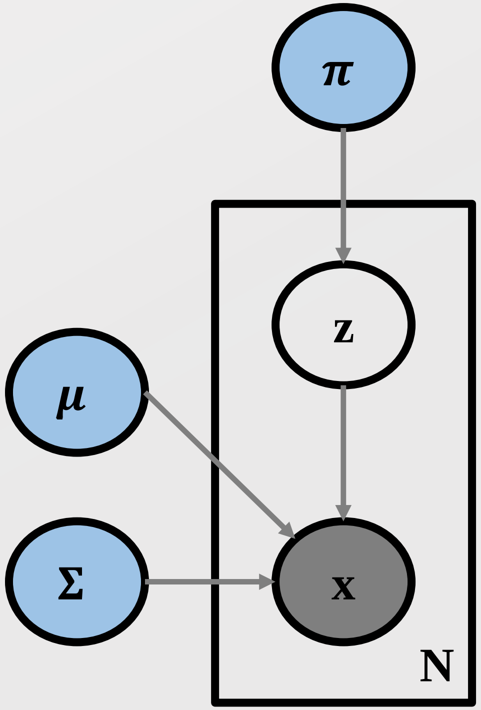
A	P(J|A)
T	0.90
F	0.05

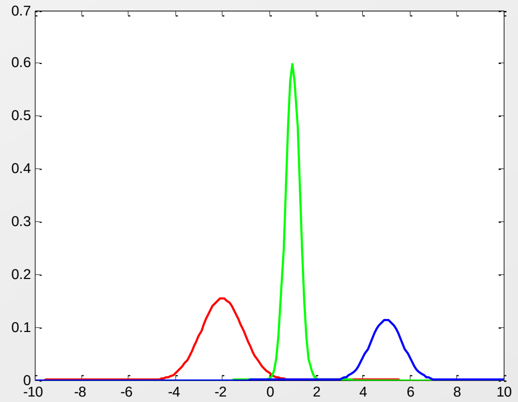
A	P(M|A)
T	0.70
F	0.01

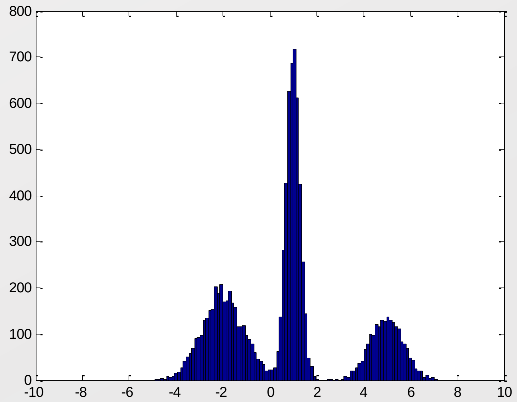
Forward Sampling in GMM

- Forward sampling of GMM
  - Sample z from π
    - z is the indicator of the mixture distribution
  - With selected z, sample x from $\mathrm{N}(\mu_z, \Sigma_z)$
- After many, many sampling, you can draw the histogram of the mixture distribution
- You have an empirical PDF, so you can ask a query like $P(0 \le x \le 5|\pi, \mu, \Sigma)$

$$P(x) = \sum_{k=1}^{K} P(z_k)P(x|z)$$
$$= \sum_{k=1}^{K} \pi_k N(x|\mu_k, \Sigma_k)$$





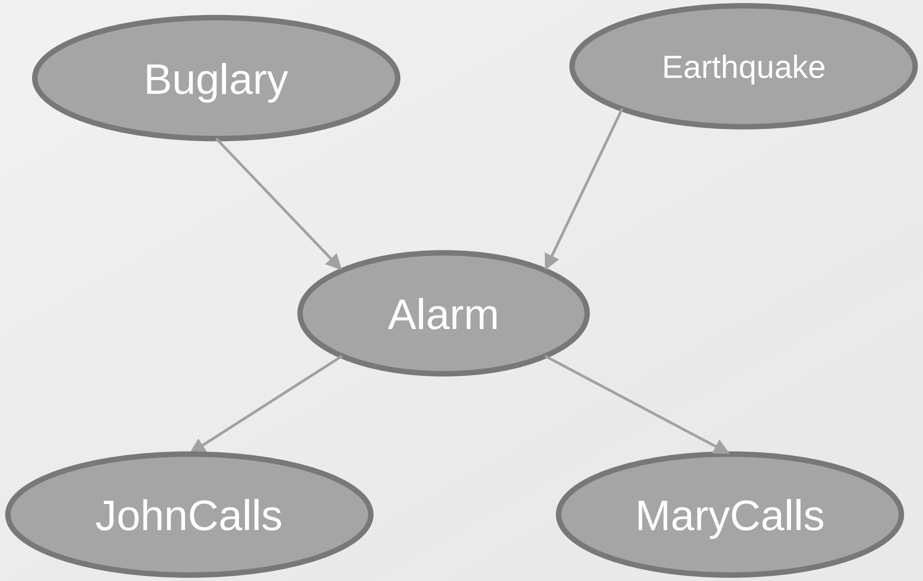


Rejection Sampling

- P(E=T|MC=T,A=F)=?
- RejectionSampling
  - Iterate many times
    - Generate a sample from the Bayesian network
      - Buglary → false
      - Earthquake → false
      - Alarm|B=F,E=F → true
        - If the sample does not follow MC=T, A=F, reject the sampling procedure, and repeat
      - JC|A=T → true
      - MC|A=T → false
  - Return Count(E=T,MC=T,A=F)/# of Samples
- Any problem?

P(B)=0.001

P(E)=0.002



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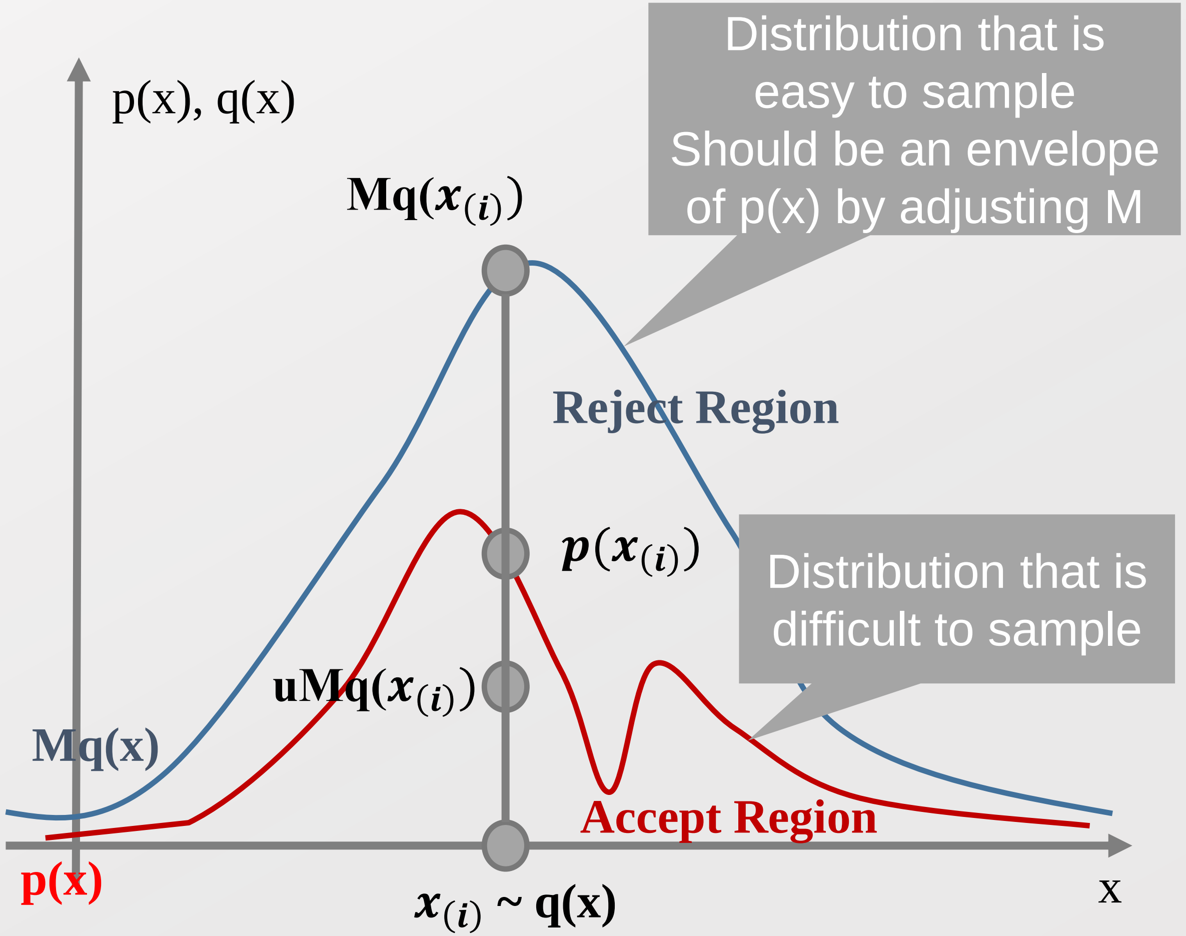
F	0.01

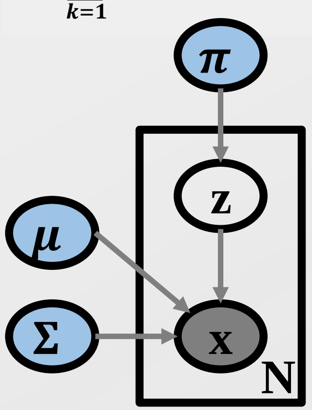
Rejection Sampling from Numerical View

- count = 0
- while count < N
  - Sample $x_{(i)}$ ~ q(x)
  - Sample u ~ Unif(0,1)
  - If $u < \frac{p(x_{(i)})}{Mq(x_{(i)})}$
    - Accept $x_{(i)}$
    - Increase count
  - Else
    - Reject and re-sample



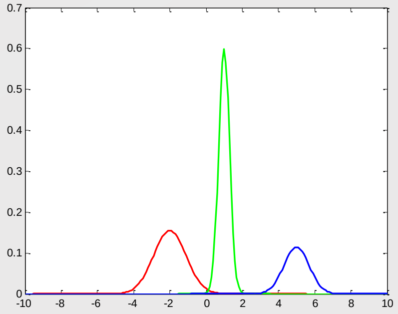
Rejection Sampling in GMM

$$P(x) = \sum_{k=1}^{K} P(z_k)P(x|z) = \sum_{k=1}^{K} \pi_k N(x|\mu_k, \Sigma_k)$$

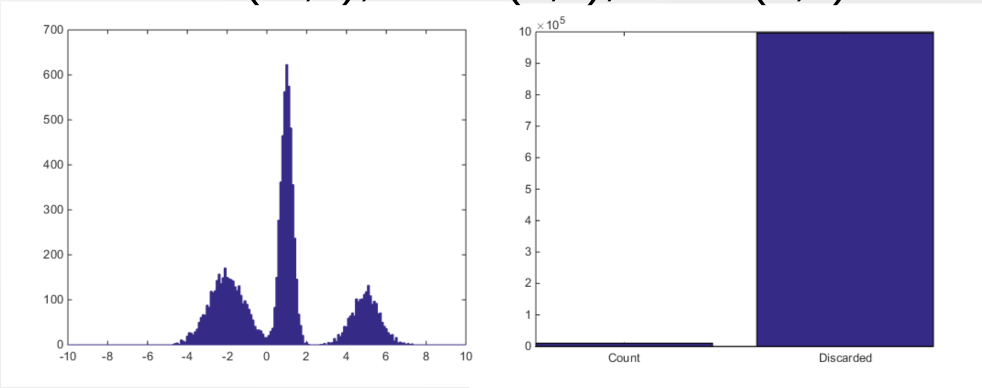


- Rejection sampling of GMM
  - Sample z from {1, 2, 3} with 1/3 change each
  - Sample x from N($\mu_{q(z)}, \Sigma_{q(z)}$)
    - $q(x)$ = The probability drawing x from N($\mu_{q(z)}, \Sigma_{q(z)}$)
  - Sample u from Uniform(0,1)
  - If $M \times u \times q(x) < p(x)$
    - Accept the sample of (z, x)
  - Else
    - Discard the sample

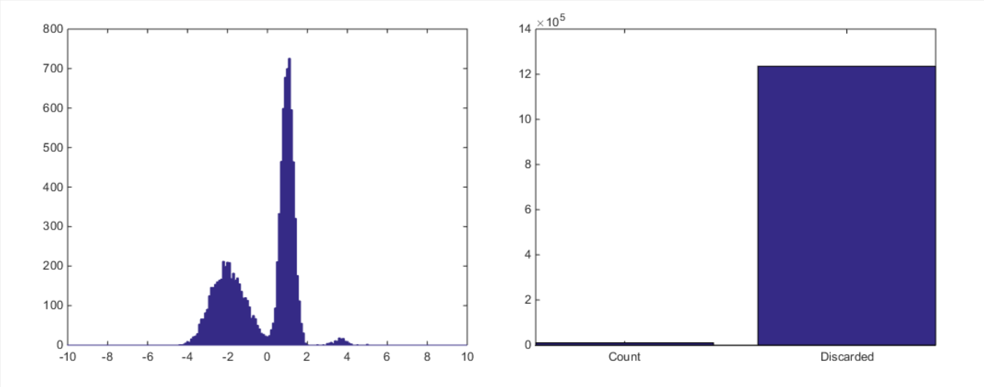
P Mixture
= 0.35*N(-2,0.9),
0.45*N(1,0.3),
0.2*N(5,0.8)



Q Mixture
= 1/3*N(-2,1), 1/3*N(1,1), 1/3*N(5,1)



Q Mixture
= 3 * (1/3 * N(0,1))

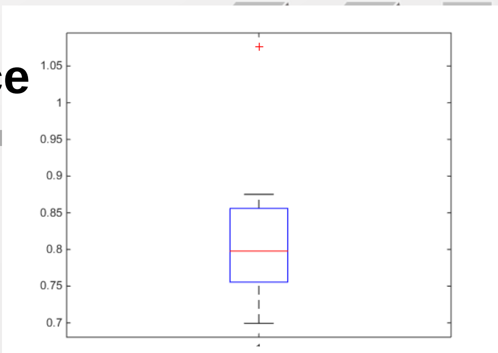


Importance Sampling

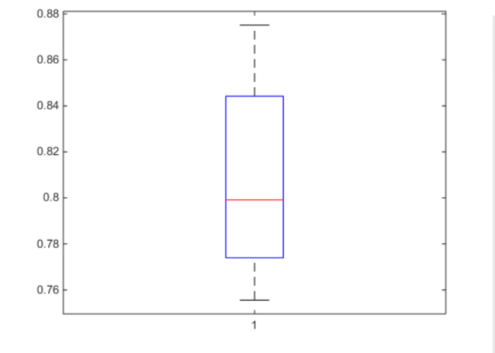
- Huge waste from the rejection
- Is generating the PDF the end goal?
  - No… Usually, the question follows
    - Calculating the expectation of PDF
    - Calculating a certain probability

- Let's use the wasted sample to answer the questions
  - $E(f) = \int f(z)p(z)dz = \int f(z)\frac{p(z)}{q(z)}q(z)dz \cong \frac{1}{L}\sum_{l=1}^{L}\frac{P(z^l)}{q(z^l)}f(z^l)$
    - L = # of samples, z^l=a sample of Z
    - Here, the importance weight plays the role
      - $r^l = \frac{P(z^l)}{q(z^l)}$
    - What if $P(z^l)$ and $q(z^l)$ is not normalized, as they should be as probability distributions
    - $E(f) \cong \frac{1}{L}\sum_{l=1}^{L}\frac{P(z^l)}{q(z^l)}f(z^l) = \frac{1}{L}\frac{Z_q}{Z_p}\sum_{l=1}^{L}\frac{\tilde{P}(z^l)}{\tilde{q}(z^l)}f(z^l)$
  - P(Z>1) = $\int_1^{\infty} 1_{z>1}p(z)dz = \int_1^{\infty} 1_{z>1}\frac{p(z)}{q(z)}q(z)dz \cong \frac{1}{L}\sum_{l=1}^{L}\frac{P(z^l)}{q(z^l)}1_{z^l>1}$

Importance Sampling Prone to Extreme Values



Filtered Extreme Values

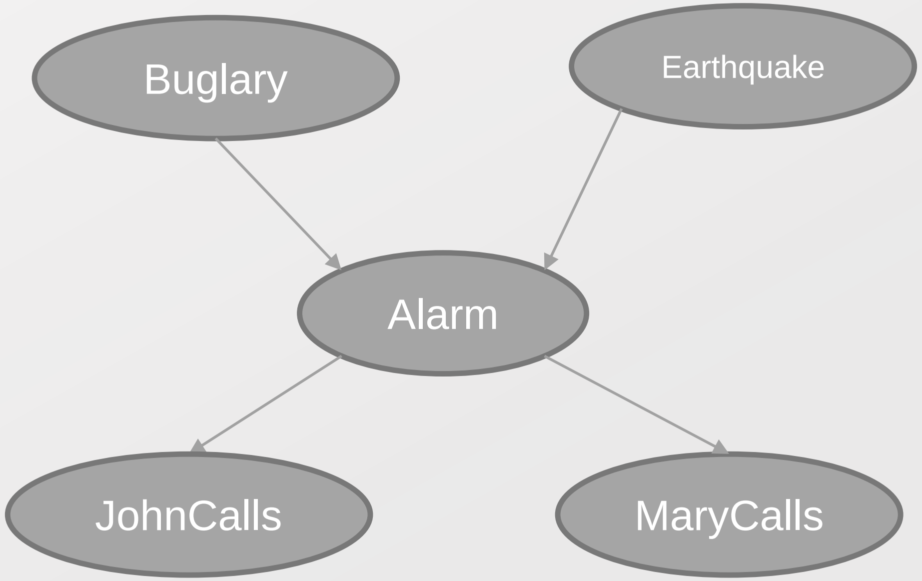


Likelihood Weighting Algorithm

- P(E=T|MC=T,A=F)=?
- LikelihoodWeighting
  - SumSW=NormSW=0
  - Iterate many times
    - SW=SampleWeight = 1
    - Generate a sample from the Bayesian network
      - Buglary → false
      - Earthquake → false
      - Alarm=F|B=F,E=F
        - P(A=F|B=F,E=F)=0.999
        - SW=1*0.999
      - JC|A=T → true
      - MC=T|A=F
        - P(MC=T|A=F)=0.01
        - SW=1*0.999*0.01
    - If the sample has E=T, then SumSW+=SW
    - NormSW+=SW
  - Return SumSW/NormSW
- Any further improvement?
- These samples are….

P(B)=0.001

P(E)=0.002



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Detour: EM Algorithm

$$l(\theta) = \ln P(X|\theta) = \ln\left\{\sum_Z q(Z)\frac{P(X,Z|\theta)}{q(Z)}\right\} \geq \sum_Z q(Z)\ln\frac{P(X,Z|\theta)}{q(Z)} = Q(\theta,q)$$

$$Q(\theta,q) = E_{q(Z)}\ln P(X,Z|\theta) + H(q)$$

$$L(\theta,q) = \ln P(X|\theta) - \sum_Z\{q(Z)\ln\frac{q(Z)}{P(Z|X,\theta)}\}$$

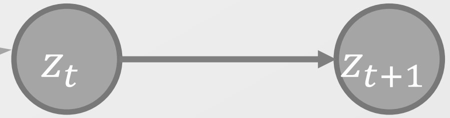
- EM algorithm
  - Finds the maximum likelihood solutions for models with latent variables
  - $P(X|\theta) = \sum_Z P(X,Z|\theta) \rightarrow \ln P(X|\theta) = \ln\{\sum_Z P(X,Z|\theta)\}$
- EM algorithm
  - Initialize θ^0 to an arbitrary point
  - Loop until the likelihood converges
    - Expectation step
      - $q^{t+1}(z) = argmax_q Q(\theta^t,q) = argmax_q L(\theta^t,q) = argmin_q KL(q||P(Z|X,\theta^t))$
      - → $q^t(z) = P(Z|X,\theta)$→**Assign Z by $P(Z|X,\theta)$**
    - Maximization step
      - $\theta^{t+1} = argmax_\theta Q(\theta,q^{t+1}) = argmax_\theta L(\theta,q^{t+1})$
      - → fixed Z means that there is no unobserved variables
      - → Same optimization of ordinary MLE

Computing Expectation…. Sometimes, it can be hard

Detour: Markov Chain

- Markov chain
  - Each node has a probability distribution of states
    - i.e.) The probability that a state is the current state of a system
      - Concrete observation of a system: [1 0 0] → the system is at the first state
      - Stochastic observation of a system: [0.7 0.2 0.1] → the system is likely at the first state
    - The node has a vector of state probability distribution
  - Each link suggests a probabilistic state transition
    - If a system is at the first state, the probability distribution of the next state is [0.3 0.4 0.3]
    - The link has a matrix of state transition probability distribution.

$z_t = [0.5 \quad 0.2 \quad 0.3]$



$$P(z_{t+1}) = P(z_t)P(z_{t+1}|z_t) = z_t T_{i,j}$$
$$= [0.5 \quad 0.2 \quad 0.3] \begin{bmatrix} 0.7 & 0.2 & 0.1 \\ 0.2 & 0.3 & 0.5 \\ 0.4 & 0.2 & 0.4 \end{bmatrix}$$
$$= [0.51 \quad 0.22 \quad 0.27]$$

- The system has three states, a, b, and c.
- Transition matrix is

$$\mathrm{P}(z_j|z_i) = T_{i,j} = \begin{bmatrix} 0.7 & 0.2 & 0.1 \\ 0.2 & 0.3 & 0.5 \\ 0.4 & 0.2 & 0.4 \end{bmatrix}$$

Detour: Properties of Markov Chain

- Accessible
  - **i→j:** State **j** is **accessible** from **i** if $T_{i,j}^{k} > 0 \; and \; k \geq 0$
  - $\boldsymbol{i} \leftrightarrow \boldsymbol{j}$: State **i** and **j** **communicate** if **i→j** and **j→i**
- Reducibility
  - A Markov chain is **irreducible** if $\boldsymbol{i} \leftrightarrow \boldsymbol{j}, \forall \boldsymbol{i} \in \boldsymbol{S}, \forall \boldsymbol{j} \in \boldsymbol{S}$
- Periodicity
  - State **i** has **period d** if $d = \gcd\{n: T_{i,i}^{n} > 0\}$
  - If **d**=1, State **i** is **aperiodic**.
- Transience
  - State **j** is **recurrent** if $\mathrm{P}(\inf(t \geq 1: X_t = j) < \infty | X_0 = j) = 1$
  - States which are not **recurrent** are **transient**.
- Ergodicity
  - A state is **ergodic** if the state is (positive) **recurrent** and **aperiodic**.
  - Markov chain is ergodic if all states are ergodic.

Detour: Stationary Distribution

- $RT_i = \min\{n > 0 : X_n = i | X_0 = i\}$
  - Return time to state **i** after the departure from state **i**
- Limit theorem of Markov chain
  - A friend in ISE dept. told me…..
  - If a Markov chain is irreducible and ergodic
    - $\pi_i = \lim_{n\to\infty} T_{i,j}^{(n)} = \frac{1}{E[RT_i]}$
    - π_i is uniquely determined by the set of equations
      - $\pi_i \geq 0, \sum_{i\in S}\pi_i = 1, \pi_j = \sum_{i\in S}\pi_i T_{i,j}$
  - How to compute $\boldsymbol{\pi}$ given $\boldsymbol{T}$
    - $\pi\left(I_{|S|,|S|} - T + 1_{|S|,|S|}\right) = 1_{1,|S|}$
      - $\pi_j = \sum_{i\in S}\pi_i T_{i,j} \to \pi_j - \sum_{i\in S}\pi_i T_{i,j} = 0 \to \pi\left(I_{|S|,|S|} - T\right) = 0$
        - To the above formula, apply $\sum_{i\in S}\pi_i = 1 \to \pi 1_{|S|,|S|} = 1_{1,|S|}$ to both sides
      - $\pi\left(I_{|S|,|S|} - T + 1_{|S|,|S|}\right) = 1_{1,|S|}$
  - Here, $\boldsymbol{\pi}$ is the stationary distribution!

```
>> T

T =

    0.7000    0.2000    0.1000
    0.2000    0.3000    0.5000
    0.4000    0.2000    0.4000

>> pi = ones(1,3) / (eye(3,3)-T+ones(3,3))

pi =

    0.5079    0.2222    0.2698

>> pi*T

ans =

    0.5079    0.2222    0.2698

>> pi(1)*T(1,2)

ans =

    0.1016

>> pi(2)*T(2,1)

ans =

    0.0444
```

Irreversible MC

```
>> T2 = [0 0.5 0.5 ; 0.25 0.5 0.25; 0.25 0.

T2 =

         0    0.5000    0.5000
    0.2500    0.5000    0.2500
    0.2500    0.2500    0.5000

>> pi2 = ones(1,3)/(eye(3,3)-T2+ones(3,3))

pi2 =

    0.2000    0.4000    0.4000

>> pi2*T2

ans =

    0.2000    0.4000    0.4000

>> pi2(1)*T2(1,2)

ans =

    0.1000

>> pi2(2)*T2(2,1)

ans =

    0.1000
```

Reversible MC

$\boldsymbol{\pi}$ is the stationary distribution

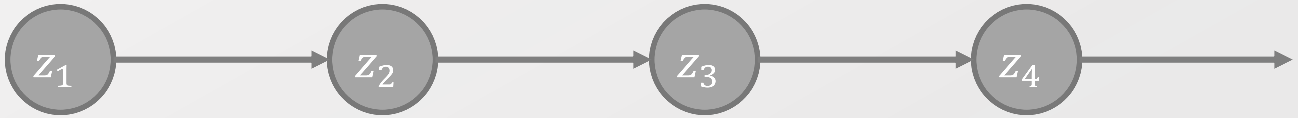
Reversible Markov chain

$\pi_i T_{i,j} = \pi_j T_{j,i}$

Detailed Balance, or **Balance Equation**

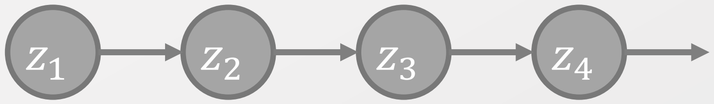
Markov Chain for Sampling

- Problem of the previous samplings?
  - No use of the past records → every sampling is independent
- Assigning Z values is a key in the inference
  - Let's assign the values by sampling result
    - Calculate P(E|MC=T,A=F) → Toss a biased coin to assign a value to E
- Sequence of random variables such a process moves through, with the Markov property defining serial dependence only between adjacent periods (as in a "chain")
- A Markov chain is a stochastic process with the Markov property
  - Example) First-order Markov chain



    - $p\left(\mathbf{z}^{(m+1)} \,|\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(m)}\right) = p\left(\mathbf{z}^{(m+1)} \mid \mathbf{z}^{(m)}\right), m \in \{1, \dots, M-1\}$
- Describing systems that follow a chain of linked events, where what happens next depends only on the current state of the system

Markov chain theory vs. Markov Chain Monte Carlo

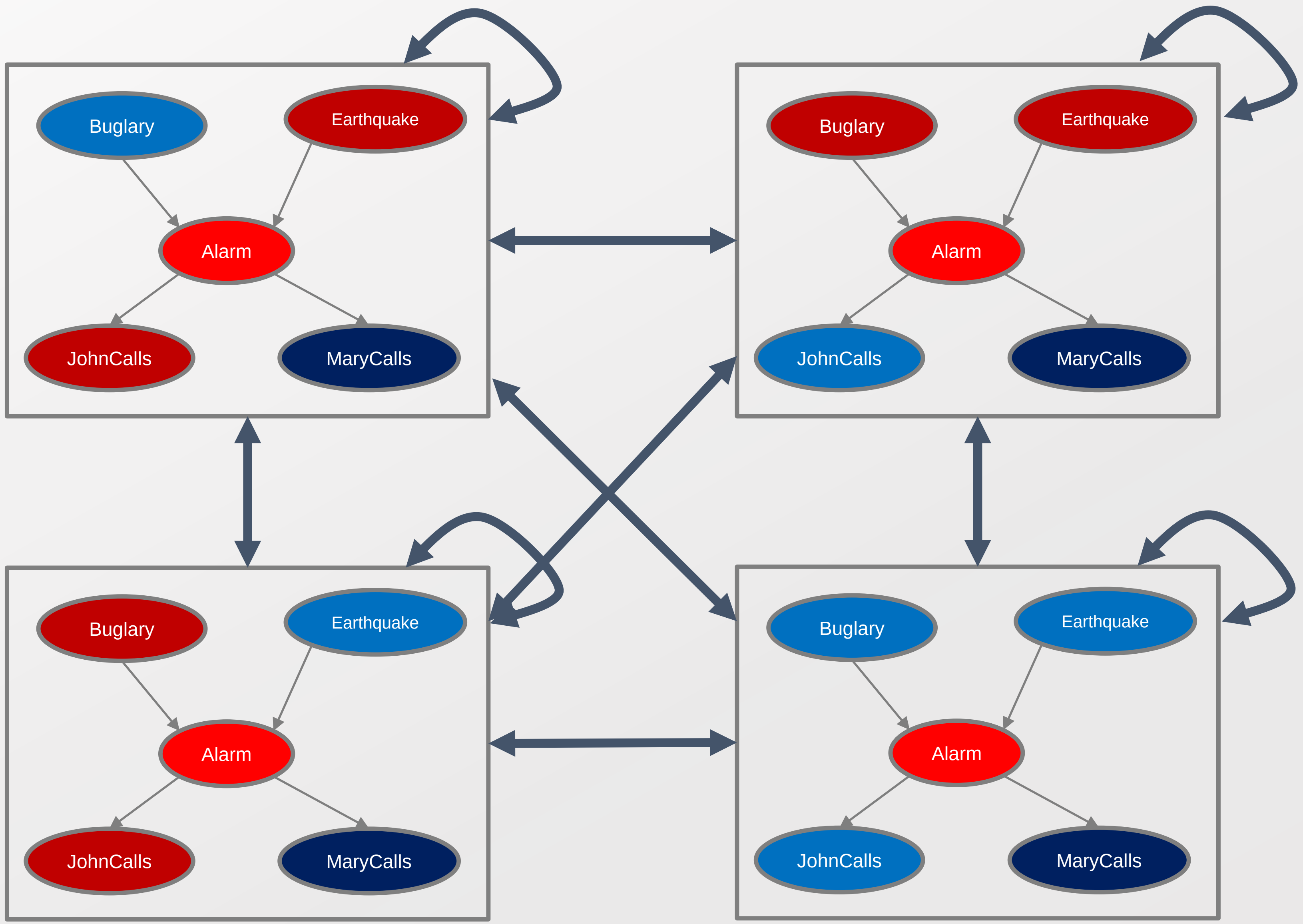


- Traditional Markov Chain analysis :
  - A transition rule, $p\left(z^{(t+1)} \mid z^{(t)}\right)$, is given,
  - Interested in finding the stationary distribution $\pi(z)$

- Markov chain Monte Carlo(MCMC) :
  - A target stationary distribution $\pi(z)$ is known,
  - Interested in prescribing an efficient transition rule to reach the stationary distribution
  - Algorithms for sampling from probability distributions based on constructing a Markov chain that has the desired distribution $\pi(z)$
  - Starting from an arbitrary state, the Markov chain proceeds

$$\underbrace{z^{(1)} \to z^{(2)} \to \cdots \to z^{(m)}}_{Burn-in\ period} \to \underbrace{z^{(m+1)} \to z^{(m+2)} \to \cdots \to z^{(m+n)}}_{Treat\ them\ as\ samples\ from\ \pi(x)}$$

Markov Chain of Z



Metropolis-Hastings Algorithm

$q(z^t|z^*)P(z^*) < q(z^*|z^t)P(z^t)$ → Movement from z^t to z^* is too often

- General algorithm of MCMC
  - Current value: z^t
  - Propose a candidate $z^* \sim q(z^*|z^t)$ where q_t is a proposal distribution
    - Same as importance and rejection samplings, yet the difference is the Markov property idea in the proposal distribution
  - With an acceptance probability, α
    - Accept → $z^{t+1} = z^*$
    - Reject → $z^{t+1} = z^t$
- Metropolis-Hastings algorithm
  - Given the general algorithm of MCMC
  - Consider a ratio, $r(z^*|z^t) = \frac{q(z^t|z^*)P(z^*)}{q(z^*|z^t)P(z^t)}$, we want this to be 1
    - $q(z^t|z^*)P(z^*)r_{z^*\to z^t} = q(z^*|z^t)P(z^t)r_{z^t\to z^*}$
    - $r(z^*|z^t) < 1 \to q(z^t|z^*)P(z^*) < q(z^*|z^t)P(z^t)$
      - Increase $r_{z^*\to z^t}$=1, degrease $r_{z^t\to z^*} = r(z^*|z^t)$
    - $r(z^*|z^t) > 1 \to q(z^t|z^*)P(z^*) > q(z^*|z^t)P(z^t)$
      - Decrease $r_{z^*\to z^t}$=$r(z^t|z^*)$, increase $r_{z^t\to z^*} = 1$
  - Acceptance probability $\alpha(z^*|z^t) = \min\{1, r(z^*|z^t)\}$

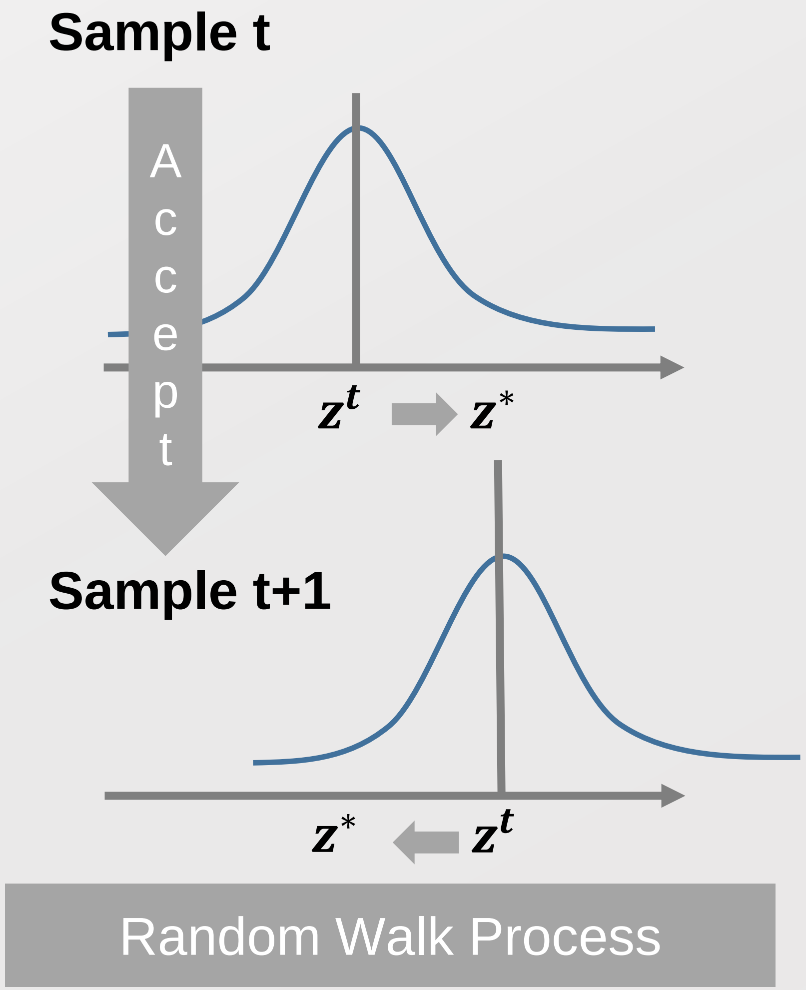
We want the stationary distribution, $\pi(z)$, of our MCMC sampling to be $\mathrm{P}(z)$

Reversible Markov chain
$\pi_i T_{i,j} = \pi_j T_{j,i}$

q is not well-designed to be the reversible MC, so we adjust by **r**

Random Walk M-H Algorithm

- $T_{t,*}^{MH} = q(z^*|z^t)\alpha(z^*|z^t)$
  - Transition probability to satisfy the balance equation with $\mathrm{P}(z)$ as the stationary distribution
  - $\alpha(z^*|z^t) = \min\left\{1, \frac{q(z^t|z^*)P(z^*)}{q(z^*|z^t)P(z^t)}\right\}$
  - Here, we already assumed, so far, the easy calculation of $P(z)$
  - What we miss is the definition of $q(z^*|z^t)$, but this is a proposal that any probability distribution can be
    - Surely, there are better and worse proposal probability distributions.
    - Choosing $q(z^*|z^t)$ determines the type of M-H algorithm
- Random walk M-H algorithm
  - $T_{t,*}^{MH} = q(z^*|z^t)\alpha(z^*|z^t)$
  - $z^* \sim N(z^t, \sigma^2)$
  - $q(z^*|z^t) = \frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{(z^*-z^t)^2}{2\sigma^2})$



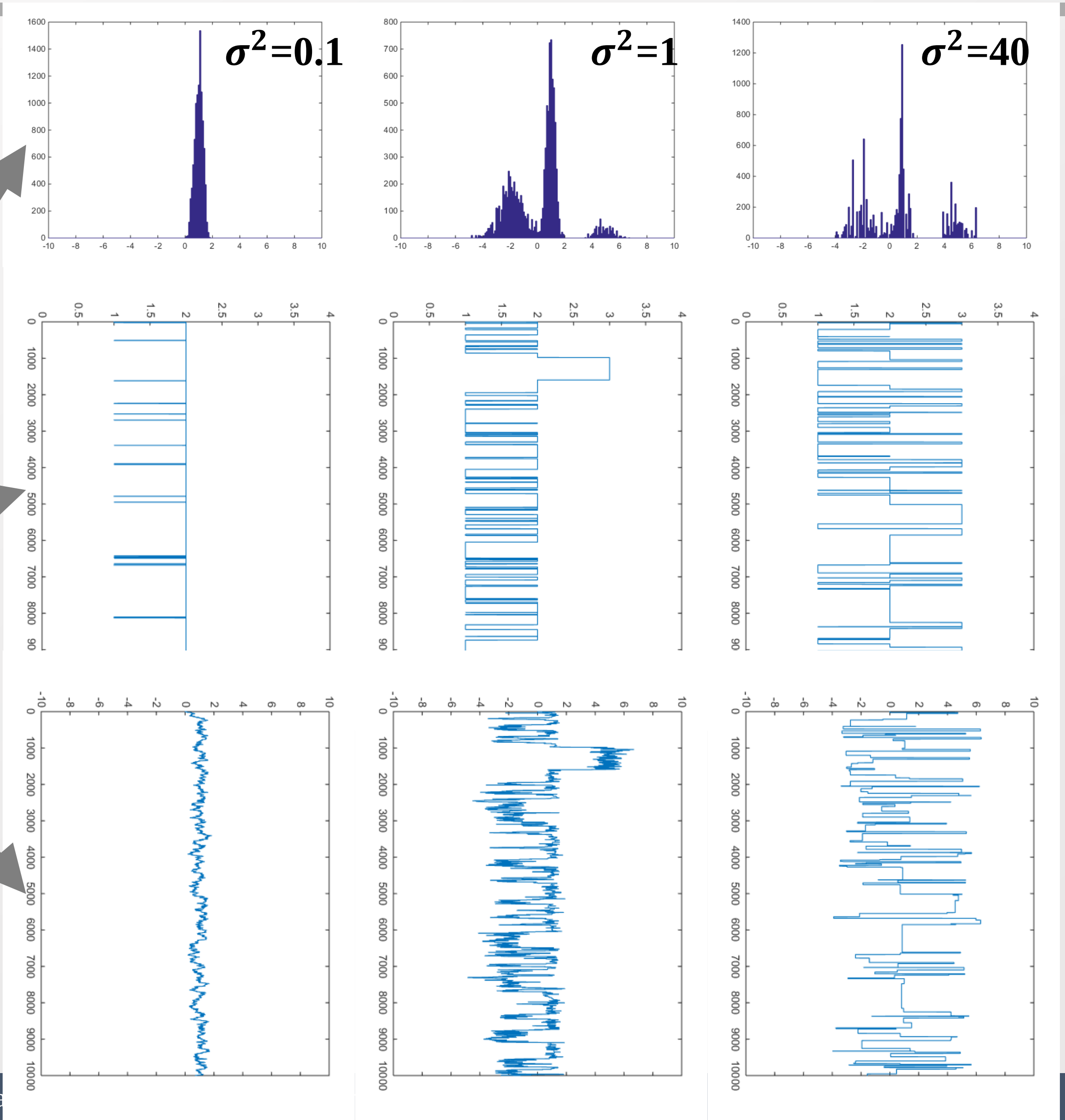
Result of Random Walk M-H

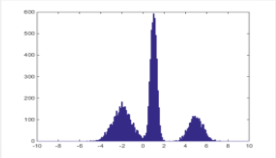
Sampling Result of Random Walk M-H

Overall Sampling

Latent Mode Selection Sampling

Observed Variable Sampling



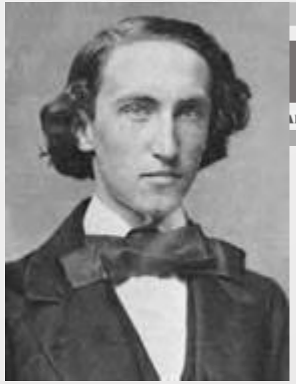


Target Mixture Distribution $T^{MH}_{t,*} = q(z^*|z^t)\alpha(z^*|z^t)$

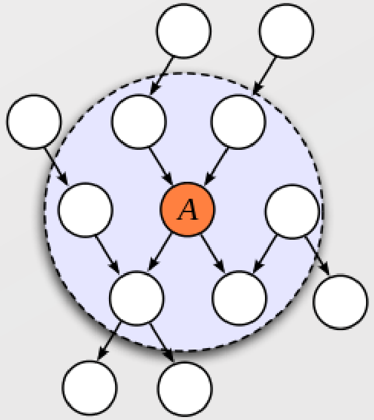
$z^* \sim N(z^t, \sigma^2)$

Gibbs Sampling

Josiah Willard Gibbs
(1839 - 1903)
- physicist

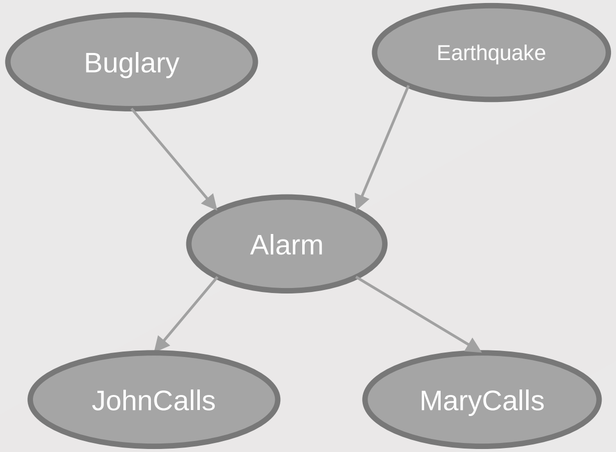


- Gibbs Sampling: A special case of M-H algorithm
  - Let's suppose $z^t = (z_k^t, z_{-k}^t) \rightarrow z^* = (z_k^*, z_{-k}^t)$
    - $T_{t,*}^{MH} = q(z^*|z^t)\alpha(z^*|z^t)$
    - $q(z^*|z^t) = P(z_k^*, z_{-k}^t | z_{-k}^t) = P(z_k^* | z_{-k}^t)$
  - Let's observe the balance equation
    - Should hold $\mathrm{P}(z^t)q(z^*|z^t) = \mathrm{P}(z^*)q(z^t|z^*)$
    - $\mathrm{P}(z^t)q(z^*|z^t) = \mathrm{P}(z_k^t, z_{-k}^t)P(z_k^*|z_{-k}^t) = \mathrm{P}(z_k^t|z_{-k}^t)P(z_{-k}^t)P(z_k^*|z_{-k}^t)$
      $= \mathrm{P}(z_k^t|z_{-k}^t)P(z_k^*, z_{-k}^t) = q(z^t|z^*)P(z^*)$
    - Always hold the balance equation!
  - Then, the acceptance probability becomes $\alpha(z^*|z^t) = 1$



- Example of Gibbs sampling
  - When the joint distribution is not known explicitly or is difficult to sample from directly, but the conditional distribution of each variable is known and is easy
    - P(E,JC,B|A=F,MC=T)=?
      - Hard to sample directly. Why?
    - Consider a conditional distribution $p(z_i|z_{-i}, e)$
      - P(E|B,A,JC,MC)=P(E|A)
      - P(JC|B,E,A,MC)=P(JC|A)
      - P(B|E,A,JC,MC)=P(B|A,E)
  - Update one random variable at a time

Can simplify using the Markov blanket



Concept of Gibbs Sampling

- Each step involves **replacing** the value of one of the variables by a value drawn from the distribution of that variable conditioned on the values of the remaining variables
- Repeated either by cycling through the variables in some particular order or by choosing the variable to be updated at each step at random from some distribution
- Example
  1. Full joint probability : $p(z_1, z_2, z_3)$
  2. Sample $z_1 \sim p\left(z_1 \mid z_2^{(\tau)}, z_3^{(\tau)}\right)$ → Obtain a value $z_1^{(\tau+1)}$
  3. Sample $z_2 \sim p\left(z_2 \mid z_1^{(\tau+1)}, z_3^{(\tau)}\right)$ → Obtain a value $z_2^{(\tau+1)}$
  4. Sample $z_3 \sim p\left(z_3 \mid z_1^{(\tau+1)}, z_2^{(\tau+1)}\right)$ → Obtain a value $z_3^{(\tau+1)}$

$\left\{z_1^{(\tau)}, z_2^{(\tau)}, z_3^{(\tau)}\right\}$ $\left\{z_1^{(\tau+1)}, z_2^{(\tau)}, z_3^{(\tau)}\right\}$ $\left\{z_1^{(\tau+1)}, z_2^{(\tau+1)}, z_3^{(\tau)}\right\}$ $\left\{z_1^{(\tau+1)}, z_2^{(\tau+1)}, z_3^{(\tau+1)}\right\}$

Gibbs Sampling Algorithm

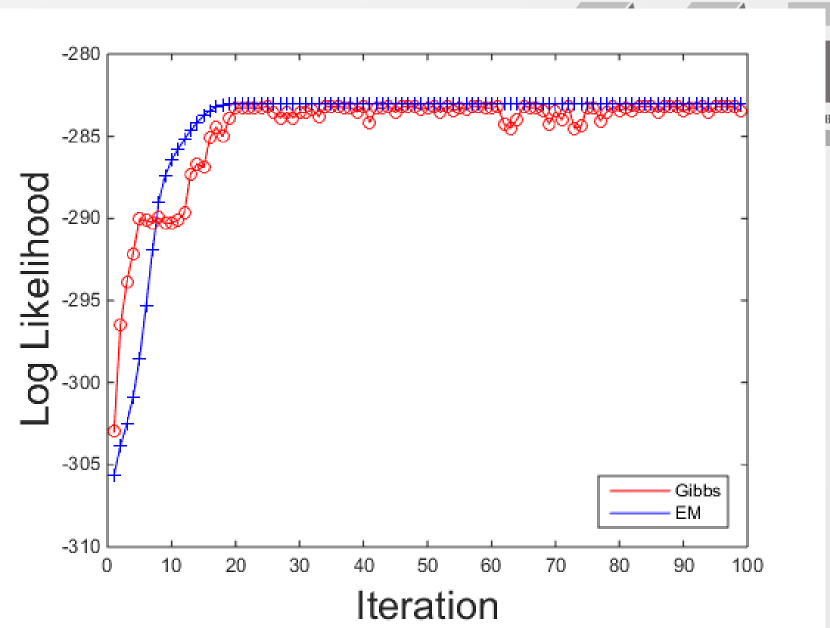
- Full joint distribution, $p(\boldsymbol{z}) = p(z_1, \dots, z_M)$
- State = $\{z_i : i = 1, \dots, M\}$
- Algorithm
  1. Initialize $\{z_i : i = 1, \dots, M\}$
  2. For step $\tau = 1, \dots, T$:
     - Sample $z_1^{(\tau+1)} \sim p\left(z_1 \,|z_2^{(\tau)}, z_3^{(\tau)}, \dots, z_M^{(\tau)}\right)$
     - Sample $z_2^{(\tau+1)} \sim p\left(z_2 \,|z_1^{(\tau+1)}, z_3^{(\tau)}, \dots, z_M^{(\tau)}\right)$

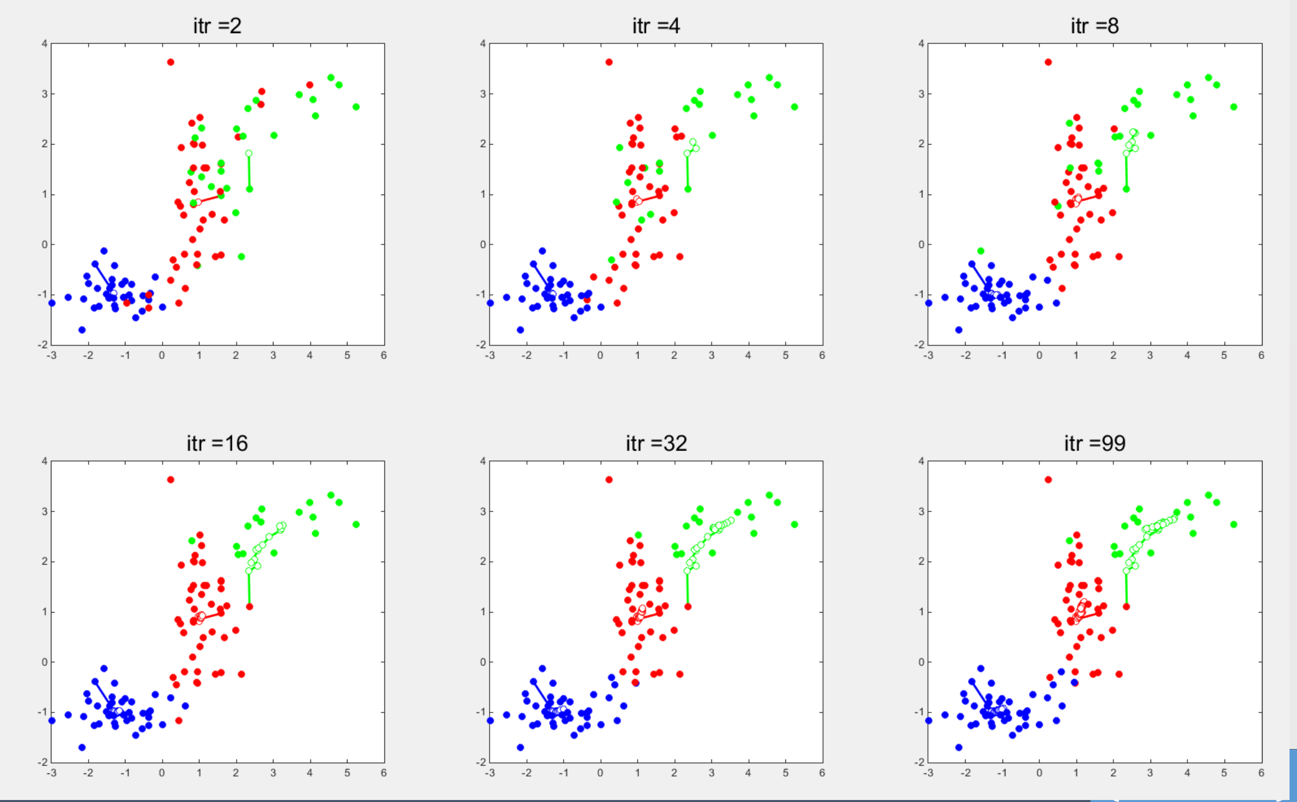
       $\vdots$
     - Sample $z_j^{(\tau+1)} \sim p\left(z_j \,|z_1^{(\tau+1)}, \dots, z_{j-1}^{(\tau+1)}, z_{j+1}^{(\tau)}, \dots, z_M^{(\tau)}\right)$

       $\vdots$
     - Sample $z_M^{(\tau+1)} \sim p\left(z_M \,|z_1^{(\tau+1)}, z_2^{(\tau+1)}, \dots, z_{M-1}^{(\tau+1)}\right)$

Gibbs Sampling based GMM

- Hard to tell the performance with the simple GMM
  - Sampling based inference
    - Simulation based
  - EM based inference
    - Optimization based
- Real power of Gibbs sampler comes from collapsing! → Collapsed Gibbs Sampler
  - Let's look at more sophisticated model for collapsing technique

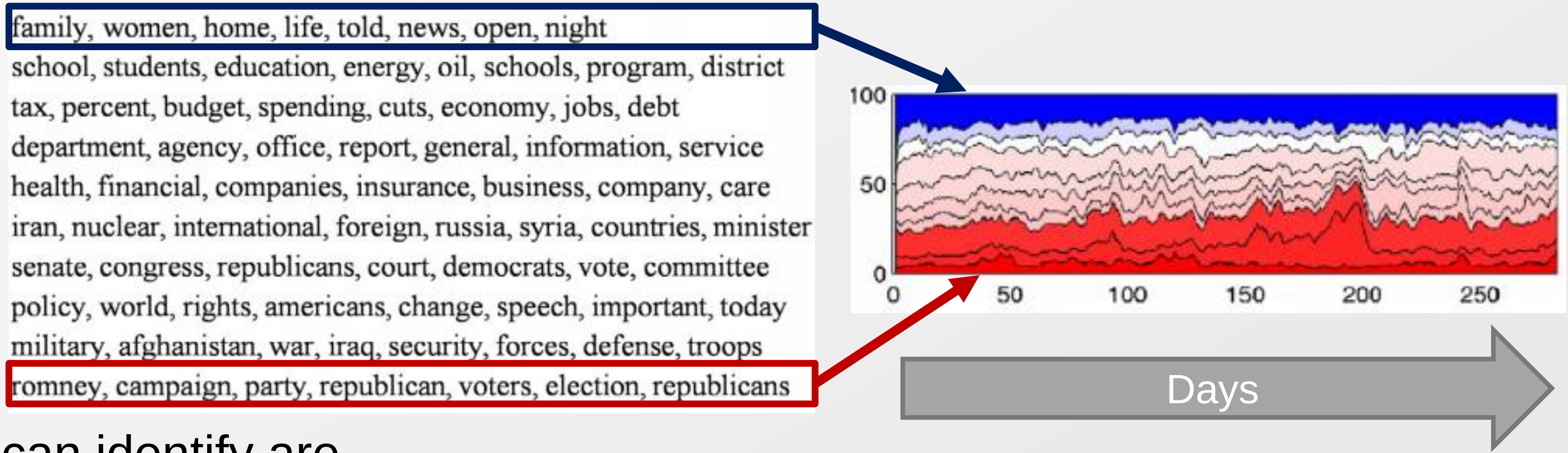




LATENT DIRICHLET ALLOCATION

Topic Modeling

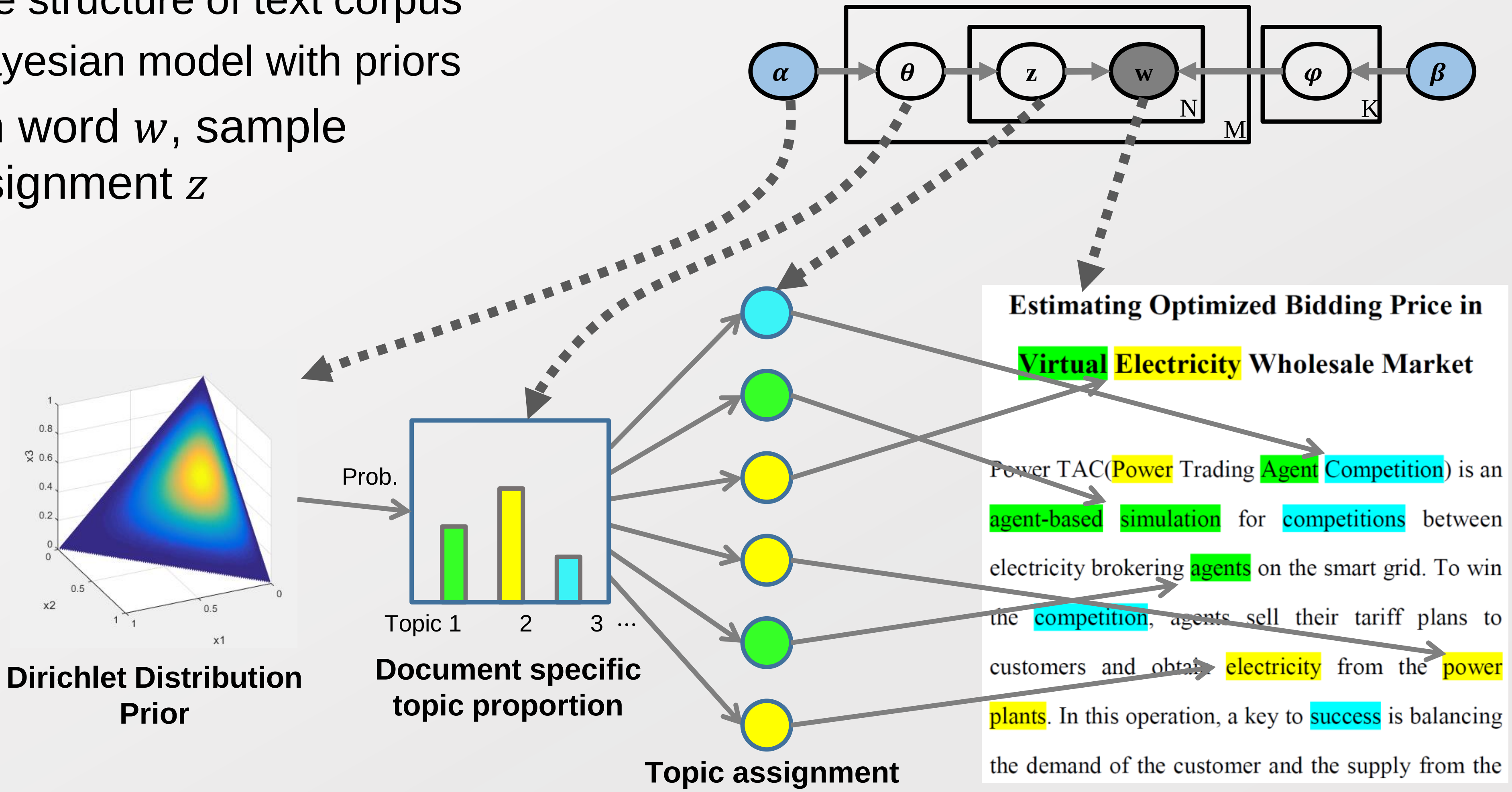
- Sample results of topic modeling on News paper searched by ‘Obama’



- What we can identify are
  - Topics
  - The proportion of topics
  - The most probable words in topics
- Text analysis without reading the whole corpus

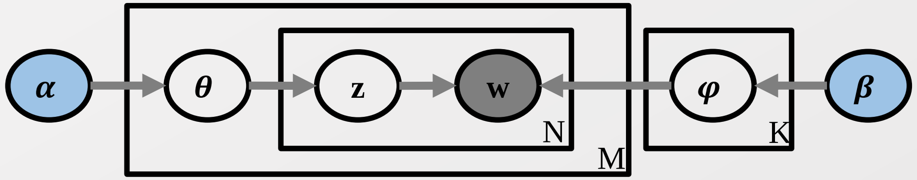
Latent Dirichlet Allocation

- Latent Dirichlet Allocation
  - Soft clustering in text data
  - Has the structure of text corpus
  - Is a Bayesian model with priors
- For each word w, sample topic assignment z



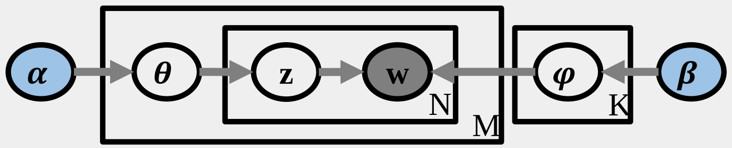
Finding Topic Assignment Per Word

- Let's treat this as a Bayesian network
  - Do you remember the story of "Alarm and call"?
    - There was a story of **generating** Mary's call from the event
  - **Generative Process**
    - $\theta_i \sim Dir(\alpha), i \in \{1, \ldots, M\}$
    - $\varphi_k \sim Dir(\beta), k \in \{1, \ldots, K\}$
    - $z_{i,l} \sim Mult(\theta_i), i \in \{1, \ldots, M\}, l \in \{1, \ldots, N\}$
    - $w_{i,l} \sim Mult\left(\varphi_{z_{i,l}}\right), i \in \{1, \ldots, M\}, l \in \{1, \ldots, N\}$



  - A word **w** is generated from the distribution of $\boldsymbol{\varphi_z}$ word-topic distribution
  - **z** topic is generated from the distribution of $\boldsymbol{\theta}$ document-topic distribution
  - $\boldsymbol{\theta}$ document topic distribution is generated from the distribution of $\boldsymbol{\alpha}$
  - $\boldsymbol{\varphi}$ word-topic distribution is generated from the distribution of $\boldsymbol{\beta}$
- If we have Z distribution, we can find the most likely θ and φ
  - θ: Topic distribution in a document
  - φ: Word distribution in a topic
  - Finding the most likely allocation of Z is the key of inference on θ and φ

Gibbs Sampling on Z (1)



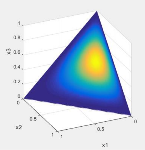
- Finding the most likely assignment on Z →Gibbs Sampling
- Start with the factorization
  - $P(W, Z, \theta, \varphi; \alpha, \beta)$

$$= \prod_{i=1}^{K} P(\varphi_i; \beta) \prod_{j=1}^{M} P(\theta_j; \alpha) \prod_{l=1}^{N} P(Z_{j,l}|\theta_j) P(W_{j,l}|\varphi_{Z_{j,l}})$$

- We are going to collapse θ and φ to leave only W, Z, α and β
  - Why? W (Data point), Z (Sampling Target), α and β (priors)
  - Collapsed Gibbs sampling!
- $P(W, Z; \alpha, \beta) = \int_\theta \int_\varphi P(W, Z, \theta, \varphi; \alpha, \beta) d\varphi d\theta = \int_\varphi \prod_{i=1}^{K} P(\varphi_i; \beta) \prod_{j=1}^{M} \prod_{l=1}^{N} P(W_{j,l}|\varphi_{Z_{j,l}})\, d\varphi \times \int_\theta \prod_{j=1}^{M} P(\theta_j; \alpha) \prod_{l=1}^{N} P(Z_{j,l}|\theta_j)\, d\theta$

1. Independence between two integrals
2. Need to remove the integrals and come up with the sampling distribution

Gibbs Sampling on Z (2)



$$x \sim Dir(\alpha)$$

$$\mathrm{P}(\mathrm{X}|\alpha) = \frac{\Gamma(\sum_{i=1}^{K} \alpha_i)}{\prod_{i=1}^{K} \Gamma(\alpha_i)} \prod_{i=1}^{K} x_i^{\alpha_i - 1}$$

- $P(W,Z;\alpha,\beta) = \int_\theta \int_\varphi P(W,Z,\theta,\varphi;\alpha,\beta) d\varphi d\theta = \int_\varphi \prod_{i=1}^{K} P(\varphi_i;\beta) \prod_{j=1}^{M} \prod_{l=1}^{N} P(W_{j,l}|\varphi_{Z_{j,l}})\, d\varphi \times \int_\theta \prod_{j=1}^{M} P(\theta_j;\alpha) \prod_{l=1}^{N} P(Z_{j,l}|\theta_j)\, d\theta = (1) \times (2)$
- $(1) = \int_\varphi \prod_{i=1}^{K} P(\varphi_i;\beta) \prod_{j=1}^{M} \prod_{l=1}^{N} P(W_{j,l}|\varphi_{Z_{j,l}})\, d\varphi = \prod_{i=1}^{K} \int_{\varphi_i} P(\varphi_i;\beta) \prod_{j=1}^{M} \prod_{l=1}^{N} P(W_{j,l}|\varphi_{Z_{j,l}})\, d\varphi_i = \prod_{i=1}^{K} \int_{\varphi_i} \frac{\Gamma(\sum_{v=1}^{V} \beta_v)}{\prod_{v=1}^{V} \Gamma(\beta_v)} \prod_{v=1}^{V} {\varphi_{i,v}}^{\beta_v - 1} \prod_{j=1}^{M} \prod_{l=1}^{N} P(W_{j,l}|\varphi_{Z_{j,l}})\, d\varphi_i$
  - We introduce a new count of $n_{j,r}^{i}$: number of words assigned to i-th topic in j-th document with r-th unique word
- $= \prod_{i=1}^{K} \int_{\varphi_i} \frac{\Gamma(\sum_{v=1}^{V} \beta_v)}{\prod_{v=1}^{V} \Gamma(\beta_v)} \prod_{v=1}^{V} {\varphi_{i,v}}^{\beta_v - 1} \prod_{v=1}^{V} {\varphi_{i,v}}^{n_{(.),v}^{i}}\, d\varphi_i$
- $= \prod_{i=1}^{K} \int_{\varphi_i} \frac{\Gamma(\sum_{v=1}^{V} \beta_v)}{\prod_{v=1}^{V} \Gamma(\beta_v)} \prod_{v=1}^{V} {\varphi_{i,v}}^{n_{(.),v}^{i} + \beta_v - 1}\, d\varphi_i$
- $= \prod_{i=1}^{K} \frac{\prod_{v=1}^{V} \Gamma(n_{(.),v}^{i} + \beta_v) \Gamma(\sum_{v=1}^{V} \beta_v)}{\prod_{v=1}^{V} \Gamma(\beta_v) \Gamma(\sum_{v=1}^{V} n_{(.),v}^{i} + \beta_v)} \int_{\varphi_i} \frac{\Gamma(\sum_{v=1}^{V} n_{(.),v}^{i} + \beta_v)}{\prod_{v=1}^{V} \Gamma(n_{(.),v}^{i} + \beta_v)} \prod_{v=1}^{V} {\varphi_{i,v}}^{n_{(.),v}^{i} + \beta_v - 1}\, d\varphi_i$
- $= \prod_{i=1}^{K} \frac{\prod_{v=1}^{V} \Gamma(n_{(.),v}^{i} + \beta_v) \Gamma(\sum_{v=1}^{V} \beta_v)}{\prod_{v=1}^{V} \Gamma(\beta_v) \Gamma(\sum_{v=1}^{V} n_{(.),v}^{i} + \beta_v)}$

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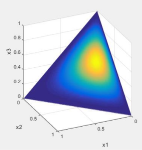
KAIST

Gibbs Sampling on Z (3)



$$x \sim Dir(\alpha)$$

$$\mathrm{P}(\mathrm{X}|\alpha) = \frac{\Gamma(\sum_{i=1}^{K}\alpha_i)}{\prod_{i=1}^{K}\Gamma(\alpha_i)}\prod_{i=1}^{K} x_i^{\alpha_i-1}$$

- $P(W,Z;\alpha,\beta) = \int_\theta \int_\varphi P(W,Z,\theta,\varphi;\alpha,\beta)d\varphi d\theta = \int_\varphi \prod_{i=1}^{K} P(\varphi_i;\beta)\prod_{j=1}^{M}\prod_{l=1}^{N} P(W_{j,l}|\varphi_{Z_{j,l}})\,d\varphi \times \int_\theta \prod_{j=1}^{M} P(\theta_j;\alpha)\prod_{l=1}^{N} P(Z_{j,l}|\theta_j)\,d\theta = (1)\times(2)$
- $(2) = \int_\theta \prod_{j=1}^{M} P\left(\theta_j;\alpha\right)\prod_{l=1}^{N} P\left(Z_{j,l}\middle|\theta_j\right)d\theta = \prod_{j=1}^{M}\int_{\theta_j} P\left(\theta_j;\alpha\right)\prod_{l=1}^{N} P\left(Z_{j,l}\middle|\theta_j\right)d\theta_j = \prod_{j=1}^{M}\int_{\theta_j}\frac{\Gamma(\sum_{k=1}^{K}\alpha_k)}{\prod_{k=1}^{K}\Gamma(\alpha_k)}\prod_{k=1}^{K}\theta_{j,k}{}^{\alpha_k-1}\prod_{l=1}^{N} P\left(Z_{j,l}\middle|\theta_j\right)d\theta_j$
  - We introduce a new count of $n_{j,r}^{i}$: number of words assigned to i-th topic in j-th document with r-th unique word
- $= \prod_{j=1}^{M}\int_{\theta_j}\frac{\Gamma(\sum_{i=1}^{K}\alpha_i)}{\prod_{i=1}^{K}\Gamma(\alpha_i)}\prod_{i=1}^{K}\theta_{j,i}{}^{\alpha_i-1}\prod_{k=1}^{K}\theta_{j,k}{}^{n_{j,(.)}^{k}}\,d\theta_j$
- $= \prod_{j=1}^{M}\int_{\theta_j}\frac{\Gamma(\sum_{i=1}^{K}\alpha_i)}{\prod_{i=1}^{K}\Gamma(\alpha_i)}\prod_{i=1}^{K}\theta_{j,k}{}^{n_{j,(.)}^{i}+\alpha_k-1}\,d\theta_j$
- $= \prod_{j=1}^{M}\frac{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_k)\Gamma(\sum_{i=1}^{K}\alpha_k)}{\prod_{i=1}^{K}\Gamma(\alpha_i)\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{i}+\alpha_k)}\int_{\theta_j}\frac{\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{i}+\alpha_k)}{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_k)}\prod_{i=1}^{K}\theta_{j,i}{}^{n_{j,(.)}^{i}+\alpha_k-1}\,d\theta_j$
- $= \prod_{j=1}^{M}\frac{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_i)\Gamma(\sum_{i=1}^{K}\alpha_i)}{\prod_{i=1}^{K}\Gamma(\alpha_i)\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{i}+\alpha_i)}$

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Collapse from Conjugacy

- Same mechanism to remove θ and φ
  - $=\prod_{i=1}^{K}\frac{\prod_{v=1}^{V}\Gamma(n_{(.),v}^{i}+\beta_v)\Gamma(\sum_{v=1}^{V}\beta_v)}{\prod_{v=1}^{V}\Gamma(\beta_v)\Gamma(\sum_{v=1}^{V}n_{(.),v}^{i}+\beta_v)}\int_{\varphi_i}\frac{\Gamma(\sum_{v=1}^{V}n_{(.),v}^{i}+\beta_v)}{\prod_{v=1}^{V}\Gamma(n_{(.),v}^{i}+\beta_v)}\prod_{v=1}^{V}\varphi_{i,v}{}^{n_{(.),v}^{i}+\beta_v-1}\,d\varphi_i$
  - $=\prod_{j=1}^{M}\frac{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_k)\Gamma(\sum_{i=1}^{K}\alpha_k)}{\prod_{i=1}^{K}\Gamma(\alpha_i)\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{i}+\alpha_k)}\int_{\theta_j}\frac{\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{i}+\alpha_k)}{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_k)}\prod_{i=1}^{K}\theta_{j,i}{}^{n_{j,(.)}^{i}+\alpha_k-1}\,d\theta_j$
- This is a multiplication of the Dirichlet distribution and the multinomial distribution. After multiplication, another Dirichlet distribution emerges.
  - In LDA: i.e. $\int_{\theta}\prod_{j=1}^{M}P(\theta_j;\alpha)\prod_{l=1}^{N}P(Z_{j,l}|\theta_j)\,d\theta$
  - In general: $\mathrm{P}(X|\theta)\times P(\theta)$
  - Likelihood and prior multiplication results in the prior distribution → Conjugate prior
- LDA utilizes the multinomial distribution and the Dirichlet distribution
  - Dirichlet distribution is the conjugate prior of the multinomical distribution
  - Enables sum to one technique!

Gibbs Sampling Formula (1)

- $P(W,Z;\alpha,\beta) = \prod_{i=1}^{K} \frac{\prod_{v=1}^{V}\Gamma(n_{(.),v}^{i}+\beta_v)\Gamma(\sum_{v=1}^{V}\beta_v)}{\prod_{v=1}^{V}\Gamma(\beta_v)\Gamma(\sum_{v=1}^{V}n_{(.),v}^{i}+\beta_v)} \prod_{j=1}^{M} \frac{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_i)\Gamma(\sum_{i=1}^{K}\alpha_i)}{\prod_{i=1}^{K}\Gamma(\alpha_i)\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{i}+\alpha_i)}$
- Here, W, α and β are assumed or data-points, and Z is the target of sampling.
  - Gibbs sampling iterates the element of Z, one by one.
  - Therefore, we need to derive a formula of a single element Z when all other element of Z, W, α and β are given.
- $P\left(Z_{(m,l)} = k \middle| Z_{-(m,l)}, W; \alpha, \beta\right) = \frac{P\left(Z_{(m,l)}=k, Z_{-(m,l)}, W; \alpha, \beta\right)}{P(Z_{-(m,l)}, W; \alpha, \beta)}$

$$\propto P\left(Z_{(m,l)} = k, Z_{-(m,l)}, W; \alpha, \beta\right)$$

  - $Z_{(m,l)}$ is the topic assignment on the l-th word of m-th document

$\left\{z_1^{(\tau)}, z_2^{(\tau)}, z_3^{(\tau)}\right\}$ $\left\{z_1^{(\tau+1)}, z_2^{(\tau)}, z_3^{(\tau)}\right\}$ $\left\{z_1^{(\tau+1)}, z_2^{(\tau+1)}, z_3^{(\tau)}\right\}$ $\left\{z_1^{(\tau+1)}, z_2^{(\tau+1)}, z_3^{(\tau+1)}\right\}$

Gibbs Sampling Formula (2)

- $P(W,Z;\alpha,\beta)=\prod_{i=1}^{K}\frac{\prod_{v=1}^{V}\Gamma(n_{(.),v}^{i}+\beta_v)\Gamma(\sum_{v=1}^{V}\beta_v)}{\prod_{v=1}^{V}\Gamma(\beta_v)\Gamma(\sum_{v=1}^{V}n_{(.),v}^{i}+\beta_v)}\prod_{j=1}^{M}\frac{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_i)\Gamma(\sum_{i=1}^{K}\alpha_i)}{\prod_{i=1}^{K}\Gamma(\alpha_i)\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{k}+\alpha_i)}$
  - $=\left(\frac{\Gamma(\sum_{v=1}^{V}\beta_v)}{\prod_{v=1}^{V}\Gamma(\beta_v)}\right)^{K}\left(\frac{\Gamma(\sum_{i=1}^{K}\alpha_i)}{\prod_{i=1}^{K}\Gamma(\alpha_i)}\right)^{M}\prod_{i=1}^{K}\frac{\prod_{v=1}^{V}\Gamma(n_{(.),v}^{i}+\beta_v)}{\Gamma(\sum_{v=1}^{V}n_{(.),v}^{i}+\beta_v)}\prod_{j=1}^{M}\frac{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_i)}{\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{i}+\alpha_i)}$
  - $\propto\prod_{i=1}^{K}\frac{\prod_{v=1}^{V}\Gamma(n_{(.),v}^{i}+\beta_v)}{\Gamma(\sum_{v=1}^{V}n_{(.),v}^{i}+\beta_v)}\prod_{j=1}^{M}\frac{\prod_{i=1}^{K}\Gamma(n_{j,(.)}^{i}+\alpha_i)}{\Gamma(\sum_{i=1}^{K}n_{j,(.)}^{i}+\alpha_i)}$
- Now, apply that $P\left(Z_{(m,l)}=k,Z_{-(m,l)},W;\alpha,\beta\right)$
  - $\propto\prod_{i=1}^{K}\frac{\prod_{v=1}^{V}\Gamma(n_{(.),v}^{i}+\beta_v)}{\Gamma(\sum_{v=1}^{V}n_{(.),v}^{i}+\beta_v)}\times\frac{\prod_{i=1}^{K}\Gamma(n_{m,(.)}^{i}+\alpha_i)}{\Gamma(\sum_{i=1}^{K}n_{m,(.)}^{i}+\alpha_i)}$: Fixing document by **m**
  - $\propto\prod_{i=1}^{K}\frac{\Gamma(n_{(.),v}^{i}+\beta_v)}{\Gamma(\sum_{r=1}^{V}n_{(.),r}^{i}+\beta_r)}\times\frac{\prod_{i=1}^{K}\Gamma(n_{m,(.)}^{i}+\alpha_i)}{\Gamma(\sum_{i=1}^{K}n_{m,(.)}^{i}+\alpha_i)}$: Fixing word by **l**
  - $\propto\prod_{i=1}^{K}\frac{\Gamma(n_{(.),v}^{i}+\beta_v)}{\Gamma(\sum_{r=1}^{V}n_{(.),r}^{i}+\beta_r)}\times\prod_{i=1}^{K}\Gamma(n_{m,(.)}^{i}+\alpha_i)$: Remove a constant $\Gamma(\sum_{i=1}^{K}n_{m,(.)}^{i}+\alpha_i)$

Gibbs Sampling Formula (3)

- $P\left(Z_{(m,l)} = k \middle| Z_{-(m,l)}, W; \alpha, \beta\right) \propto P\left(Z_{(m,l)} = k, Z_{-(m,l)}, W; \alpha, \beta\right)$
  - $\propto \prod_{i=1}^{K} \frac{\Gamma(n_{(.),v}^{i}+\beta_v)}{\Gamma(\sum_{r=1}^{V} n_{(.),r}^{i}+\beta_r)} \times \prod_{i=1}^{K} \Gamma(n_{m,(.)}^{i} + \alpha_k)$
- Now, we set $n_{j,r}^{i,-(m,l)}$ as $n_{j,r}^{i}$ excluding the count from the topic assignment of $Z_{(m,l)}$
  - $\propto \prod_{i=1,i\neq k}^{K} \frac{\Gamma\left(n_{(.),v}^{i,-(m,n)}+\beta_v\right)}{\Gamma\left(\sum_{r=1}^{V} n_{(.),r}^{i,-(m,n)}+\beta_r\right)} \times \prod_{i=1,i\neq k}^{K} \Gamma(n_{m,(.)}^{i,-(m,n)} + \alpha_k)$
    $\times \frac{\Gamma\left(n_{(.),v}^{k,-(m,n)} + \beta_v + 1\right)}{\Gamma\left((\sum_{r=1}^{V} n_{(.),r}^{k,-(m,n)} + \beta_r) + 1\right)} \times \Gamma(n_{m,(.)}^{k,-(m,n)} + \alpha_k + 1)$
    - Take out the k-th topic assignment because, the count of the k-th topic assignment count will be increased by 1 compared to $n_{(.),(.)}^{k,-(m,l)}$
    - Notice the increment of 1 in the separated multiplication
  - $\propto \prod_{i=1,i\neq k}^{K} \frac{\Gamma\left(n_{(.),v}^{i,-(m,n)}+\beta_v\right)}{\Gamma\left(\sum_{r=1}^{V} n_{(.),r}^{i,-(m,n)}+\beta_r\right)} \times \prod_{i=1,i\neq k}^{K} \Gamma(n_{m,(.)}^{i,-(m,n)} + \alpha_k)$
    $\times \frac{\Gamma\left(n_{(.),v}^{k,-(m,n)}+\beta_v\right)}{\Gamma\left(\sum_{r=1}^{V} n_{(.),r}^{k,-(m,n)}+\beta_r\right)} \times \Gamma(n_{m,(.)}^{k,-(m,n)} + \alpha_k) \times \frac{n_{(.),v}^{k,-(m,n)}+\beta_v}{(\sum_{r=1}^{V} n_{(.),r}^{k,-(m,n)}+\beta_r)} \times (n_{m,(.)}^{k,-(m,n)} + \alpha_k)$
    - Definition of $\Gamma(x) = (x-1)!$
    - Therefore, $\Gamma(x+1) = (x)! \times x$

Gibbs Sampling Formula (4)

- $P\left(Z_{(m,l)} = k \middle| Z_{-(m,l)}, W; \alpha, \beta\right) \propto P\left(Z_{(m,l)} = k, Z_{-(m,l)}, W; \alpha, \beta\right)$
  - $\propto \prod_{i=1, i \neq k}^{K} \frac{\Gamma\left(n_{(.),v}^{i,-(m,n)} + \beta_v\right)}{\Gamma\left(\sum_{r=1}^{V} n_{(.),r}^{i,-(m,n)} + \beta_r\right)} \times \prod_{i=1, i \neq k}^{K} \Gamma(n_{m,(.)}^{i,-(m,n)} + \alpha_k)$
  $\times \frac{\Gamma\left(n_{(.),v}^{k,-(m,n)} + \beta_v\right)}{\Gamma\left(\sum_{r=1}^{V} n_{(.),r}^{k,-(m,n)} + \beta_r\right)} \times \Gamma(n_{m,(.)}^{k,-(m,n)} + \alpha_k) \times \frac{n_{(.),v}^{k,-(m,n)} + \beta_v}{(\sum_{r=1}^{V} n_{(.),r}^{k,-(m,n)} + \beta_r)} \times (n_{m,(.)}^{k,-(m,n)} + \alpha_k)$
  - $\propto \prod_{i=1}^{K} \frac{\Gamma\left(n_{(.),v}^{i,-(m,n)} + \beta_v\right)}{\Gamma\left(\sum_{r=1}^{V} n_{(.),r}^{i,-(m,n)} + \beta_r\right)} \times \prod_{i=1}^{K} \Gamma(n_{m,(.)}^{i,-(m,n)} + \alpha_k)$
  $$\times \frac{n_{(.),v}^{k,-(m,n)} + \beta_v}{(\sum_{r=1}^{V} n_{(.),r}^{k,-(m,n)} + \beta_r)} \times (n_{m,(.)}^{k,-(m,n)} + \alpha_k)$$
    - Absolved the $i = k$ case in to the large operator of multiplications
    - The topic assignment count used for the large multiplication is same to the assignment of any **k** on the word assignment of $\boldsymbol{Z_{(m,l)}}$
    - Therefore, only the meaningful proportion is the separated single multiplications

- $P\left(Z_{(m,l)} = k \middle| Z_{-(m,l)}, W; \alpha, \beta\right) \propto \frac{n_{(.),v}^{k,-(m,n)} + \beta_v}{(\sum_{r=1}^{V} n_{(.),r}^{k,-(m,n)} + \beta_r)} \times (n_{m,(.)}^{k,-(m,n)} + \alpha_k)$
  - Finally, this formula is simplified enough to calculate the likelihood of assigning $\boldsymbol{k}$ to $\boldsymbol{Z_{(m,l)}}$
  - To become a probability, we need to normalize the above formula.

LDA Model Parameter Inference Routine with Gibbs

- LDA(TextCorpus T, α, β)
  - Randomly, initialize Z assignment on T
  - Count $n_{j,r}^{i}$ with the initial Z assignment
  - While performance measure (i.e. perplexity) converges
    - For **m** = 1 to T's document number
      - For **l** = 1 to T_m's document word length
        - Sampling **k** from $P\left(Z_{(m,l)} = k \middle| Z_{-(m,l)}, W; \alpha, \beta\right) \propto \frac{n_{(.),v}^{k,-(m,n)} + \beta_v}{\left(\sum_{r=1}^{V} n_{(.),r}^{k,-(m,n)} + \beta_r\right)} \times \left(n_{m,(.)}^{k,-(m,n)} + \alpha_k\right)$
        - Adjust $\boldsymbol{n_{j,r}^{i}}$ by assigning $\boldsymbol{Z}_{(\boldsymbol{m},\boldsymbol{l})} = \boldsymbol{k}$
  - Calculate the most likely estimation on $\boldsymbol{\theta}$ and $\boldsymbol{\varphi}$
  - Return $\boldsymbol{\theta}$ and $\boldsymbol{\varphi}$

- Note
  - θ represents the document-topic probability
  - φ represents the topic-word probability
  - Perplexity is the measurement on the quality of the soft-clustering, and calculating it may take some time. Hence, many cases, we just set the iteration number.