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Particle-Based Approximate Inference

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➤ 临渊羡鱼，不如退而结网。——《汉书》

➤ 当局者迷，旁观者清。——《旧唐书》



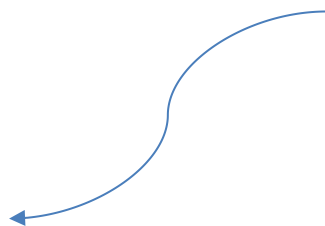
- ✓ Motivation
- ✓ Some Basic Methods
 1. Naive Sampling/Forward Sampling
 2. Rejection Sampling
 3. Importance Sampling
 - 3.1 Unnormalized Importance Sampling
 - 3.2 Normalized Importance Sampling
 - 3.2.1 Likelihood Weighting
- ✓ MCMC(Markov Chain Monte Carlo)
 1. MCMC
 2. Gibbs Sampling



01 Motivation

- Representation, Learning, Inference

Inference: response to queries (what we want to know)



- $P(z|e)$
- $E(f(z))$

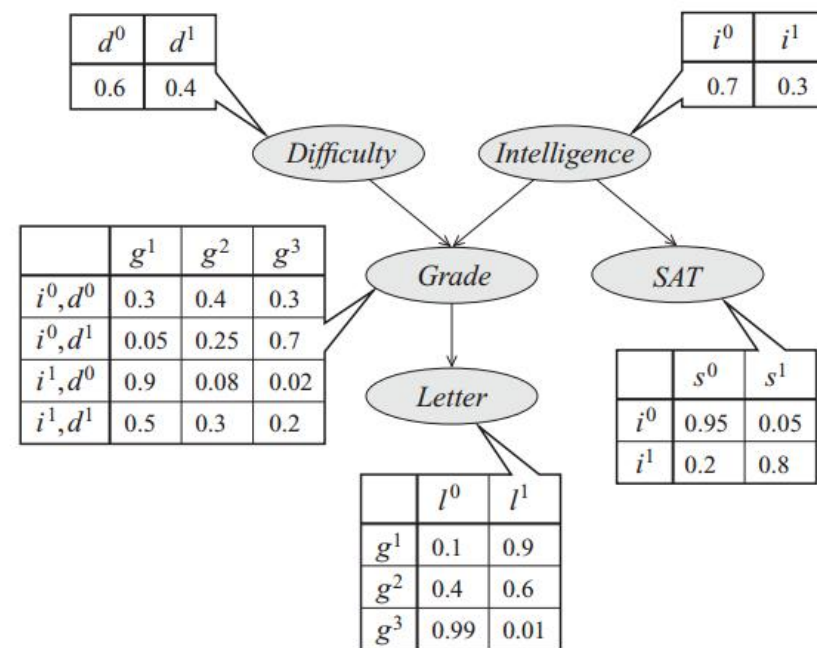
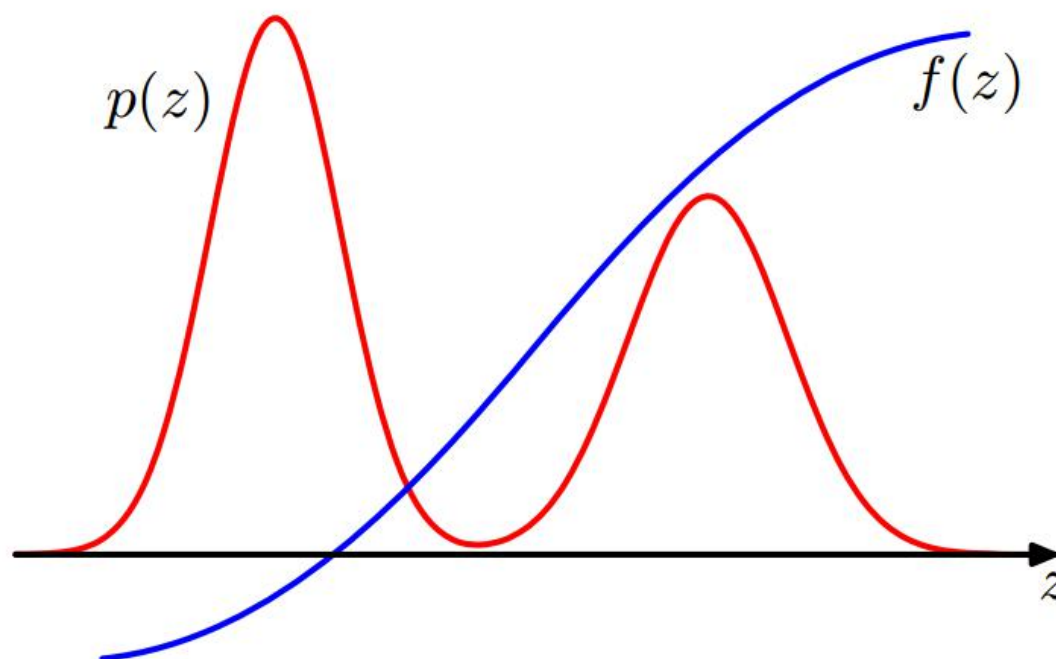


Figure 1: Student Bayesian network $B_{student}$ with CPDs

From a high level, it appears that **sampling methods are the ultimate general-purpose inference algorithm**. They are the **only** method that can be applied to **arbitrary probabilistic models** and that is guaranteed to **achieve the correct results at the large sample limit**.



- How to sample?

In most case, we want to find $E(f(z)) = \int f(z)p(z)dz$

- We draw samples $\{z^i\}_M$ from $f(z)$ i.i.d.

And we set

$$E(\hat{f}(z)) = \frac{1}{M} \sum_{i=1}^M f(z^i)$$



$$\hat{P}_D(z) = \frac{1}{M} \sum_{i=1}^M I(z^m = z)$$

- Why sampling work?
 - Hoeffding bound:

$$P_D(\hat{P}_D(z) \notin [P(z) - \varepsilon, P(z) + \varepsilon]) \leq 2e^{-2M\varepsilon^2} \leq \delta$$



$$M \geq \frac{\ln(2/\delta)}{2\varepsilon^2}$$

- Common transformation:

Target: generate random numbers from simple nonuniform distribution.

- Method(Transformation technique):

given $z \sim Uniform(0, 1)$ using some function $f(\cdot)$ to transform z so that $y = f(z)$

➡ the distribution of y is: $p(y) = p(z) \left| \frac{dz}{dy} \right|$

➡ $p(z) = 1$ $z = h(y) = \int_{-\infty}^y p(\hat{y}) d\hat{y}$

➡ $y = h^{-1}(z) = f(z)$

- One example:

draw samples from exponential distribution

$$p(y) = \lambda \exp(-\lambda y) \quad 0 \leq \lambda < \infty$$



$$h(y) = 1 - \exp(-\lambda y)$$



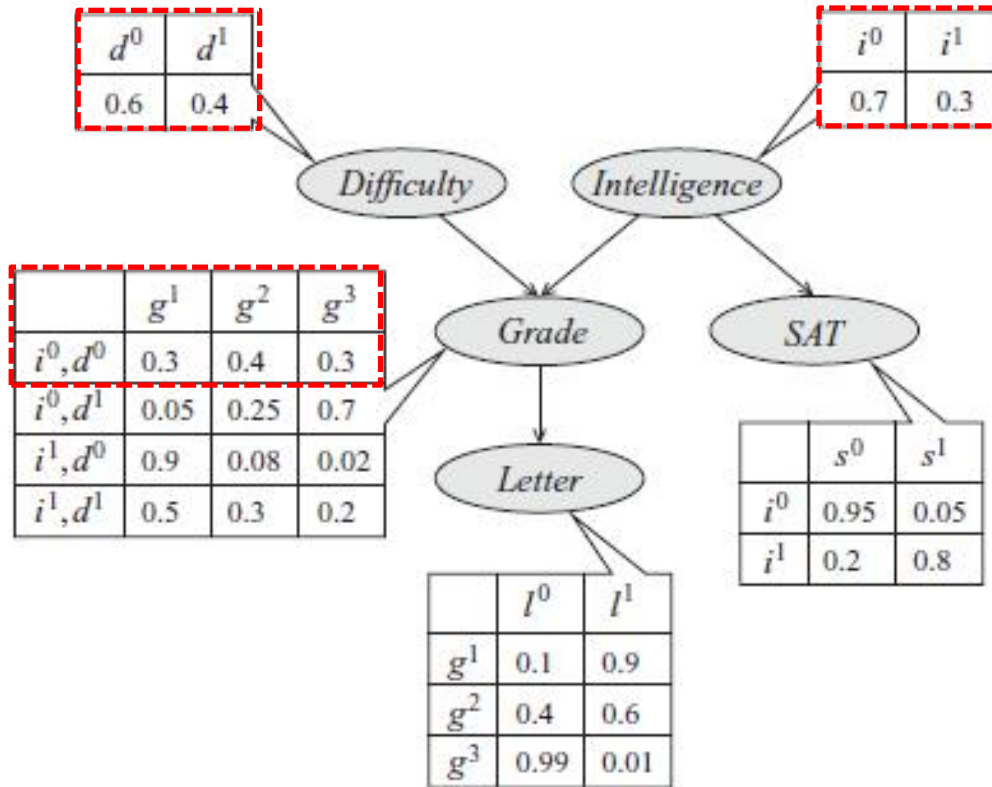
$$y = -\lambda^{-1} \ln(1 - z)$$

Thus, if we transform the uniformly distributed variable z using $y = -\lambda^{-1} \ln(1 - z)$, then y will have an exponential distribution.



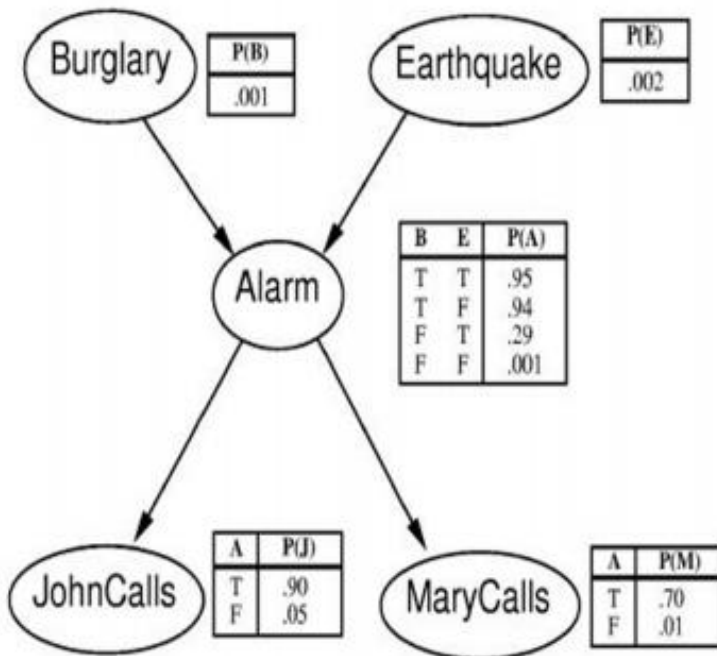
2 Some Basic Methods

- In the BN:



- First, figuratively toss a coin to draw the sample from D. Assume we get d^0 .
- Similarly, toss a coin to draw the sample from I. Assume we get i^0 .
- Then we sample for G given d^0 and i^0 .
- The process continues similarly for S and L.

- The problems:
 - Apply (at least in their simple form) only to Bayesian networks, in undirected models, even generating a sample from the prior distribution is a difficult task.
 - For a model with hundreds or more variables, rare events will be very hard to gain enough samples even after a long time for sampling.



| | | | | |
|----|----|----|----|----|
| E0 | B0 | A0 | M0 | J0 |
| E0 | B0 | A0 | M0 | J0 |
| E0 | B0 | A0 | M0 | J1 |
| E0 | B0 | A0 | M0 | J0 |
| E0 | B0 | A0 | M0 | J0 |
| E0 | B0 | A0 | M0 | J0 |
| E0 | B0 | A0 | M0 | J0 |
| E1 | B0 | A1 | M1 | J1 |
| E0 | B0 | A0 | M0 | J0 |
| E0 | B0 | A0 | M0 | J0 |
| E0 | B0 | A0 | M0 | J0 |
| E0 | B0 | A0 | M0 | J0 |

$$P(J|B1) = P(J, B1) / P(B1)$$

can not defined

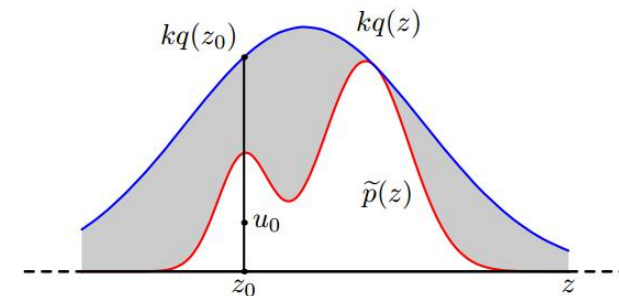
- Suppose we wish to sample from :

$$p(x) = p'(x)/\alpha$$

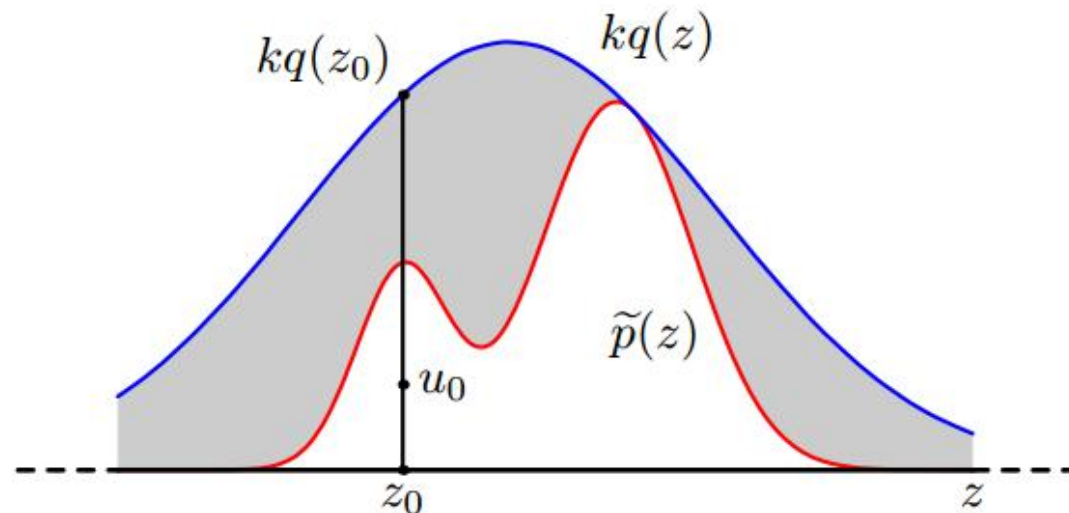
- It's common that $p(x)$ is difficult to sample or even to compute, But $p'(x)$ is easy to evaluate. $p(x)$ is often called the **target distribution**.

- Sample from a simple distribution $q(x)$, known as the **proposal distribution**.

- Introduce a constant k who guarantees that $kq(z) \geq \tilde{p}(z)$ for all values of z .

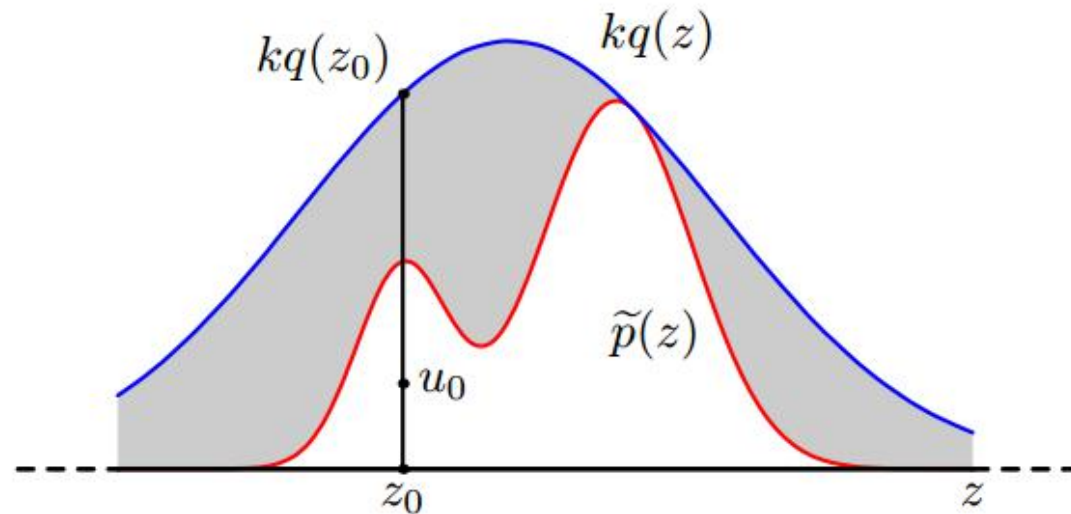


- Three steps for each sample:
 - First, generate a number z_0 from the distribution $q(z)$.
 - Next, generate a number u_0 from the uniform distribution over $[0, kq(z_0)]$.
 - Finally, if $u_0 > \tilde{p}(z_0)$ then the sample is rejected, otherwise z_0 is retained.

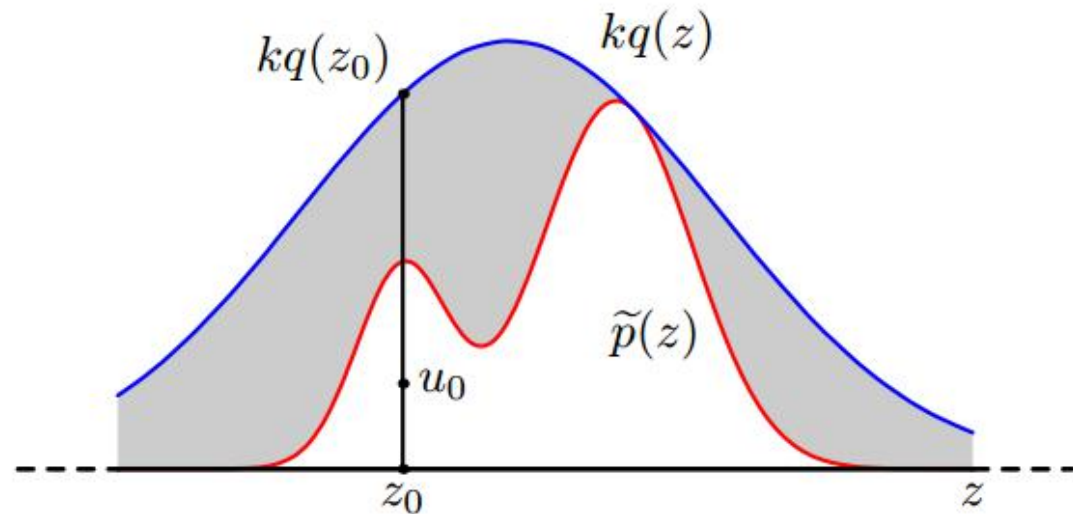


- Correctness:

$$\begin{aligned} p_D(z) &\propto \frac{[p'(z)/k q(z)]q(z)}{\int [p'(z)/k q(z)]q(z)dx} \\ &= \frac{p'(z)}{\int p'(z)dx} \\ &= p(z) \end{aligned}$$



- Drawbacks:
 - In low dimensions, the shape of $p'(x)$ and $q(x)$ need to be similar with each other, otherwise we will reject lots of samples.
 - In high dimensions, even if the shapes of these two distributions are similar, the rejection rate is really high. (leave out the proof)

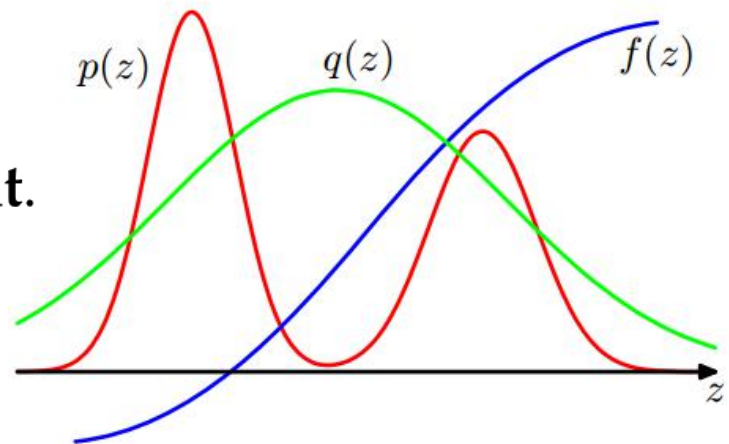


- Suppose sampling from $P(x)$ is hard, but we can sample from a simpler proposal distribution $Q(x)$.
- If Q dominates P (i.e., $Q(x) > 0$ whenever $P(x) > 0$), the procedure to compute $E(f(x))$ is:

- Sample $x^m \sim Q(x)$ for $m = 1, 2, 3, \dots, M$

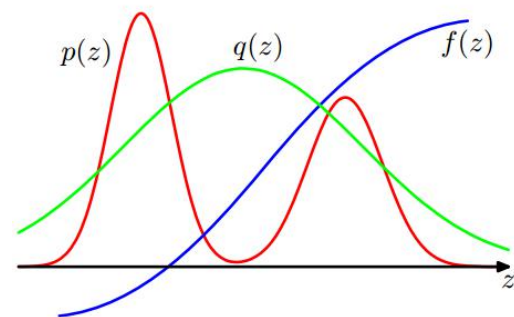
- Compute $\hat{f} = \frac{1}{M} \sum_{m=1}^M f(x^m) \frac{P(x^m)}{Q(x^m)}$

$\frac{P(x^m)}{Q(x^m)}$ is known as **importance weight**.



- Claim: \hat{f} is an unbiased estimator of $\mathbb{E}_P[f(x)]$:

$$\begin{aligned}\mathbb{E}_Q[\hat{f}] &= \mathbb{E}_Q\left[\frac{1}{M} \sum_{m=1}^M f(x^m) \frac{P(x^m)}{Q(x^m)}\right] \\ &= \frac{1}{M} \sum_{m=1}^M \mathbb{E}_Q\left[f(x^m) \frac{P(x^m)}{Q(x^m)}\right] \\ &= \mathbb{E}_{x \sim Q}\left[f(x) \frac{P(x)}{Q(x)}\right] \quad \text{as } x^m \text{ are i.i.d drawn from } Q \\ &= \int f(x) \frac{P(x)}{Q(x)} Q(x) dx \\ &= \int f(x) P(x) dx \\ &= \mathbb{E}_P[f(x)]\end{aligned}$$



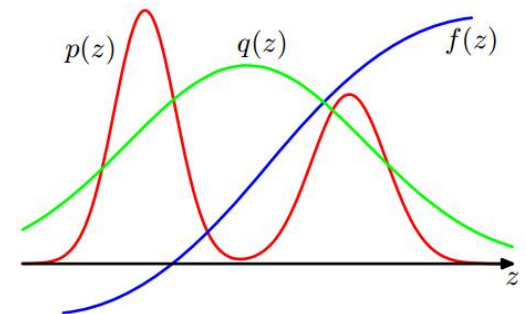
- Suppose we can only evaluate $P'(x) = \alpha P(x)$ for some unknown scaling factor $\alpha > 0$. (e.g. for an MRF)
- We can eliminate the nasty normalization constant α as follows:

- Let $r(x) = \frac{P'(x)}{Q(x)}$

➔
$$\mathbb{E}_Q[r(x)] = \mathbb{E}_Q\left[\frac{P'(x)}{Q(x)}\right] = \int \frac{P'(x)}{Q(x)} Q(x) dx = \int P'(x) dx = \alpha$$

↓

$$\hat{\alpha} = \frac{1}{M} \sum_{m=1}^M r(x^m)$$



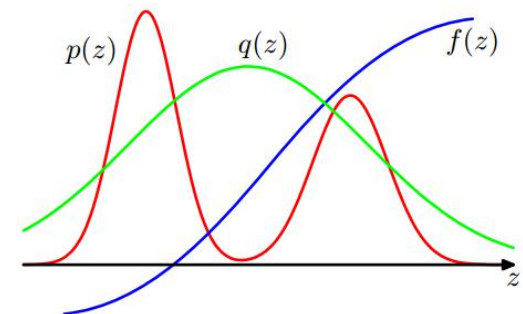
- The procedure to compute $E(f(x))$ is:

- Sample $x^m \sim Q(x)$ for $m = 1, 2, 3, \dots, M$

- Compute scaling factor estimator $\hat{\alpha} = \frac{1}{M} \sum_{m=1}^M r(x^m)$

- Compute

$$\hat{f} = \frac{1}{\hat{\alpha}} \frac{1}{M} \sum_{m=1}^M f(x^m) \frac{P'(x^m)}{Q(x^m)} = \frac{\sum_{m=1}^M f(x^m) r(x^m)}{\sum_{m=1}^M r(x^m)}$$



- Correctness:

$$P(x) = \frac{P'(x)}{\alpha}$$

$$E_P(f(x)) = \int f(x)P(x)dx = \frac{1}{\alpha} \int f(x) \frac{P'(x)}{Q(x)} Q(x)dx$$

$$= \frac{\int f(x) r(x) Q(x)dx}{\int r(x) Q(x)dx}$$

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

$$\alpha = \int r(x) Q(x)dx$$

$$\frac{1}{M} \approx \frac{\sum_m f(x^m) r^m}{\sum_m r^m}$$

where $x^m \sim Q(x)$

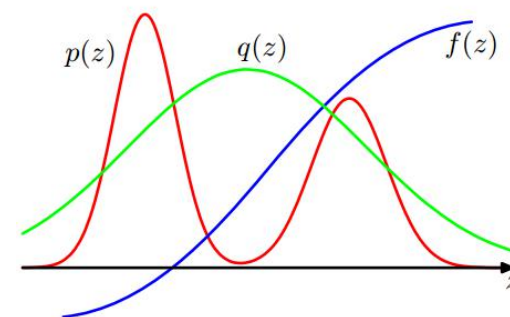
$$= \sum_m f(x^m) w^m \quad \text{where } w^m = \frac{r^m}{\sum_m r^m}$$

- Claim: Normalized importance sampling is biased.

To show this, suppose we sampled only once, that is, $M = 1$:

$$\hat{f} = \frac{f(x_1)r(x_1)}{r(x_1)} = f(x_1)$$

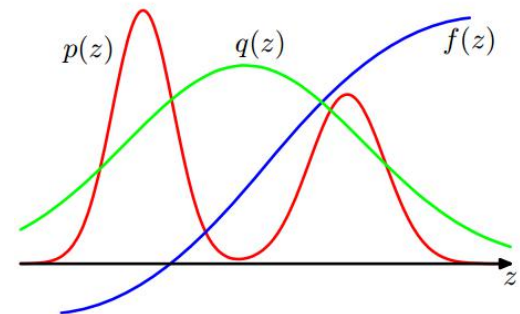
$$\mathbb{E}_Q[\hat{f}] = \mathbb{E}_Q[f(x_1)] \neq \mathbb{E}_P[f(x_1)] \text{ in general}$$



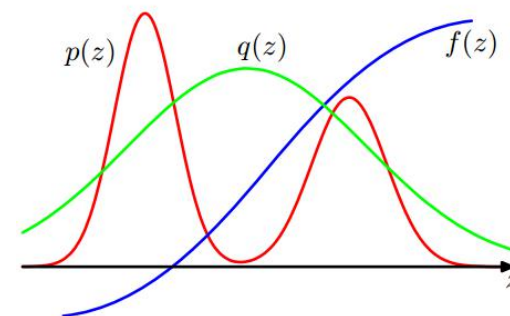
Unnormalized vs Normalized Importance Sampling



- Bias: Unnormalized importance sampling is unbiased, but normalized importance sampling is biased.
- Variance: in practice, the variance of the estimator in the unnormalized case is usually higher than that in the normalized case.
- Requirement : Unnormalized importance sampling need to calculate $P(x)$, however, it is common to have $P'(x)$ available instead of $P(x)$.



- The success of this approach depends crucially on how well the sampling distribution $Q(x)$ matches the desired distribution $P(x)$. As is often the case, $P(x)f(x)$ is strongly varying and has a significant proportion of its mass concentrated over relatively small regions of x space, then the set of importance weights may be dominated by a few weights having large values, with the remaining weights being relatively insignificant. Thus the effective sample size can be much smaller than the apparent sample size M .



- Normalized importance sampling is applied in the Bayes net.
 - The proposal distribution $Q(x)$ (suppose we have gotten the evidence $e = \{I = i^1 \text{ and } G = g^2\}$):

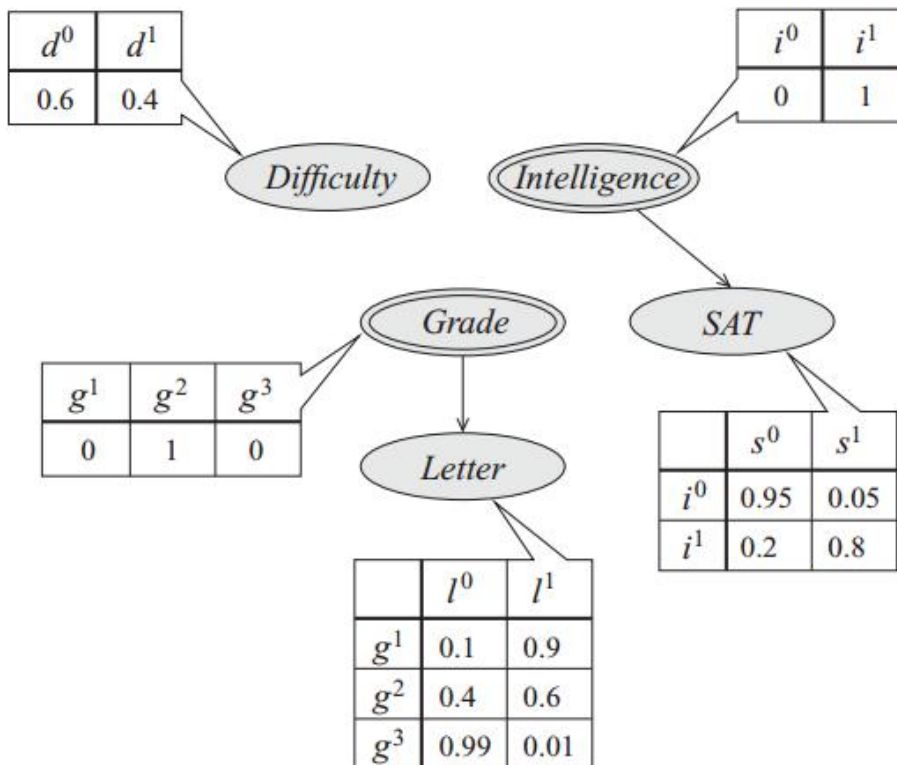


Figure 2: the mutilated(多片段) network

- Define $P'(D, S, L|e) = \frac{P(D, S, L, e)}{P(e)}$ to be the density of the mutilated network.
- But sometimes it's difficult to evaluate $\frac{P'(x) = P(x, e)}{P(e)}$ so that

$$P(x|e) = \frac{P(x, e)}{P(e)} = \frac{P'(x)}{P(e)}$$

- Based on the idea of normalized importance sampling, compute:

$$\hat{P}(X_i = x_i|e) = \frac{\sum_{m=1}^M I(x_i^m)r(x^m)}{\sum_{m=1}^M r(x^m)}$$

where $r(x^m) = \frac{P'(x^m)}{P_M(x^m)}$

- how to calculate $r(x^m) = \frac{P'(x^m)}{P_M(x^m)}$?

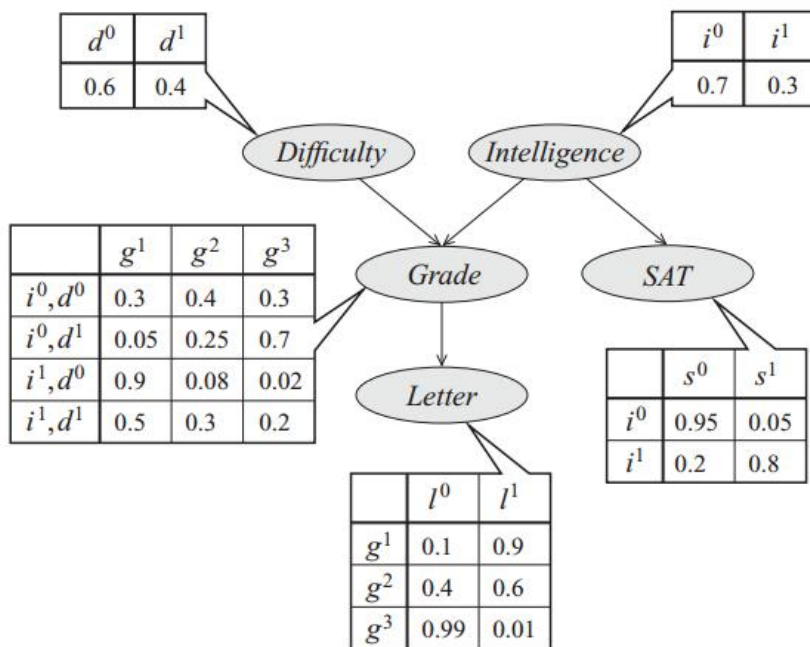


Figure 3: the original network

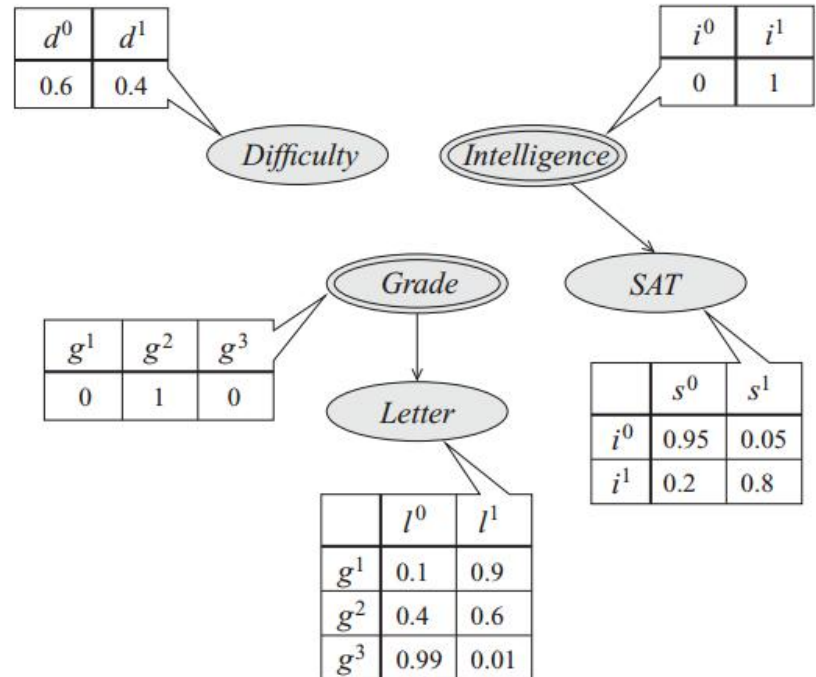


Figure 4: the mutilated network

$$r(x^m) = P'(x^m) / P_M(x^m)$$

$$P(D, I, G, S, L) = P(D)P(I)P(G|D, I)P(S|L)P(L|G)$$

$$P(D, S, L) = P(D)P(S|I)P(L|G)$$

Thus

$$r(x^m) = P(I)P(G|D, I)$$

Algorithm 12.2 Likelihood-weighted particle generation

Procedure LW-Sample (

\mathcal{B} , // Bayesian network over \mathcal{X}

$Z = z$ // Event in the network

)

1 Let X_1, \dots, X_n be a topological ordering of \mathcal{X}

2 $w \leftarrow 1$

3 **for** $i = 1, \dots, n$

4 $\mathbf{u}_i \leftarrow \mathbf{x}\langle \text{Pa}_{X_i} \rangle$ // Assignment to Pa_{X_i} in x_1, \dots, x_{i-1}

5 **if** $X_i \notin Z$ **then**

6 Sample x_i from $P(X_i | \mathbf{u}_i)$

7 **else**

8 $x_i \leftarrow z\langle X_i \rangle$ // Assignment to X_i in z

9 $w \leftarrow w \cdot P(x_i | \mathbf{u}_i)$ // Multiply weight by probability of desired value

10 **return** $(x_1, \dots, x_n), w$

LW indicates that the weights of different samples are derived from the likelihood of the evidence accumulated throughout the sampling process.

不同样本的权重来自于采样过程中累积的证据的似然

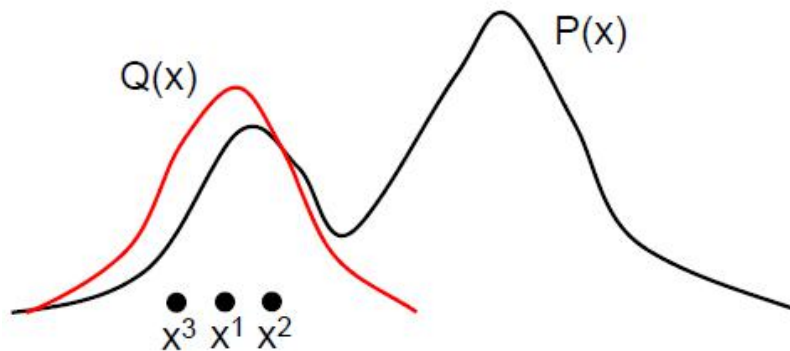


03 MCMC

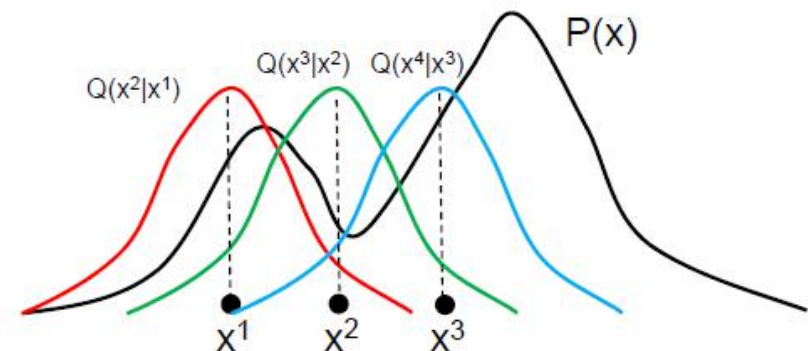
• Intuition:

- Instead of $Q(x)$, we 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 $Q(x'|x)$

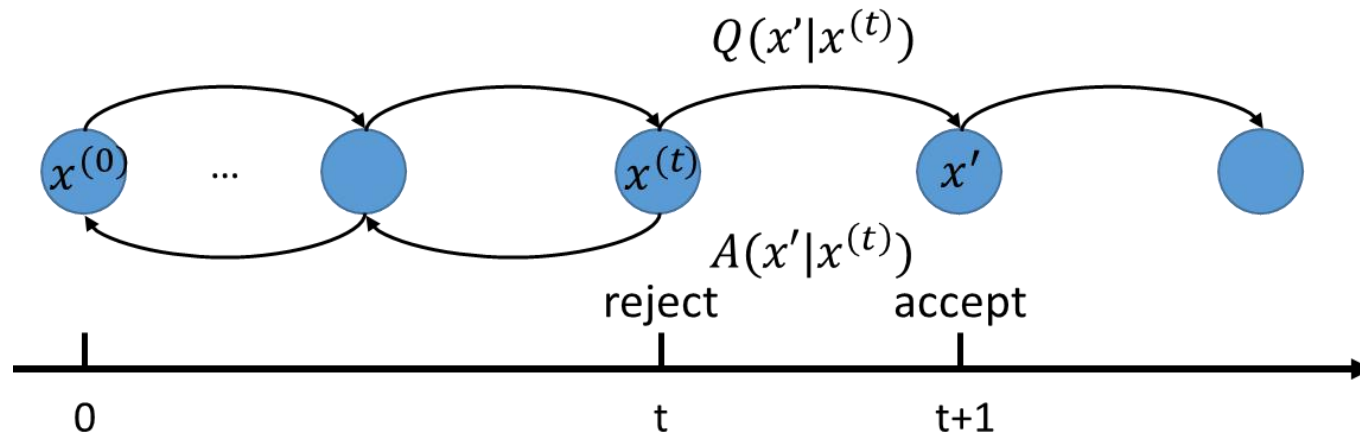


- Metropolis-Hastings(MH) Algorithm:

1. Initialize the starting state $x^{(t)}$ at $t = 0$.
2. Draws a sample x' from the proposal $Q(x'|x^{(t)})$. Note that this proposal is now a function of the previously drawn sample $x^{(t)}$ (at time step t).
3. The new sample x' is accepted with the probability:

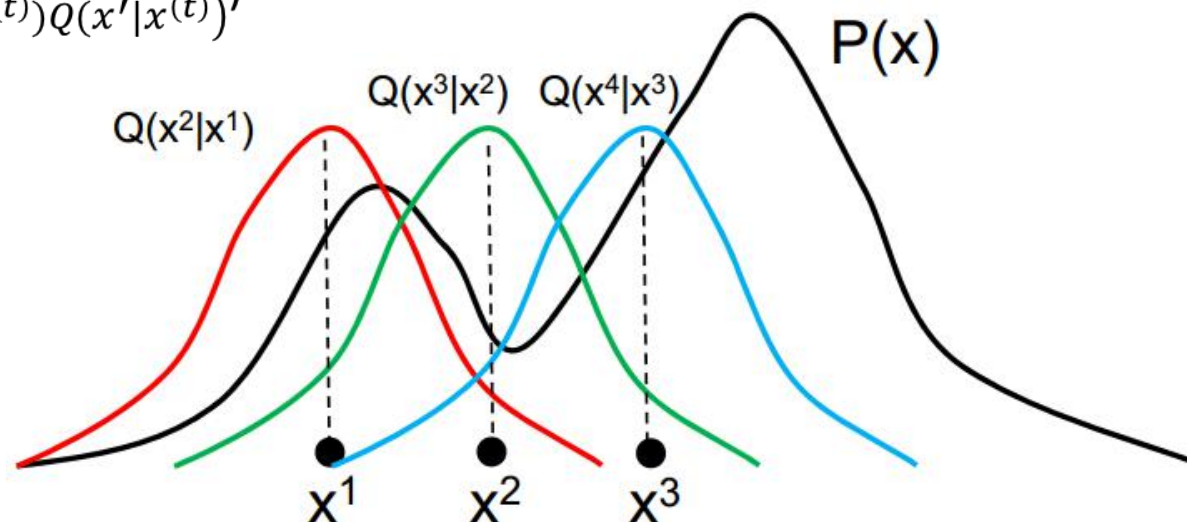
$$A(x'|x^{(t)}) = \min\left(1, \frac{P(x')Q(x^{(t)}|x')}{P(x^{(t)})Q(x'|x^{(t)})}\right)$$

4. Repeat steps 2 and 3 until the samples “converge”.



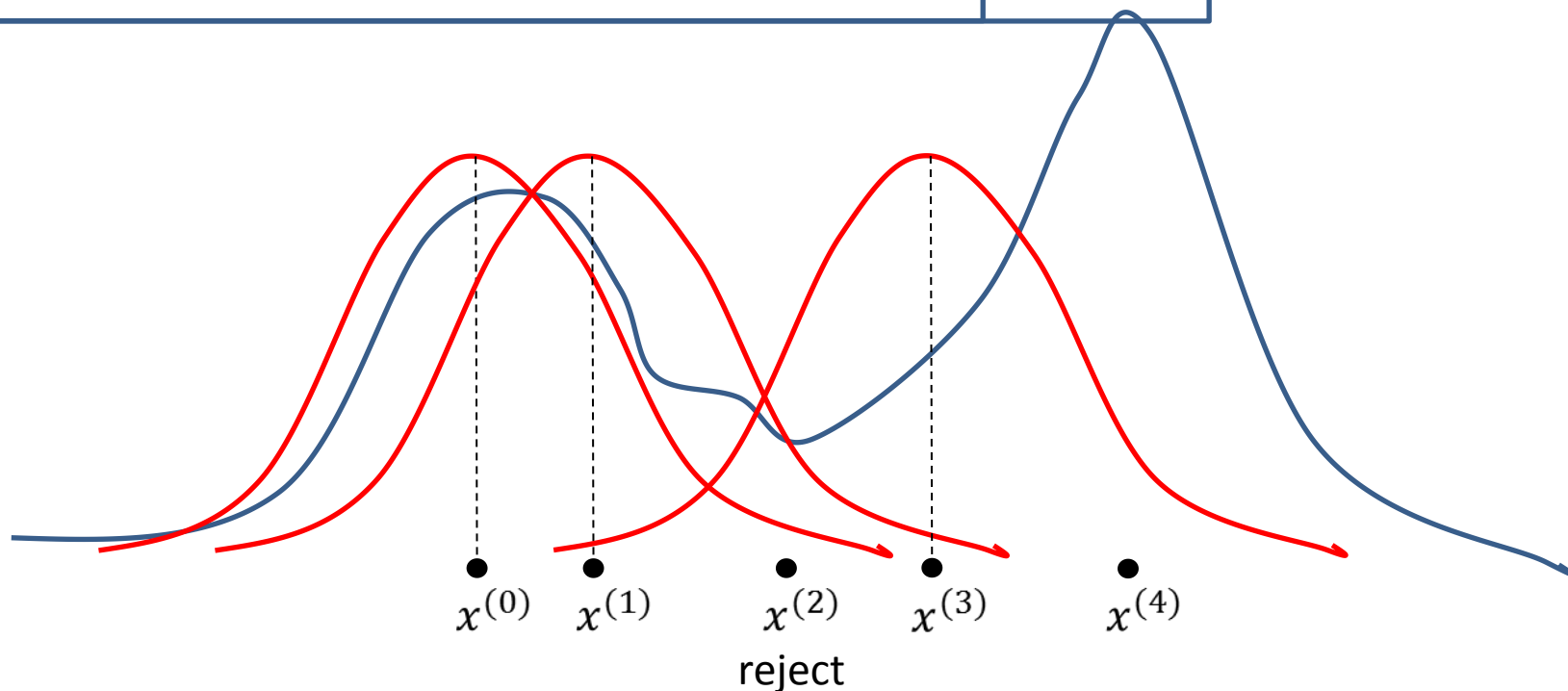
- Note that because P is in both the numerator and denominator, we can use the unnormalized P' and there is no need to find the partition function α .
- The acceptance probability $A(x'|x^{(t)})$ is like a ratio of importance sampling weights. $P(x')/Q(x'|x^{(t)})$ is the importance weight for x' , $P(x^{(t)})/Q(x^{(t)}|x')$ is the importance weight for $x^{(t)}$. So it just like that We divide the importance weight for x' by that of x .

$$A(x'|x^{(t)}) = \min\left(1, \frac{P(x')Q(x^{(t)}|x')}{P(x^{(t)})Q(x'|x^{(t)})}\right)$$



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

When adaptive proposal $Q(x^{(2)}|x^{(1)})$ allows us to sample $Q(x^{(1)}|x^{(2)}) > 1$,
 hence $A(x^{(2)}|x^{(1)})$ is close to zero

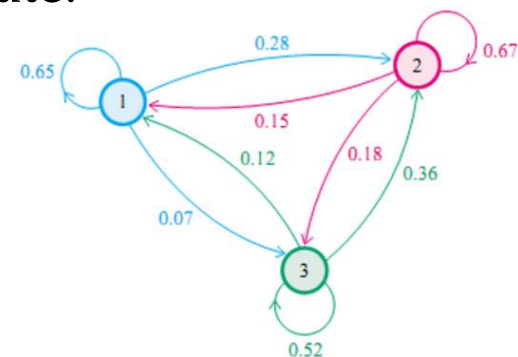


- MC(Markov Chain) concepts:

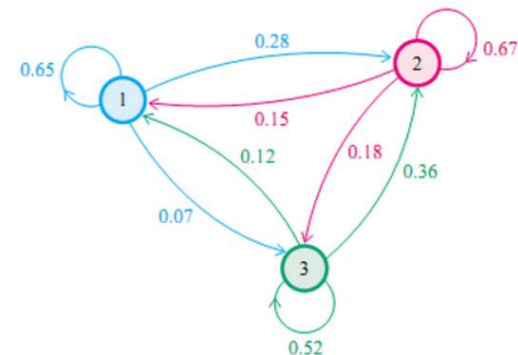
- A Markov Chain is a sequence of random variables $x^{(1)}, x^{(2)}, \dots, x^{(n)}$ with the Markov Property:

$$P(x^{(n)} = x | x^{(1)}, x^{(2)}, \dots, x^{(n-1)}) = P(x^{(n)} = x | x^{(n-1)})$$

- $x^{(i)}$ is the i -th sample of **all** variables in a graphical model.
- $x^{(i)}$ represents **the entire state** of the graphical model at time i .
- $P(x^{(n)} = x | x^{(n-1)})$ is known as the **transition kernel**.
- The next state depends only on the preceding state.



- We study homogeneous Markov Chains, in which the transition kernel $P(x^{(n)} = x | x^{(n-1)})$ is fixed with time:
 - For convenience, we call the kernel $T(x' | x)$, where x is the previous state and x' is the next state.
- When dealing with MCs, we don't think of the system as being in one state, but as having a distribution over states.
 - Probability distributions over states: $\pi^{(t)}(x)$ is a distribution over the state of the model, at time t .

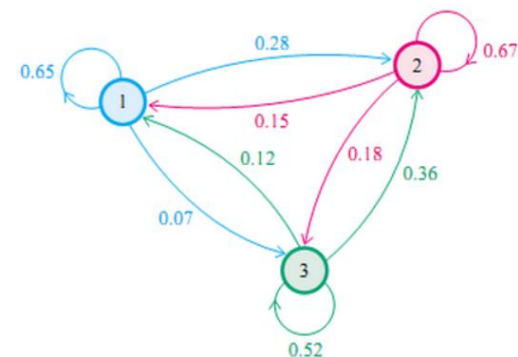


- Transitions: recall that states transition from $x^{(t)}$ to $x^{(t+1)}$ according to the transition kernel $T(x'|x)$. We can also transition entire distributions:

$$\Pi^{(t+1)}(x') = \sum_x \Pi^{(t)}(x) T(x'|x) \quad \text{for all } x'$$

- **Stationary distributions**: is stationary if it does not change under the transition kernel:

$$\Pi(x') = \sum_x \Pi(x) T(x'|x) \quad \text{for all } x'$$



- Stationary distributions are of great importance in MCMC. To understand them, we need to define some notions:
 - **Irreducible(不可约)**: 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.
 - **Aperiodic(非周期)**: an MC is aperiodic if you can return to any state x at any time.
 - **Ergodic(遍历)**: 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 $\pi^{(0)}(x)$.

- **Reversible(可逆)/Detailed balance(细致平稳)**: an MC is reversible if there exists a distribution such that the detailed balance condition is satisfied:

$$\Pi(x')T(x|x') = \Pi(x)T(x'|x)$$

- **Reversibility** guarantees to have a **Stationary distribution**:

$$\Pi(x')T(x|x') = \Pi(x)T(x'|x)$$

$$\sum_x \Pi(x')T(x|x') = \sum_x \Pi(x)T(x'|x)$$

$$\Pi(x') \sum_x T(x|x') = \sum_x \Pi(x)T(x'|x)$$

$$\Pi(x') = \sum_x \Pi(x)T(x'|x)$$

- Back to MH algorithm

- The proposal $Q(x'|x)$ keeps changing with the value of x ; how do we know the samples will eventually come from $P(x)$?
 - Recall that we draw a sample x' according to $Q(x'|x)$, and then accept/reject according to $A(x'|x)$.

Thus here the transition kernel is

$$T(x'|x) = Q(x'|x)A(x'|x)$$

- We can prove that MH algorithm satisfies detailed balance:

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

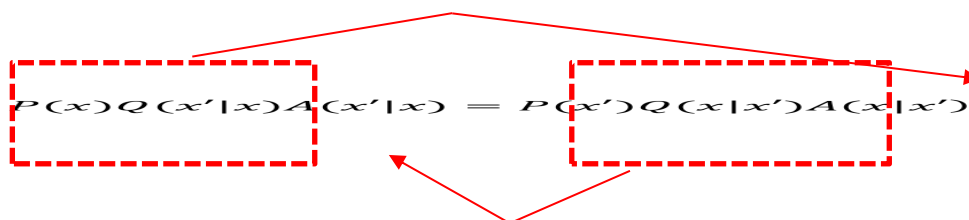
- This implies that:

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:

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

$$P(x)Q(x'|x)A(x'|x) = P(x')Q(x|x') \cdot 1$$



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

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

The structure of $A(x'|x)$ is derived from this line!

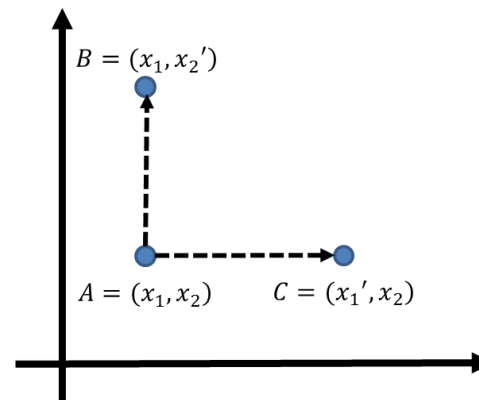
- The last line is the detailed balance condition.
- Thus, the MH algorithm eventually converges to the target distribution $P(x)$!

- In the high dimension level, the acceptance rate in MH is still not high enough, so can we find a transition matrix to directly make the acceptance rate $A(x'|x) = 1$?
- Gibbs sampling is a special case of the MH method where the proposal distributions are tractable conditional distributions on $P(x)$, which can achieve the above goal.
 - The idea is here:
 1. Suppose in a two dimensional space, here are three points:

$$A = (x_1, x_2)$$

$$B = (x_1, x_2')$$

$$C = (x_1', x_2)$$



2. We find that:

- For points A and B

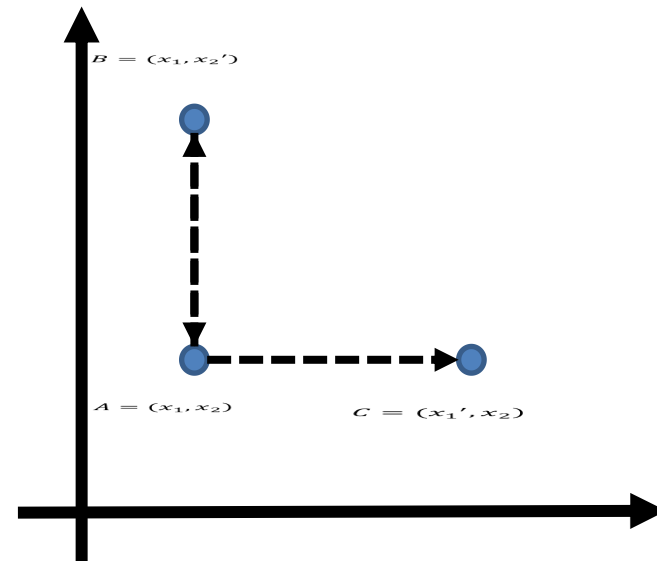
$$P(x_1, x_2)P(x_2'|x_1) = P(x_1)P(x_2|x_1)P(x_2'|x_1)$$

$$P(x_1, x_2')P(x_2|x_1) = P(x_1)P(x_2'|x_1)P(x_2|x_1)$$

➔ $P(x_1, x_2)P(x_2'|x_1) = P(x_1, x_2')P(x_2|x_1)$

➔ $P(A)P(x_2'|x_1) = P(B)P(x_2|x_1)$

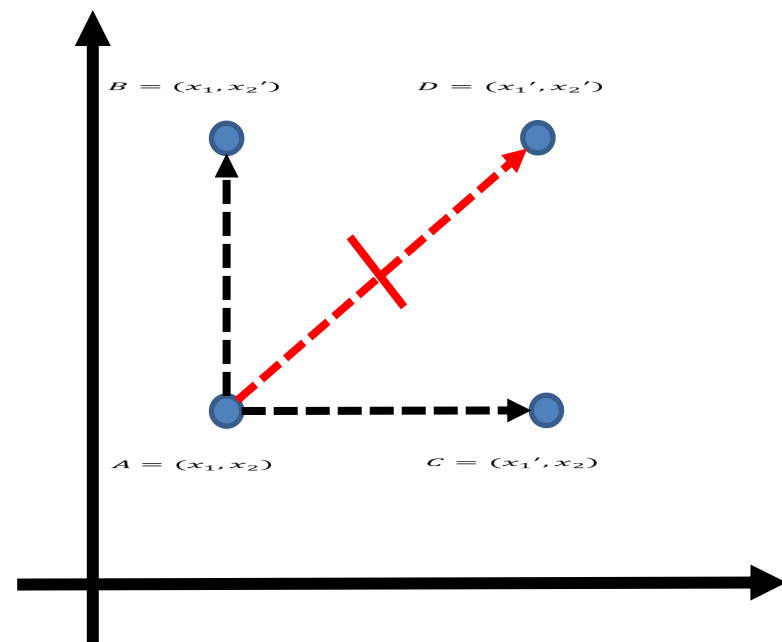
Similarly $P(A)P(x_1'|x_2) = P(C)P(x_1|x_2)$



3. Thus we can build the transition matrix:

$$\left\{ \begin{array}{ll} Q(A \rightarrow B) = P(x_2 | x_1) & \text{if } x_1(A) = x_1(B) = x_1 \\ Q(A \rightarrow C) = P(x_1 | x_2) & \text{if } x_2(A) = x_2(C) = x_2 \\ Q(A \rightarrow D) = 0 & \text{otherwise} \end{array} \right.$$

- It's easy to see that this transition matrix satisfies the detailed balance condition. So it will lead to the stationary distribution.
- Gibbs sampling 是一个“多重转移模型” (Multiple Transition Models), 每一个核就是延一个坐标轴的转移, 单个核不足以保证马尔科夫链的遍历性, 但多核则可以使其收敛于稳定分布。每次我们随机或轮转选择其中一个核。



- The pseudocode:

Algorithm 8 n维Gibbs Sampling 算法

1: 随机初始化 $\{x_i : i = 1, \dots, n\}$

2: 对 $t = 0, 1, 2, \dots$ 循环采样

1. $x_1^{(t+1)} \sim p(x_1 | x_2^{(t)}, x_3^{(t)}, \dots, x_n^{(t)})$

2. $x_2^{(t+1)} \sim p(x_2 | x_1^{(t+1)}, x_3^{(t)}, \dots, x_n^{(t)})$

3. ...

4. $x_j^{(t+1)} \sim p(x_j | x_1^{(t+1)}, \dots, x_{j-1}^{(t+1)}, x_{j+1}^{(t)}, \dots, x_n^{(t)})$

5. ...

6. $x_n^{(t+1)} \sim p(x_n | x_1^{(t+1)}, x_2^{(t)}, \dots, x_{n-1}^{(t+1)})$

- We will show the Gibbs sampling is a particular case of MH method, whose acceptance rate is 1.
 - Define x_i to be the i -th element of the feature vector x and x_{-i} to be all other elements. Gibbs sampling let

$$Q(x'|x) = Q(x_i', x_{-i} | x_i, x_{-i}) = P(x_i' | x_{-i})$$

- Then

$$\begin{aligned} A(x_i', x_{-i} | x_i, x_{-i}) &= \min\left(1, \frac{P(x_i', x_{-i})Q(x_i, x_{-i} | x_i', x_{-i})}{P(x_i, x_{-i})Q(x_i', x_{-i} | x_i, x_{-i})}\right) \\ &= \min\left(1, \frac{P(x_i', x_{-i})P(x_i | x_{-i})}{P(x_i, x_{-i})P(x_i' | x_{-i})}\right) \\ &= \min\left(1, \frac{P(x_i' | x_{-i})P(x_{-i})P(x_i | x_{-i})}{P(x_i | x_{-i})P(x_{-i})P(x_i' | x_{-i})}\right) \\ &= \min(1, 1) = 1 \end{aligned}$$

- It can be hard to move from one high probability space to another across a low probability space.
- The samples are not independent with each other truly, especially in Gibbs sampling. How to determine how two samples are “far enough” to be considered independent draws.
- Although MH algorithm will converge to the true distribution, with certain exceptions, there are no guarantees to when. In fact, it's an art to decide when to stop the algorithm.
-

More Advanced Topics of Particle-Based Methods



- The collapsed particles(坍塌的粒子).
- Deterministic Search Methods(确定性搜索方法).

- Daphne Koller and Nir Friedman. Probabilistic Graphical Models: Principles and Techniques. Ch.12.
- Christopher Bishop, et al. Pattern Recognition And Machine Learning. Ch.11.
- Eric Xin. Probabilistic Graphical Models. Lecture 16, 17, 18.
- rickjin. LDA-math-MCMC and Gibbs Sampling.
<http://cos.name/2013/01/lda-math-mcmc-and-gibbs-sampling/>

Thanks

