Probabilistic graphical models
Exact and approximate inference

22-808: Generative models
Sharif University of Technology
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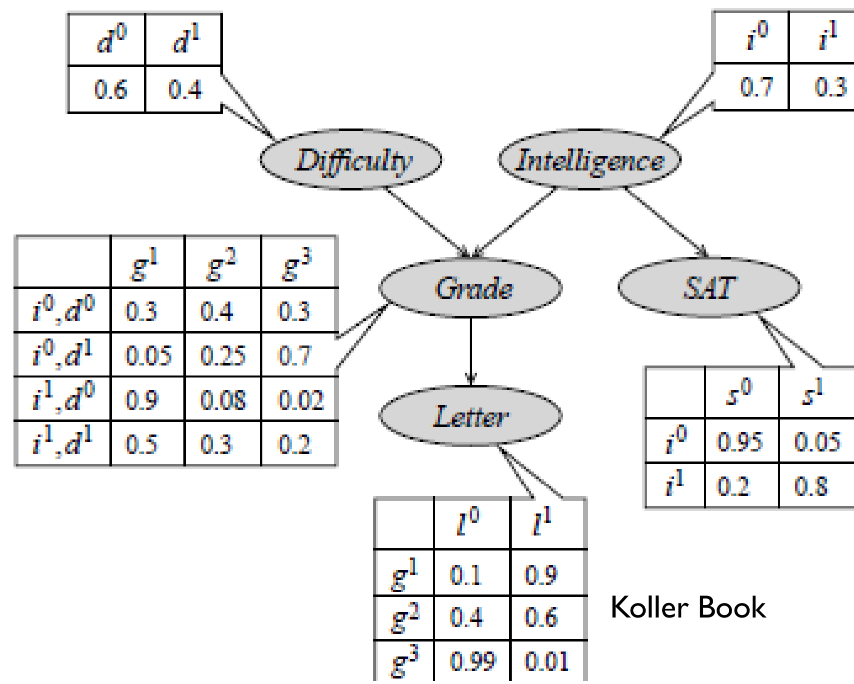
The inference problem

- Inference: answering **conditional or marginal probabilities in a joint distribution**
  - The graph structure and CPDs (in BNs) or potential functions (in MRFs) are known.
- Example:

$$p(Difficulty|Letter = 1) = ?$$
$$p(Letter|Intelligence = 1) = ?$$
$$p(SAT) = ?$$



d^0	d^1
0.6	0.4

i^0	i^1
0.7	0.3

	g^1	g^2	g^3
i^0,d^0	0.3	0.4	0.3
i^0,d^1	0.05	0.25	0.7
i^1,d^0	0.9	0.08	0.02
i^1,d^1	0.5	0.3	0.2

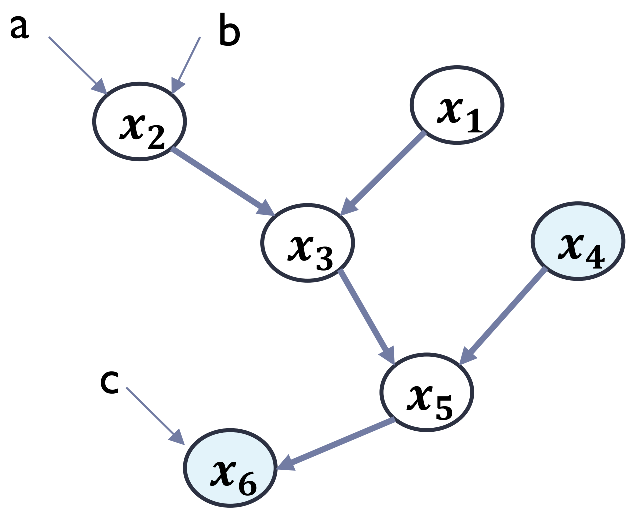
	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

	l^0	l^1
g^1	0.1	0.9
g^2	0.4	0.6
g^3	0.99	0.01

Koller Book

The inference problem

- Notation:
  - Colored nodes: observed random variables
  - White nodes: latent/hidden/unobserved random variables
  - Others not in a circle: parameters of CPDs

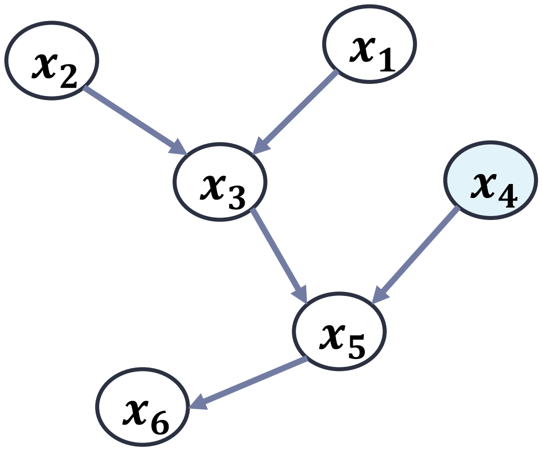


The inference problem

- Consider the following joint distribution

$$p(x_1, x_2, \dots, x_6)$$

over discrete random variables with *k possible* values.



- An inference query:

$$p(x_2 | x_4 = \overline{x_4}) = ?$$

- A naïve solution:

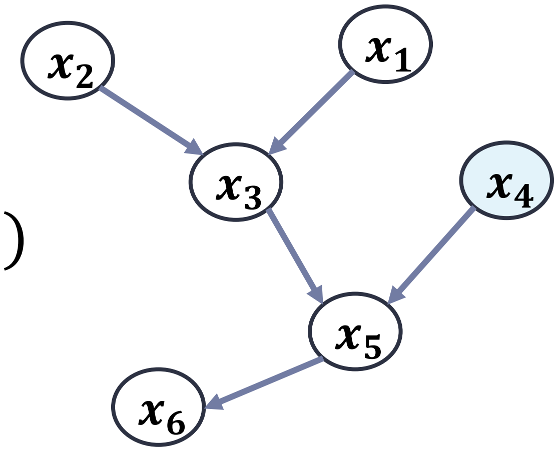
$$p(x_2 | x_4 = \overline{x_4}) = \frac{p(x_2, \overline{x_4})}{\sum_{x_2} p(x_2, \overline{x_4})}$$

$$p(x_2, \overline{x_4}) = \sum_{x_1} \sum_{x_3} \sum_{x_5} \sum_{x_6} p(x_1, x_2, x_3, \overline{x_4}, x_5, x_6)$$

The inference problem

- However, this distribution is factorized

Over this graph and we have:



$$p(x_1, x_2, \dots, x_6) =$$
$$p(x_2)p(x_1)p(x_3|x_1, x_2)p(x_5|x_4, x_3)p(x_6|x_5)$$

- A better solution:

$$p(x_2, \overline{x_4}) = \sum_{x_1}\sum_{x_3}\sum_{x_5}\sum_{x_6} p(x_1, x_2, x_3, \overline{x_4}, x_5, x_6)$$

$$= \sum_{x_1}\sum_{x_3}\sum_{x_5}\sum_{x_6} p(x_2)p(x_1)p(x_3|x_1, x_2)p(x_5|\overline{x_4}, x_3)p(x_6|x_5)$$

The inference problem

- A better solution:

$$p(x_2, \overline{x_4}) = \sum_{x_1}\sum_{x_3}\sum_{x_5}\sum_{x_6} p(x_1, x_2, x_3, \overline{x_4}, x_5, x_6)$$

$$= \sum_{x_1}\sum_{x_3}\sum_{x_5}\sum_{x_6} p(x_2)p(x_1)p(x_3|x_1, x_2)p(x_5|\overline{x_4}, x_3)p(x_6|x_5)$$

- $O(k^4)$ computation !

Distributive law: If $X \notin scope(\phi_1)$ then $\sum_X \phi_1\phi_2 = \phi_1 \sum_X \phi_2$

- Therefore, we can perform summation over the product of only a subset of factors

The inference problem

- A better solution:

$$p(x_2,\overline{x_4}) = \sum_{x_1}\sum_{x_3}\sum_{x_5}\sum_{x_6} p(x_1,x_2,x_3,\overline{x_4},x_5,x_6)$$

$$= \sum_{x_1}\sum_{x_3}\sum_{x_5}\sum_{x_6} p(x_2)p(x_1)p(x_3|x_1,x_2)p(x_5|\overline{x_4},x_3)p(x_6|x_5) =$$

$$p(x_2)\sum_{x_1} p(x_1)\sum_{x_3} p(x_3|x_1,x_2)\sum_{x_5} p(x_5|\overline{x_4},x_3)\sum_{x_6} p(x_6|x_5)$$

- $O(4k^3)$ computation !

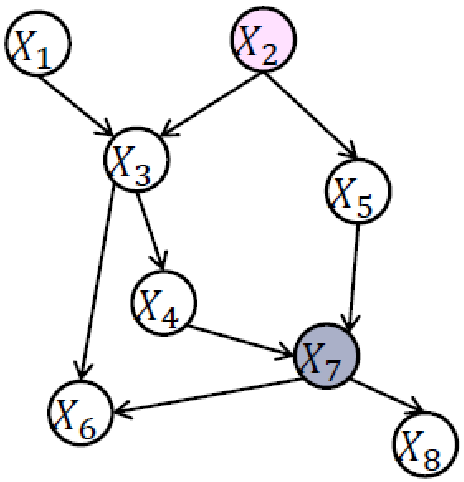
Variable elimination

- Generally, when a distribution is factorized, Variable elimination algorithm can decrease the computational complexity.

- Variable elimination algorithm for exact inference:
  - We select an elimination order of random variables
  - For each random variable, all factors containing that variable are removed from the set of factors and multiplied
  - The selected random variable is summed out from the product of factors and a new factor is obtained
  - The resulted factor is multiplied to others and algorithm is continued.

Exact inference: variable elimination Example

- Query: $P(X_2 | X_7 = \bar{x}_7)$
- $P(X_2 | \bar{x}_7) \propto P(X_2, \bar{x}_7)$



$P(x_2, \bar{x}_7)$

$$= \sum_{x_1} \sum_{x_3} \sum_{x_4} \sum_{x_5} \sum_{x_6} \sum_{x_8} P(x_1, x_2, x_3, x_4, x_5, x_6, \bar{x}_7, x_8)$$

Consider the elimination order $X_1, X_3, X_4, X_5, X_6, X_8$

$P(x_2, \bar{x}_7)$

$$= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} \sum_{x_3} \sum_{x_1} P(x_1) P(x_2) P(x_3 | x_1, x_2) P(x_4 | x_3) P(x_5 | x_2) P(x_6 | x_3, \bar{x}_7) P(\bar{x}_7 | x_4, x_5) P(x_8 | \bar{x}_7)$$

Example from Soleymani pgm-sharif

Exact inference: variable elimination Example

$$P(x_2,\bar{x}_7) = \sum_{x_8}\sum_{x_6}\sum_{x_5}\sum_{x_4}\sum_{x_3} P(x_2)P(x_4|x_3)P(x_5|x_2)P(x_6|x_3,\bar{x}_7)P(\bar{x}_7|x_4,x_5)P(x_8|\bar{x}_7)\sum_{x_1} P(x_1)P(x_3|x_1,x_2)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5}\sum_{x_4}\sum_{x_3} P(x_2)P(x_4|x_3)P(x_5|x_2)P(x_6|x_3,\bar{x}_7)P(\bar{x}_7|x_4,x_5)P(x_8|\bar{x}_7)m_1(x_2,x_3)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5}\sum_{x_4} P(x_2)P(x_5|x_2)P(\bar{x}_7|x_4,x_5)P(x_8|\bar{x}_7)\sum_{x_3} P(x_4|x_3)P(x_6|x_3,\bar{x}_7)m_1(x_2,x_3)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5}\sum_{x_4} P(x_2)P(x_5|x_2)P(\bar{x}_7|x_4,x_5)P(x_8|\bar{x}_7)m_3(x_2,x_6,x_4)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5} P(x_2)P(x_5|x_2)P(x_8|\bar{x}_7)\sum_{x_4} P(\bar{x}_7|x_4,x_5)m_3(x_2,x_6,x_4)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5} P(x_2)P(x_5|x_2)P(x_8|\bar{x}_7)m_4(x_2,x_5,x_6)$$

$$= \sum_{x_8}\sum_{x_6} P(x_2)P(x_8|\bar{x}_7)\sum_{x_5} P(x_5|x_2)m_4(x_2,x_5,x_6)$$

$$= \sum_{x_8}\sum_{x_6} P(x_2)P(x_8|\bar{x}_7)m_5(x_2,x_6)$$

$$= \sum_{x_8} P(x_2)P(x_8|\bar{x}_7)\sum_{x_6} m_5(x_2,x_6)$$

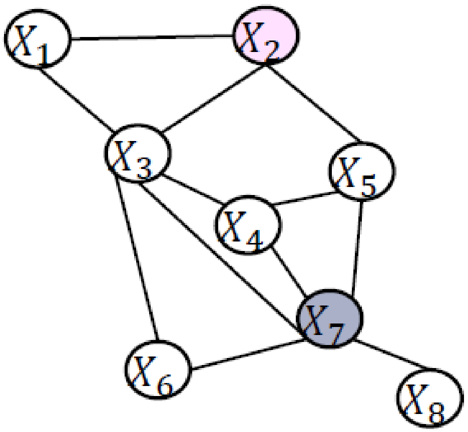
$$= \left(\sum_{x_8} P(x_2)P(x_8|\bar{x}_7)\right)m_6(x_2) = m_8(x_2)m_6(x_2)$$

Example from Soleymani pgm-sharif

Exact inference: variable elimination Example

- Query: $P(X_2|X_7 = \bar{x}_7)$

- $P(X_2|\bar{x}_7) \propto P(X_2, \bar{x}_7)$



$$P(x_2, \bar{x}_7)$$

$$= \sum_{x_1} \sum_{x_3} \sum_{x_4} \sum_{x_5} \sum_{x_6} \sum_{x_8} P(x_1, x_2, x_3, x_4, x_5, x_6, \bar{x}_7, x_8)$$

Consider the elimination order $X_1, X_3, X_4, X_5, X_6, X_8$

$$P(x_2, \bar{x}_7)$$

$$= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} \sum_{x_3} \sum_{x_1} \phi(x_3, x_4)\phi(x_2, x_5)\phi(x_3, x_6, \bar{x}_7)\phi(x_4, x_5, \bar{x}_7)\phi(\bar{x}_7, x_8)\phi(x_1, x_2, x_3)$$

Example from Soleymani pgm-sharif

Exact inference: variable elimination Example

$$P(x_2,\bar{x}_7) = \sum_{x_8}\sum_{x_6}\sum_{x_5}\sum_{x_4}\sum_{x_3}\phi(x_3,x_4)\phi(x_2,x_5)\phi(x_3,x_6,\bar{x}_7)\phi(x_4,x_5,\bar{x}_7)\phi(\bar{x}_7,x_8)\sum_{x_1}\phi(x_1,x_2,x_3)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5}\sum_{x_4}\sum_{x_3}\phi(x_3,x_4)\phi(x_2,x_5)\phi(x_3,x_6,\bar{x}_7)\phi(x_4,x_5,\bar{x}_7)\phi(\bar{x}_7,x_8)m_1(x_2,x_3)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5}\sum_{x_4}\phi(x_2,x_5)\phi(x_4,x_5,\bar{x}_7)\phi(\bar{x}_7,x_8)\sum_{x_3}\phi(x_3,x_4)\,\phi(x_3,x_6,\bar{x}_7)m_1(x_2,x_3)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5}\sum_{x_4}\phi(x_2,x_5)\phi(x_4,x_5,\bar{x}_7)\phi(\bar{x}_7,x_8)m_3(x_2,x_6,x_4)$$

$$= \sum_{x_8}\sum_{x_6}\sum_{x_5}\phi(x_2,x_5)\phi(\bar{x}_7,x_8)\sum_{x_4}\phi(x_4,x_5,\bar{x}_7)m_3(x_2,x_6,x_4)$$

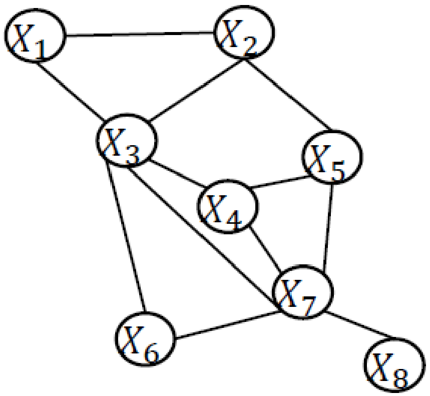
$$= \sum_{x_8}\sum_{x_6}\sum_{x_5}\phi(x_2,x_5)\phi(\bar{x}_7,x_8)m_4(x_2,x_5,x_6)$$

$$= \sum_{x_8}\sum_{x_6}\phi(\bar{x}_7,x_8)\sum_{x_5}\phi(x_2,x_5)m_4(x_2,x_5,x_6)$$

$$= \sum_{x_8}\sum_{x_6}\phi(\bar{x}_7,x_8)m_5(x_2,x_6)$$

$$= \sum_{x_8}\phi(\bar{x}_7,x_8)\sum_{x_6}m_5(x_2,x_6)$$

$$= \left(\sum_{x_8}\phi(\bar{x}_7,x_8)\right)m_6(x_2)$$



Example from Soleymani pgm-sharif

Exact inference: variable elimination

- In each elimination step, we need $O(k^m)$ computations where m is the number of variables is the product of factors containing the variable
  - k is the size of the largest scope of random variables
- With a system with n random variables, we need $O(nk^m)$ computations

Inference algorithms

- Exact inference :
  - Variable elimination
    - Can be applied on any graph
    - Responds only one query
  - Message passing
    - Sum-product
      - Only for trees
    - Junction tree
      - Can be applied on any graph

- In many real world applications these algorithms are computationally too complex to be applied

Inference algorithms

- Approximate inference:
  - Deterministic approximation
    - Variational inference
  - Stochastic simulation/sampling methods

Variational inference

- The calculus of variations (or variational calculus) is a field of mathematical analysis that uses variations, which are small changes in functions and functionals, to find maxima and minima of functionals
  - Functionals: functions of functions ☺
- Variational Bayesian methods are a family of techniques for approximating intractable integrals arising in Bayesian inference and machine learning.

Variational inference

- Generally, consider two sets of random variables in a joint distribution p:
  - X: Observed random variables
  - Z: Latent random variables

calculate $p(Z|X)$?

- $p(Z|X) = \frac{p(X,Z)}{p(X)}$, where$p(X) = \int p(X,Z)$
  - We usually have the joint distribution $p(X,Z)$.
  - However, calculating the marginal distribution $p(X)$ is interactable.

Variational inference

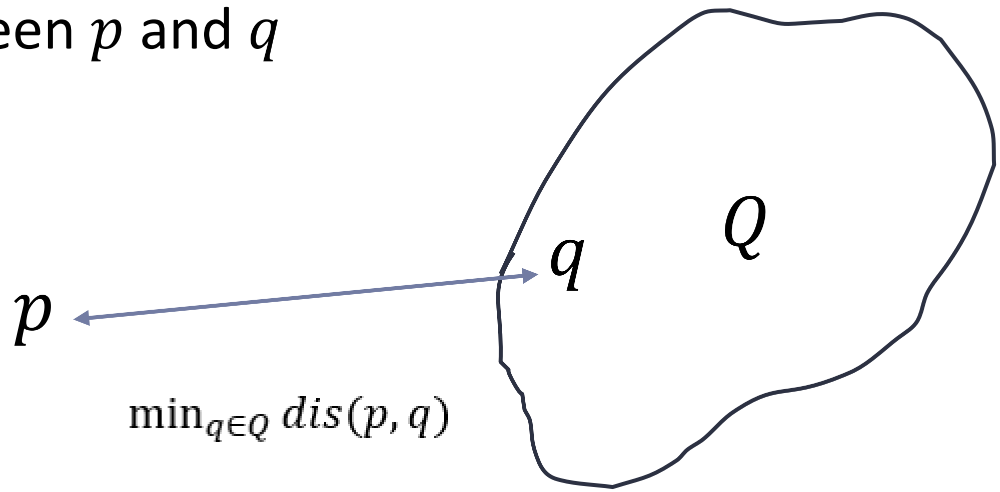
- Generally, consider two sets of random variables in a joint distribution p:
  - X: Observed random variables
  - Z: Latent random variables

calculate $p(Z|X)$?

- Solution: we select a family distribution Q in which the inference query is tractable. Then we find the best approximate of p in Q.

Variational inference

- Solution: we select a family distribution Q in which the inference query is tractable. Then we find the best approximate of p in Q.
- Converting inference to optimization over a functional (variational calculus)
  - A family distribution Q
  - A similarity metric between p and q
    - KL-divergence



Variational inference

- Kullback-Leibler divergence between two distribution:

$$KL(p \parallel q) = \int p(x) \log \frac{p(x)}{q(x)} dx$$

- This is positive for any two distributions

- $KL(p||q) = 0$ if and only if $p \equiv q$

- It is not symmetric
  - we call it divergence not distance

KL-divergence

- Suppose p is the target distribution we want to approximate it,
- I-projection: $KL(q \parallel p)$
- M-projection: $KL(p \parallel q)$
- Obviously, when $p \notin Q$ the result of following optimizations is different

$$\min_q KL(p \parallel q)$$

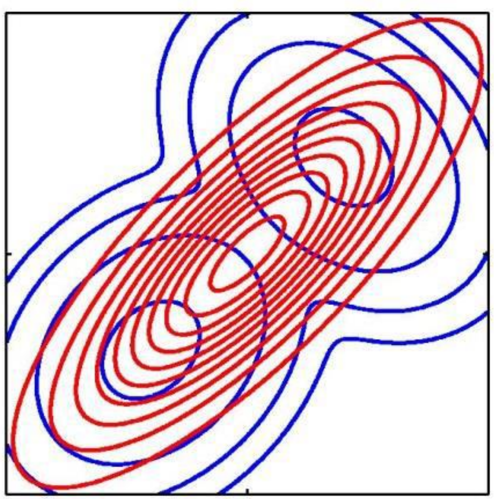
$$\min_q KL(q \parallel p)$$

KL-divergence

- p is a mixture of gaussian, Q is the family of gaussian distributions.

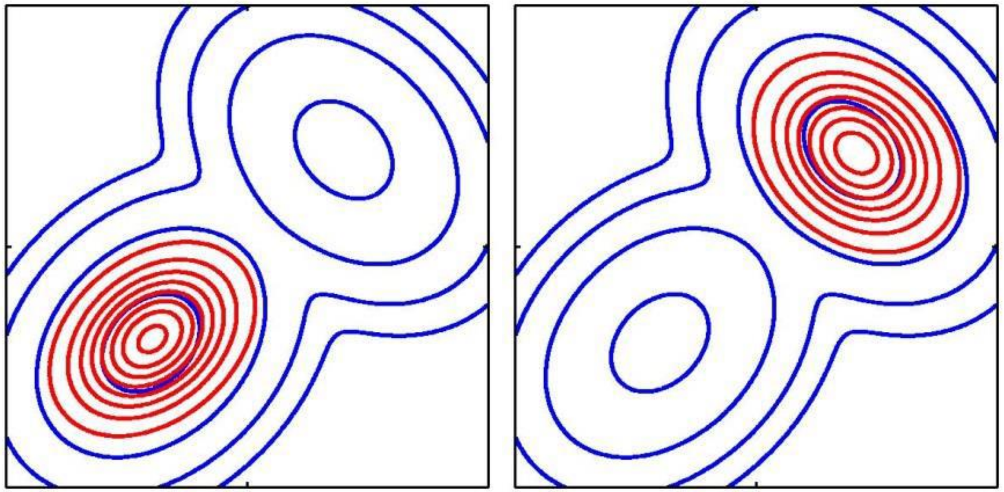
M-projection

$$\min_q KL(p \parallel q)$$



I-projection

$$\min_q KL(q \parallel \mathrm{p})$$



Bishop Book

Variational inference

- In variational inference we use the I-projection because of the computational complexity of p.

- Therefore, we should solve the following optimization to find the best q

$$\min_q KL(q(Z) \parallel p(Z|X))$$

$$KL(q(Z) \parallel p(Z|X)) = \int q(Z) \log \frac{q(Z)}{p(Z|X)} dZ = \int q(Z) \log \frac{q(Z)p(X)}{p(Z,X)} dZ$$

$$= \int q(Z) \log \frac{q(Z)p(X)}{p(Z,X)} dZ = \int q(Z) \log \frac{q(Z)}{p(Z,X)} dZ + \int q(Z) \log p(X) dZ$$

$$= KL\big(q(Z) \parallel p(Z,X)\big) + \log p(x)$$

Variational inference

- $KL(q(Z) \parallel p(Z|X)) = KL\big(q(Z) \parallel p(Z,X)\big) + \log p(x)$

- Two facts:
  - $KL(q(Z) \parallel p(Z|X)) > 0 \rightarrow \log p(x) > \underbrace{-KL\big(q(Z) \parallel p(Z,X)\big)}_{\text{Evidence lower bound (ELBO)}}$

  - $\log p(x) < 0 \rightarrow \; KL\big(q(Z) \parallel p(Z,X)\big) > \; KL(q(Z) \parallel p(Z|X))$

Variational inference

- $\log p(x) < 0 \rightarrow \underbrace{KL\big(q(Z) \parallel p(Z,X)\big)}_{\text{The upper bound}} > KL(q(Z) \parallel p(Z|X))$

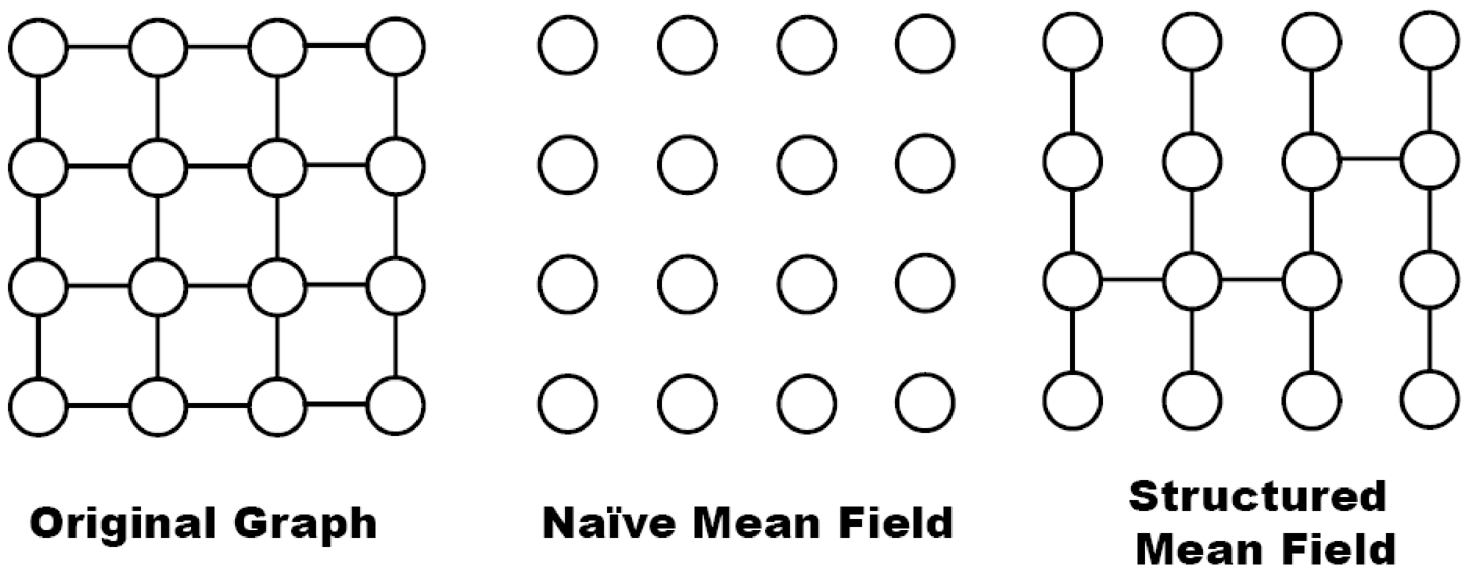
- In variational inference, we minimize the above upper bound

$$\operatorname{argmin}_{q \in Q} KL(q(Z) \parallel p(Z,X))$$

Variational mean filed approximation

- A common type of variational Bayes

Mean-field assumption: the unknown variables can be partitioned so that each partition is independent of the others



Variational mean filed approximation

Naïve mean field: the family distribution Q is fully factorized as follows:

$$q(Z) = \prod_i q_i(z_i)$$

- Variational mean field inference:

$$\underset{q \in Q}{\operatorname{argmin}} KL(q(Z) \parallel p(Z, X)) = \underset{q_1, q_2, \dots, q_n}{\operatorname{argmin}} KL(q(Z) \parallel p(Z, X))$$

Variational mean filed approximation

Naïve mean field: the family distribution Q is fully factorized as follows:

$$q(Z) = \prod_j q_j(z_j)$$

- We iteratively optimizing over one coordinate (factor) at a time, as follows,

$$\frac{\partial KL(q(Z) \| p(Z,X))}{\partial q_j} = 0 \text{ to obtain } q_j^*$$

Variational mean filed approximation

In variational naïve mean field inference, optimum factors are obtained as follows :

$$\log q_j^*(z_j) \propto \mathrm{E}_{q_{-j}}[\log p(X, Z)]$$

As each $q_j^*(z_j)$ depends on others, q_{-j}:

1. We initialize q_j^*s
2. We iteratively update each q_j^* until convergence!

Variational mean filed approximation

In variational naïve mean field inference, optimum factors are obtained as follows:

$$\log q_j^*(z_j) \propto \mathrm{E}_{q_{-j}}[\log p(X,Z)]$$

- Proof:

$$KL\big(q(Z) \parallel p(Z,X)\big) = \int q(Z)\,\log\frac{q(Z)}{p(Z,X)}\,dZ$$

$$= \mathrm{E}_{q(Z)}\left[\log\frac{q(Z)}{p(X,Z)}\right] = \underbrace{\mathrm{E}_{q(Z)}[\log q(Z)]}_{1} - \underbrace{\mathrm{E}_{q(Z)}[\log p(X,Z)]}_{2}$$

Variational mean filed approximation proof cont.

- We know,

$$q(Z) = \prod_i q_i(z_i) \rightarrow \log q(Z) = \sum_i \log q_i(z_i)$$

- Therefore,

$\mathrm{I}: \mathrm{E}_{q(Z)}[\log q(Z)] = \sum_i \mathrm{E}_{q_i(z_i)}[\log q_i(z_i)]$

- Also,

$2: \mathrm{E}_{q(Z)}[\log p(X,Z)] = \mathrm{E}_{q_j(z_j)}\left[\mathrm{E}_{q_{-j}}[\log p(X,Z)]\right]$

Variational mean filed approximation proof cont.

- Therefore,

$$KL\big(q(Z) \parallel p(Z,X)\big)$$
$$= \sum_i \mathrm{E}_{q_i(z_i)}[\log q_i(z_i)] - \mathrm{E}_{q_j(z_j)}\left[\mathrm{E}_{q_{-j}}[\log p(X,Z)]\right]$$

- and

$$\frac{\partial\, KL\big(q(Z) \parallel p(Z,X)\big)}{\partial q_j}$$
$$= \frac{\partial \int_{z_j} q_j(z_j)\left(-\mathrm{E}_{q_{-j}}[\log p(X,Z)] + \log q_j(z_j)\right) dz_j + const}{\partial q_j}$$

Variational mean filed approximation proof cont.

- According to "Euler–Lagrange equation" we can write,

$$\frac{\partial KL\big(q(Z) \parallel p(Z,X)\big)}{\partial q_j} = \frac{\partial q_j(z_j)\left(-\mathrm{E}_{q_{-j}}[\log p(X,Z)] + \log q_j(z_j)\right)}{\partial q_j}$$

- Remember the goal is:

$$q_j^* = \operatorname*{argmin}_{q_j} KL\big(q(Z) \parallel p(Z,X)\big)$$

- Therefore:

$$\frac{\partial\, q_j(z_j)\left(\mathrm{E}_{q_{-j}}[\log p(X,Z)] - \log q_j(z_j)\right)}{\partial q_j} = 0$$

$$\boxed{\rightarrow\ \log q_j^*(z_j) = \mathrm{E}_{q_{-j}}[\log p(X,Z)] + const}$$

Inference algorithms

- Approximate inference:
  - Deterministic approximation
    - Variational inference
  - Stochastic simulation/sampling methods ⟵

Sampling based approximation

- Consider the following set of i.i.d. samples from the distribution $p(x)$:

$$D = \{x^1, x^2, \dots, x^n\}$$

Monte Carlo method: for an arbitrary function $f(x)$ of random variable x, we can estimate $\mathrm{E}_p[f]$ as follows (empirical expectation),

$$\mathrm{E}_p[f] = \frac{1}{n}\sum_{i=1}^{n} f(x^i)$$

Sampling based approximation

Monte Carlo method: for an arbitrary function $f(x)$ of random variable x, we can estimate $\mathrm{E}_p[f]$ as follows (empirical expectation),

$$\mathrm{E}_p[f] = \frac{1}{n}\sum_{i=1}^{n} f(x^i)$$

- Marginal probability: $\mathrm{p}(\mathrm{x}_1 = \mathrm{k}) \rightarrow\ f = I(x_1 = k)$
- Mean of a distribution: $f = x$
- …

Forward sampling in a BN

Given a BN, and number of samples N

Choose a **topological** order on variables: $x_1, x_2, \ldots, x_M$

For $i = 1$ to N

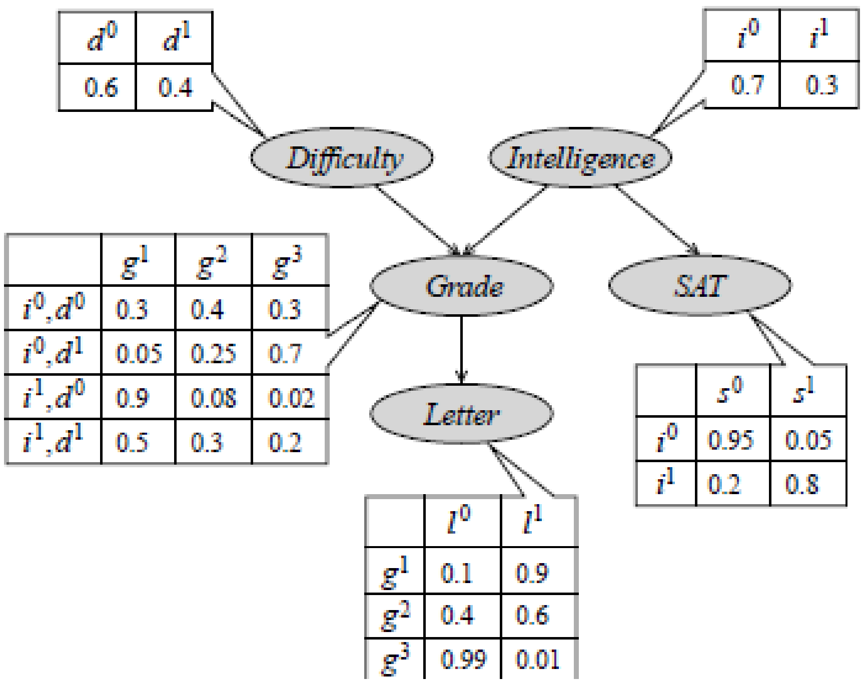
For $j = 1$ to M

Sample x_j^i from the distribution $p(x_j | parent(x_j))$

Add $\{x_1^i, x_2^i, \ldots, x_M^i\}$ to the sample set

Forward sampling in a BN

- $Sample\ D\ from\ p(D)$
- $Sample\ I\ from\ p(I)$
- $Sample\ G\ from\ p(G|D,I)$
- $Sample\ S\ from\ p(S|I)$
- $Sample\ L\ from\ p(L|G)$



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0.7	0.3

	g^1	g^2	g^3
i^0, d^0	0.3	0.4	0.3
i^0, d^1	0.05	0.25	0.7
i^1, d^0	0.9	0.08	0.02
i^1, d^1	0.5	0.3	0.2

	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

	l^0	l^1
g^1	0.1	0.9
g^2	0.4	0.6
g^3	0.99	0.01

Koller Book

Forward sampling in a BN

- Problems:
  - When the evidence rarely happens, we would need lots of samples, and most would be wasted
  - Overall probability of accepting a sample rapidly decreases when the number of observed variables and states that those variables can take increases
  - This approach is very slow and rarely used in practice.

Importance sampling

- When sampling from the target distribution p is hard, we use a proposal distribution q
  - q should dominates $p \rightarrow q(x) > 0$ whenever $p(x) > 0$

- We sample from the proposal distribution q and consider a weight for each sample:

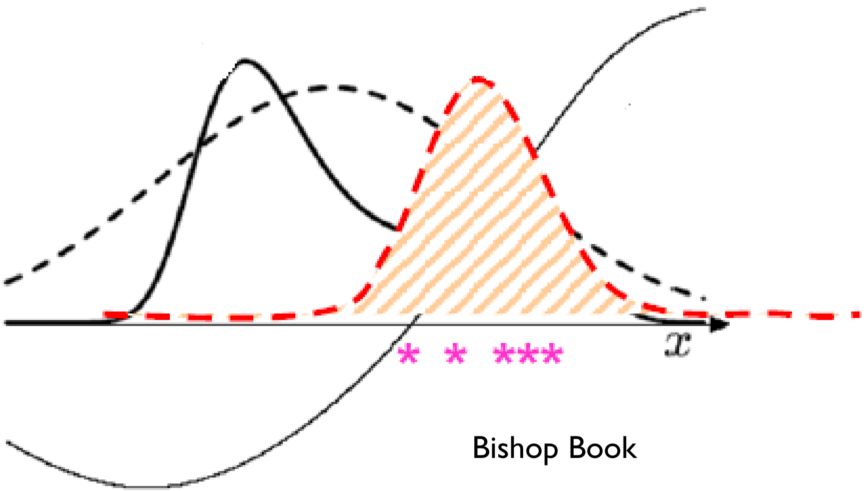
$$\mathrm{E}_p[f] = \int f(x)\, p(x)\, dx = \int f(x) \frac{p(x)}{q(x)} q(x)\, dx$$

$$\mathrm{E}_p[f] \simeq \frac{1}{n} \sum_{i=1}^{n} f(x^i) \frac{p(x^i)}{q(x^i)} \qquad x^i \sim q(x)$$

$$\mathrm{E}_p[f] \simeq \frac{1}{n} \sum_{i=1}^{n} f(x^i) w(x^i) \qquad w(x^i) = \frac{p(x^i)}{q(x^i)}$$

Importance sampling

- Importance sampling depends on how well q matches p.
  - For mismatch distributions, weights may be dominated by few samples having large weights, with the remaining weights being relatively insignificant
- It is common that $P(\boldsymbol{x})f(\boldsymbol{x})$ is strongly varying and has a significant proportion of its mass concentrated in a small region
  - The problem is more severe if none of the samples falls in the regions where $P(\boldsymbol{x})f(\boldsymbol{x})$ is large.



Bishop Book

Problems of naïve Monte Carlo method

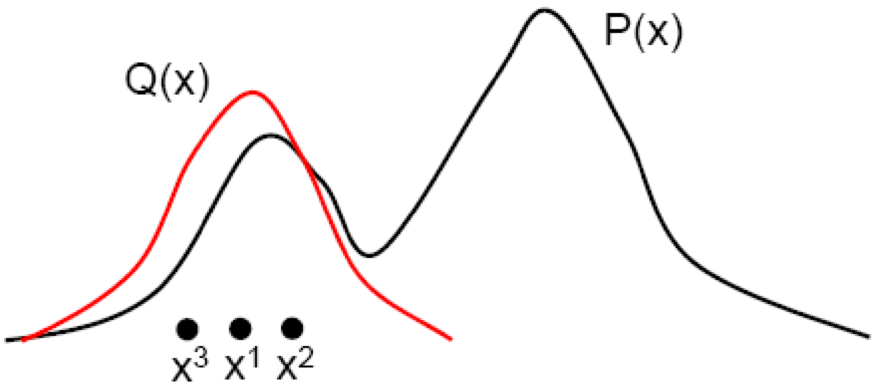
- Direct sampling: only when we can sample from $p(x)$
  - Wasteful for rare evidences

- Importance sampling: when the proposal $q(x)$ is very different from $p(x)$ most samples have very low weights.
  - In fact finding a good proposal $q(x)$ that is similar to $p(x)$ usually requires knowledge of the analytic form of $p(x)$ that is not available

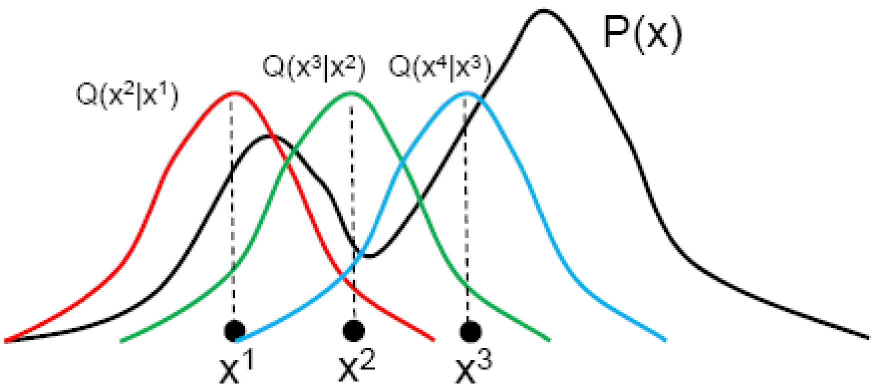
Markov chain Monte Carlo (MCMC)

- Using an adaptive distribution $q(x'|x)$ instead of a fixed distribution $q(x)$, where x is the last accepted sample and x' is the new sample.
  - During sampling process the proposal distribution changes as a function of previous sampled data

Importance sampling with a (bad) proposal Q(x)



MCMC with adaptive proposal Q(x'|x)



Bishop Book

Markov chain Monte Carlo (MCMC)

- Different methods
  - Metropolis-Hastings ⟵
  - Gibbs sampling

Markov chain Monte Carlo (MCMC)

- Metropolis-Hastings
  - Sample from $q(x'|x)$, where x is the previous sample
  - As x changes, $q(x'|x)$ can also change
  - Accept this new sample with following probability

$$A(x'|x) = \min(1, \frac{\boxed{p(x')/q(x'|x)}}{p(x)/q(x|x')})$$

importance

  - The acceptance rate $A(x'|x)$ guarantees that after sufficiently many draws, samples are generated from the target distribution $p(x)$
    - Burn-in samples: samples generated in initial iterations and hey are not from $p(x)$

Markov chain Monte Carlo (MCMC)

Metropolis-Hastings algorithm:

Initialize starting point: x^0 , set t=0

Repeat until convergence:

Sample $x^* \backsim q(x^*|x)$

$$A(x^*|x) = \min(1, \frac{p(x')/q(x'|x)}{p(x)/q(x|x')})$$

Sample $u \backsim uniform\ (0,1)$

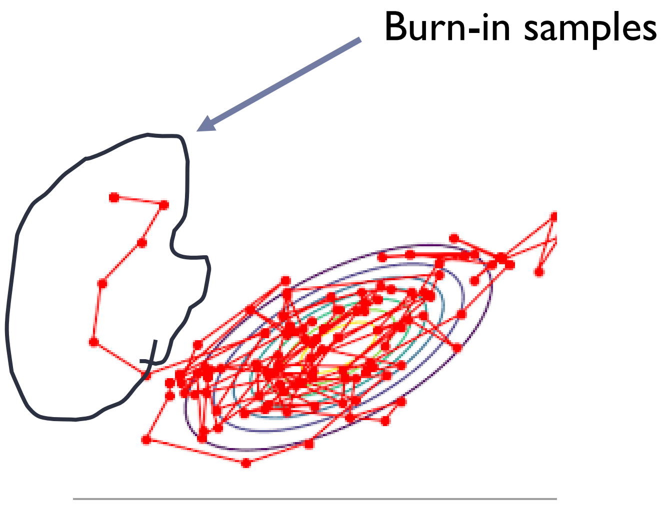
If $u < A(x^*|x)$:

$$x^{t+1} = x^*$$

Else:

$$x^{t+1} = x^t$$

Discard Burn-in samples

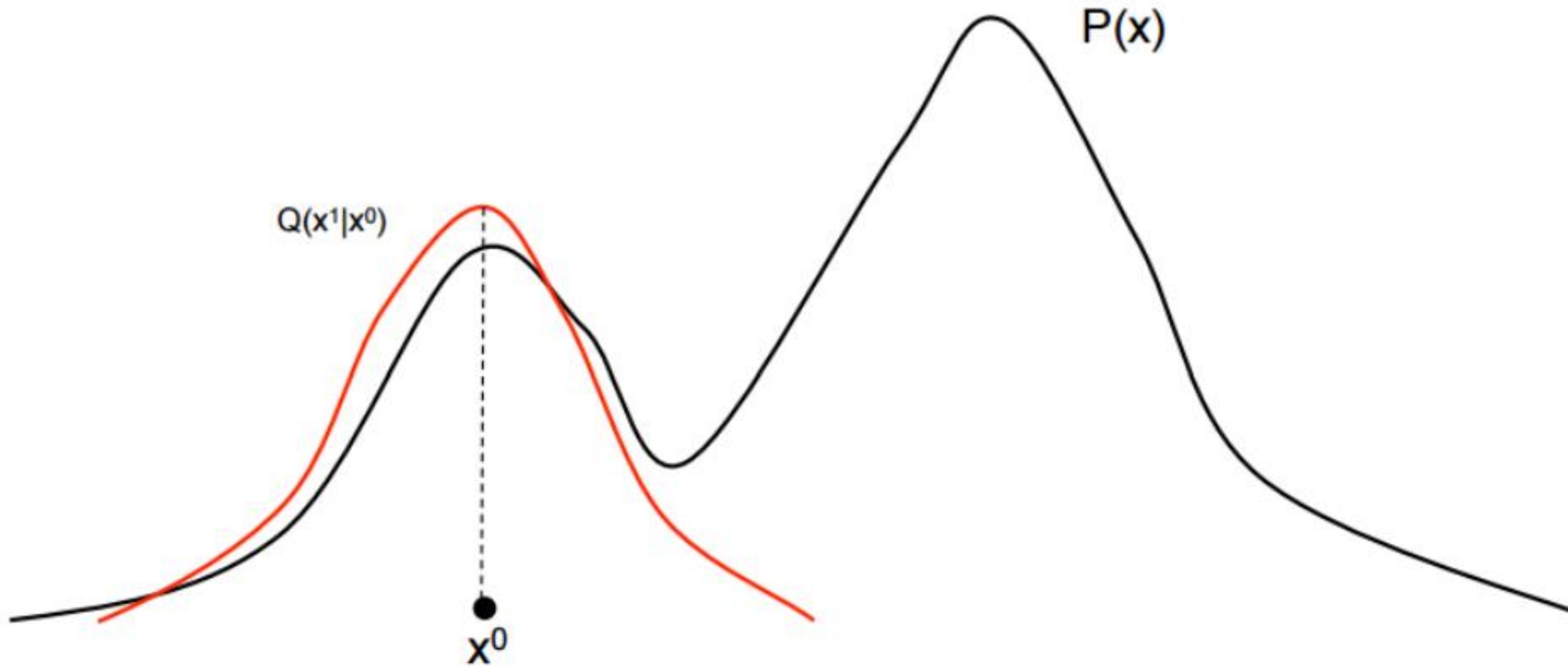


Markov chain Monte Carlo (MCMC)

- Metropolis-Hastings example:
  - The proposal distribution $q(x'|x)$ is a gaussian distribution
  - The true distribution $p(x)$ is a bimodal with two peaks!

Initialize $x^{(0)}$

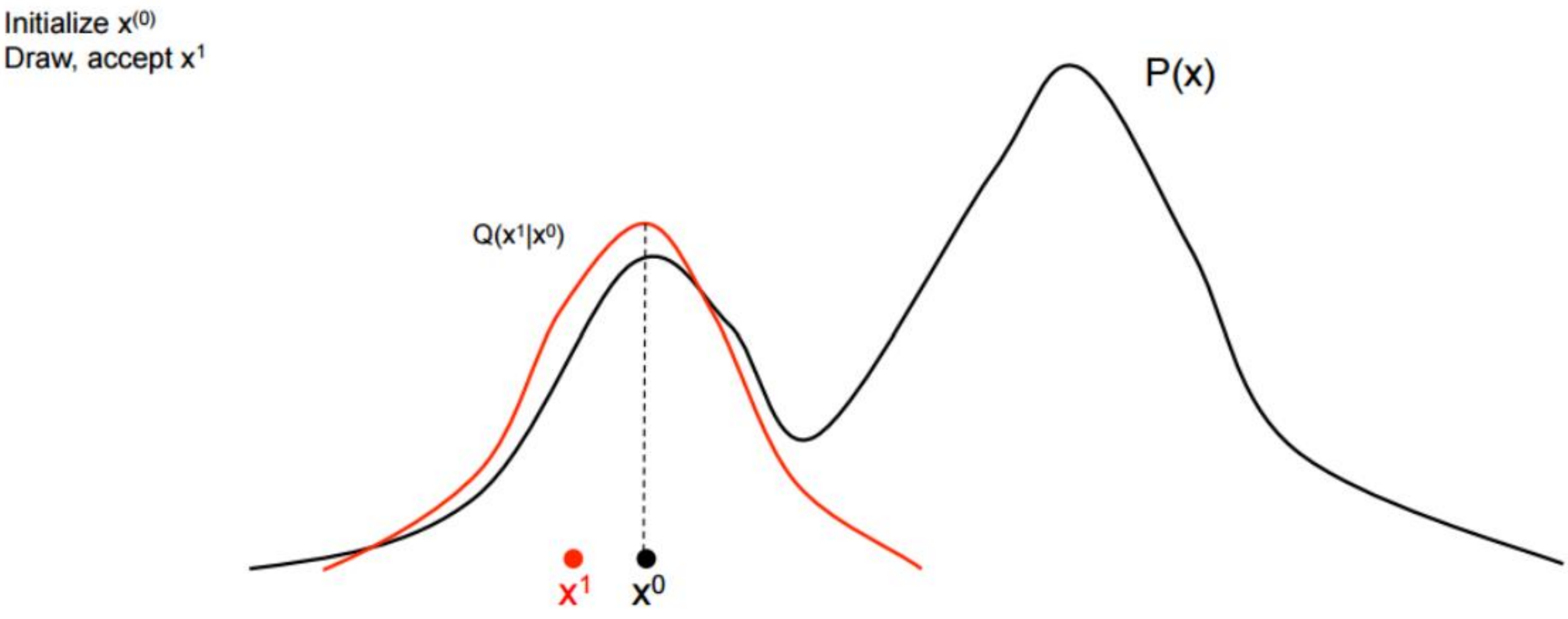
...



Jin Young Choi - SNU

Markov chain Monte Carlo (MCMC)

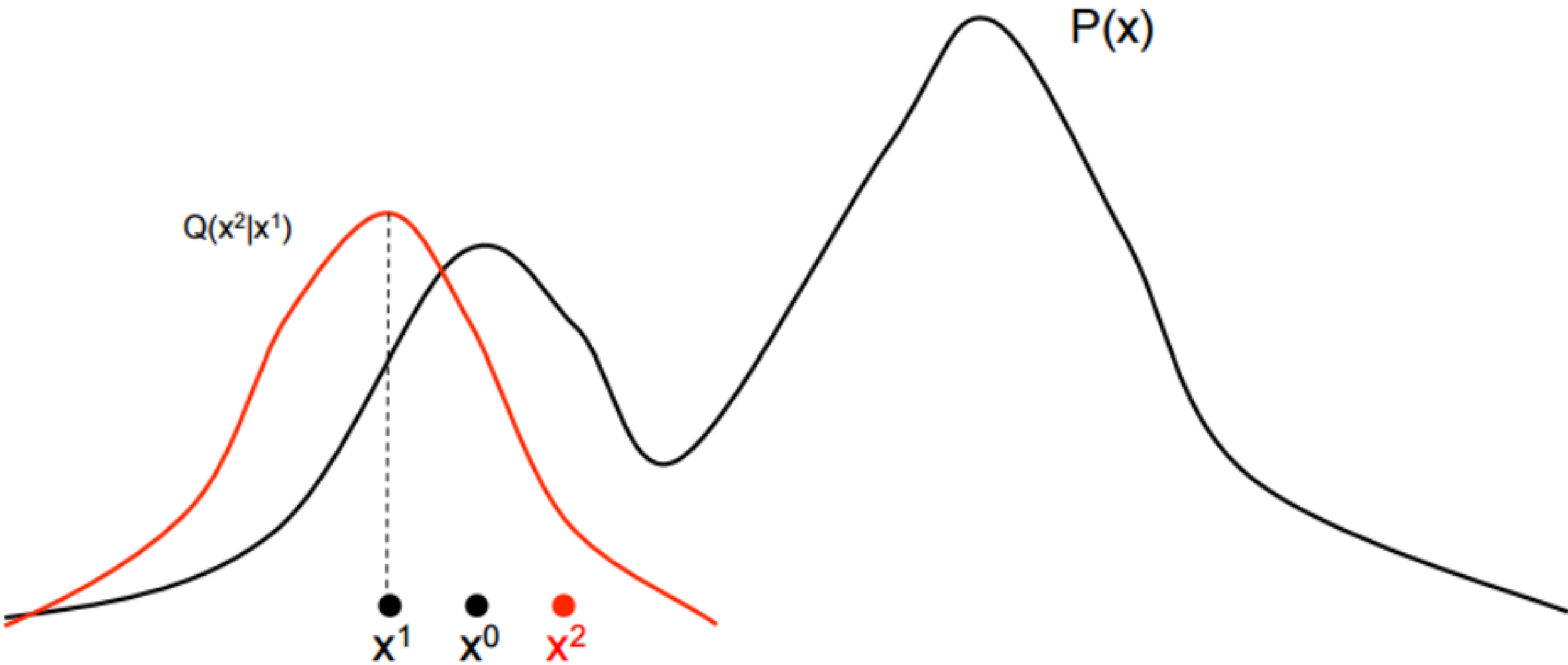
- Metropolis-Hastings example:



Markov chain Monte Carlo (MCMC)

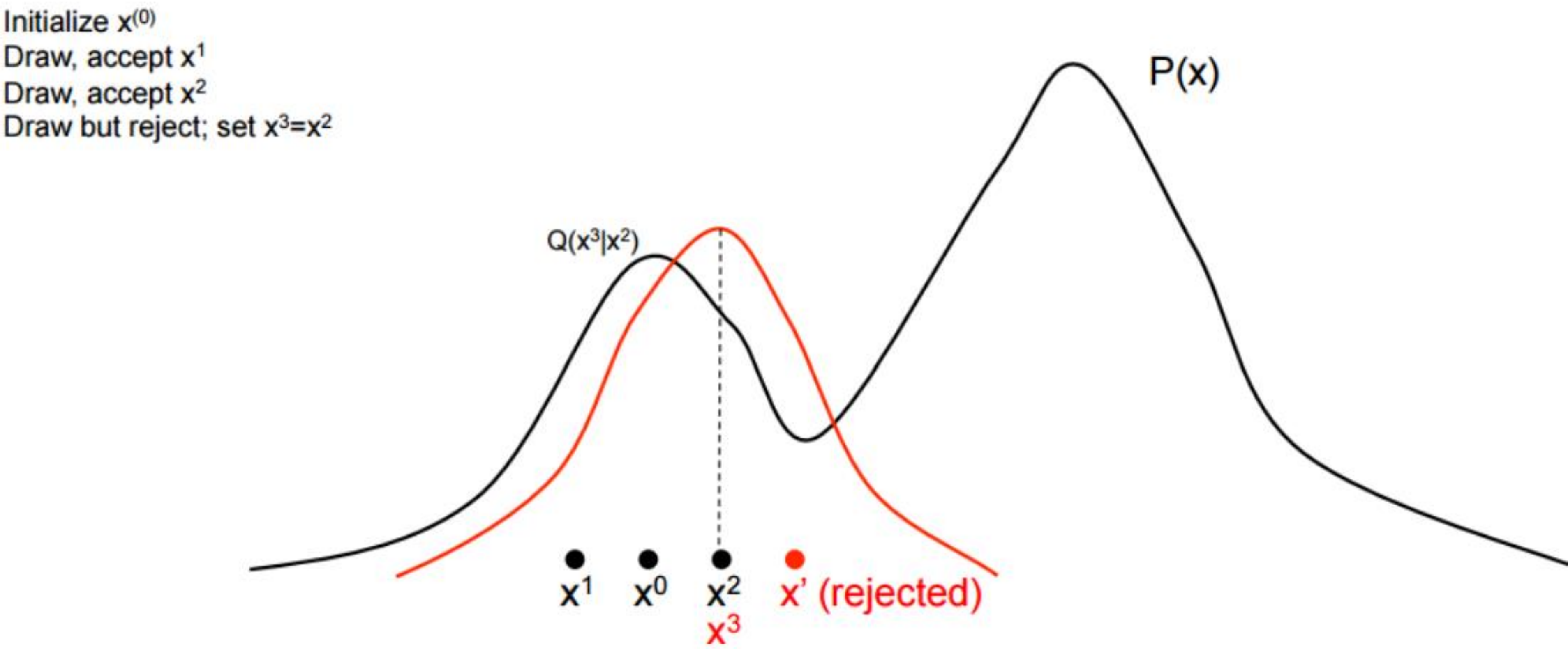
- Metropolis-Hastings example:

Initialize $x^{(0)}$
Draw, accept x^1
Draw, accept x^2



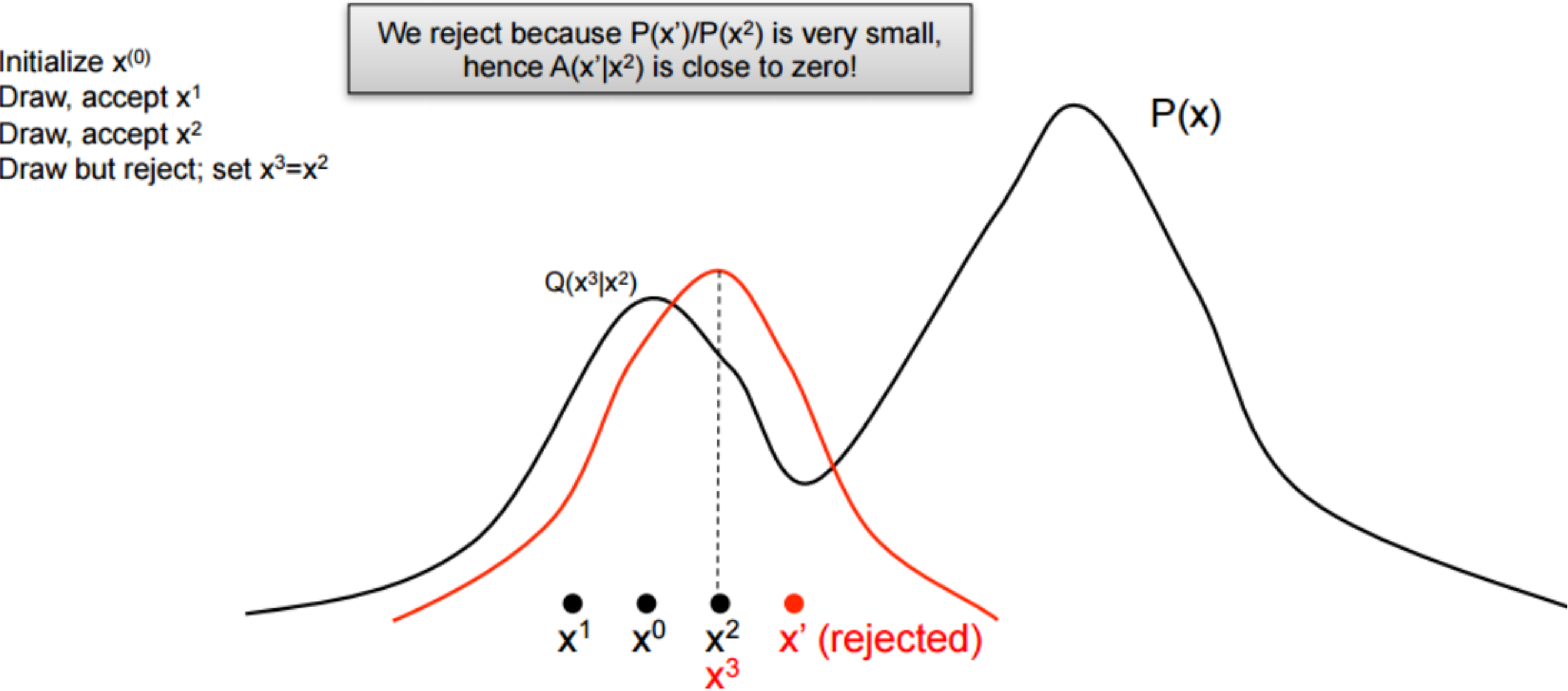
Markov chain Monte Carlo (MCMC)

- Metropolis-Hastings example:



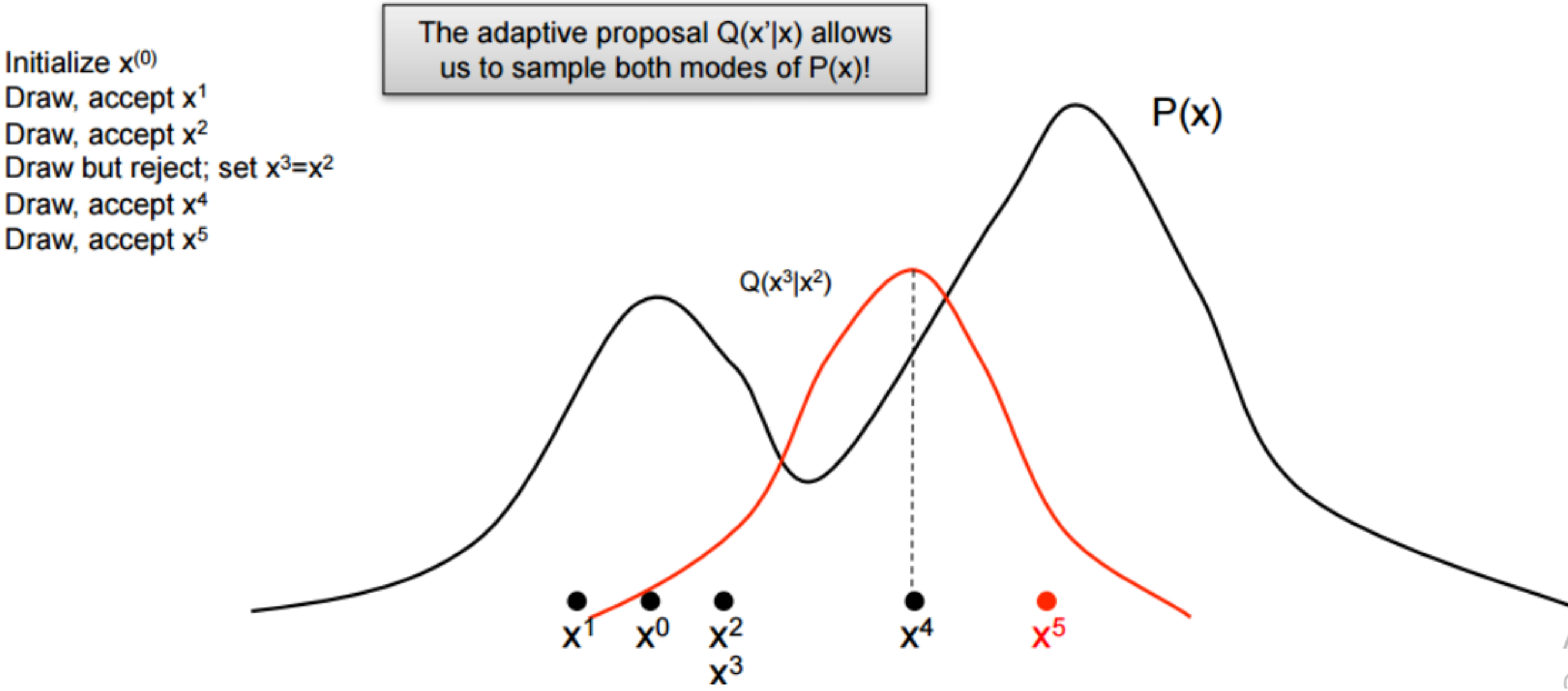
Markov chain Monte Carlo (MCMC)

- Metropolis-Hastings example:



Markov chain Monte Carlo (MCMC)

- Metropolis-Hastings example:



Next topic

- Probabilistic graphical models
  - Learning