



Probabilistic graphical models

Exact and approximate inference

22-808: Generative models
Sharif University of Technology
Fall 2025

Fatemeh Seyyedsalehi

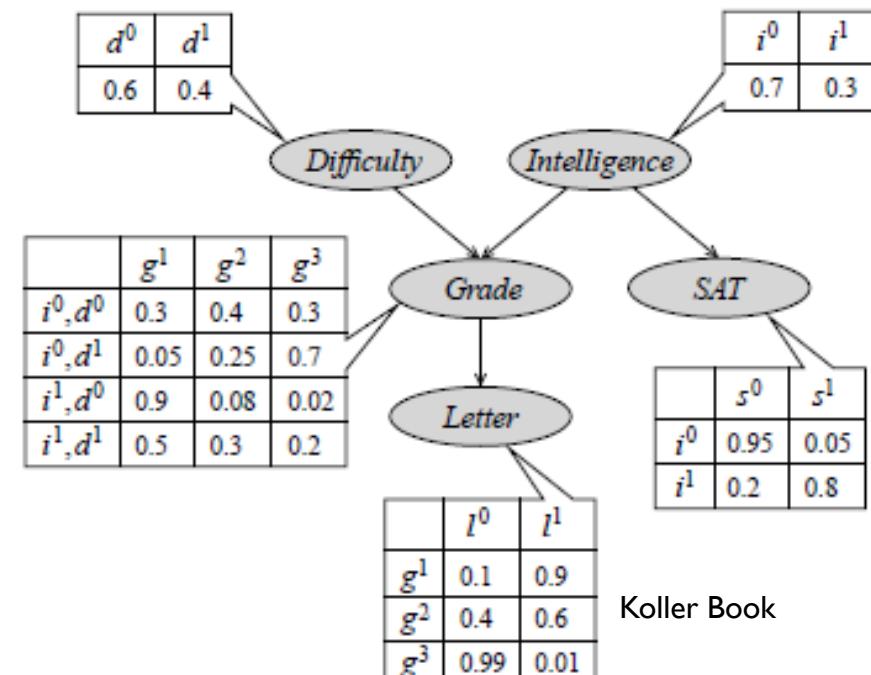
The inference problem

- ▶ 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:

$$p(\text{Difficulty} | \text{Letter} = 1) = ?$$

$$p(\text{Letter} | \text{Intelligence} = 1) = ?$$

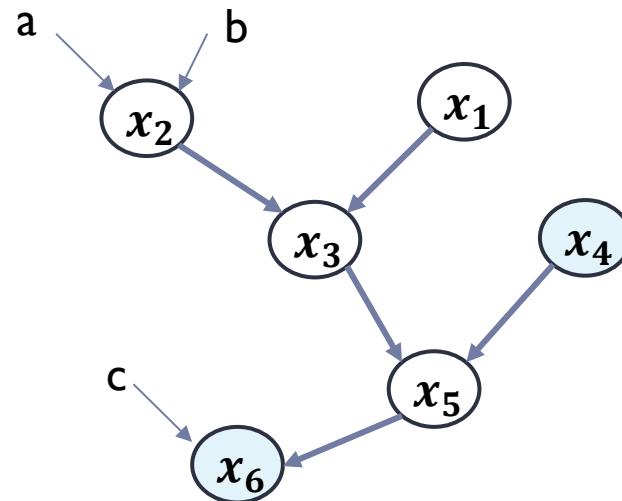
$$p(\text{SAT}) = ?$$



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.

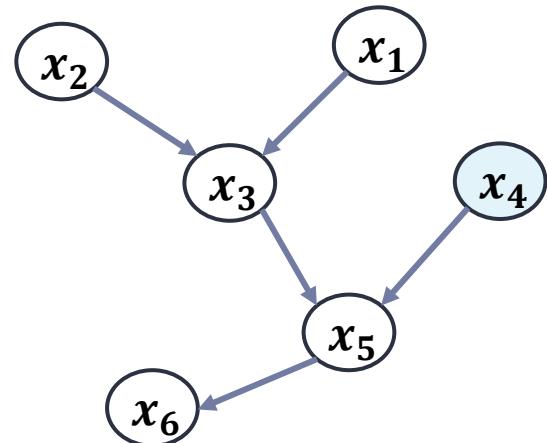
- ▶ An inference query:

$$p(x_2 | x_4 = \bar{x}_4) = ?$$

- ▶ A naïve solution:

$$p(x_2 | x_4 = \bar{x}_4) = \frac{p(x_2, \bar{x}_4)}{\sum_{x_2} p(x_2, \bar{x}_4)}$$

$$p(x_2, \bar{x}_4) = \sum_{x_1} \sum_{x_3} \sum_{x_5} \sum_{x_6} p(x_1, x_2, x_3, \bar{x}_4, x_5, x_6)$$

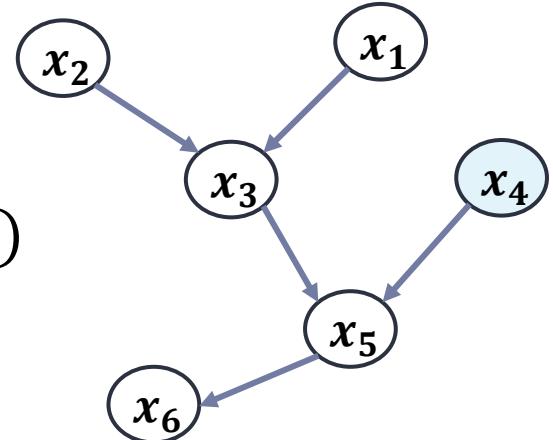


The inference problem

- ▶ 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:

$$p(x_2, \bar{x}_4) = \sum_{x_1} \sum_{x_3} \sum_{x_5} \sum_{x_6} p(x_1, x_2, x_3, \bar{x}_4, x_5, x_6) \\ = \sum_{x_1} \sum_{x_3} \sum_{x_5} \sum_{x_6} p(x_2)p(x_1)p(x_3|x_1, x_2)p(x_5|\bar{x}_4, x_3)p(x_6|x_5)$$

The inference problem

- ▶ A better solution:

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

- ▶ $O(k^4)$ computation !

Distributive law: If $X \notin \text{scope}(\phi_1)$ 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:

$$\begin{aligned} p(x_2, \overline{x_4}) &= \sum_{x_1} \sum_{x_3} \sum_{x_5} \sum_{x_6} p(x_1, x_2, x_3, \overline{x_4}, x_5, x_6) \\ &= \sum_{x_1} \sum_{x_3} \sum_{x_5} \sum_{x_6} p(x_2) p(x_1) p(x_3 | x_1, x_2) p(x_5 | \overline{x_4}, x_3) p(x_6 | x_5) = \\ &\quad p(x_2) \sum_{x_1} p(x_1) \sum_{x_3} p(x_3 | x_1, x_2) \sum_{x_5} p(x_5 | \overline{x_4}, x_3) \sum_{x_6} p(x_6 | x_5) \end{aligned}$$

- ▶ $O(4k^3)$ 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: $P(X_2|X_7 = \bar{x}_7)$

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

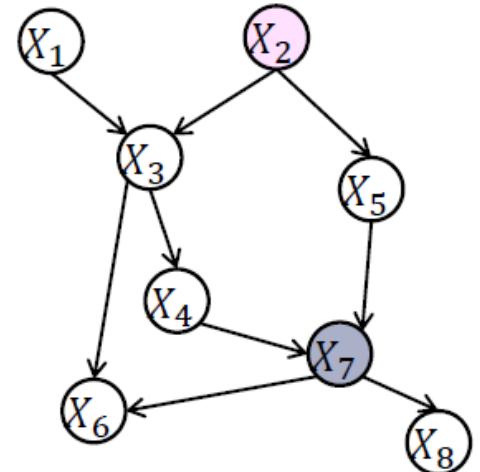
$$P(x_2, \bar{x}_7)$$

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

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

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

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



Exact inference: variable elimination

Example

$$\begin{aligned} P(x_2, \bar{x}_7) &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} \sum_{x_3} P(x_2)P(x_4|x_3)P(x_5|x_2)P(x_6|x_3, \bar{x}_7)P(\bar{x}_7|x_4, x_5)P(x_8|\bar{x}_7) \overbrace{\sum_{x_1} P(x_1)P(x_3|x_1, x_2)} \\ &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} \sum_{x_3} P(x_2)P(x_4|x_3)P(x_5|x_2)P(x_6|x_3, \bar{x}_7)P(\bar{x}_7|x_4, x_5)P(x_8|\bar{x}_7) \overbrace{m_1(x_2, x_3)} \\ &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} P(x_2)P(x_5|x_2)P(\bar{x}_7|x_4, x_5)P(x_8|\bar{x}_7) \overbrace{\sum_{x_3} P(x_4|x_3)P(x_6|x_3, \bar{x}_7)m_1(x_2, x_3)} \\ &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} P(x_2)P(x_5|x_2)P(\bar{x}_7|x_4, x_5)P(x_8|\bar{x}_7) \overbrace{m_3(x_2, x_6, x_4)} \\ &= \sum_{x_8} \sum_{x_6} \sum_{x_5} P(x_2)P(x_5|x_2)P(x_8|\bar{x}_7) \overbrace{\sum_{x_4} P(\bar{x}_7|x_4, x_5)m_3(x_2, x_6, x_4)} \\ &= \sum_{x_8} \sum_{x_6} \sum_{x_5} P(x_2)P(x_5|x_2)P(x_8|\bar{x}_7) \overbrace{m_4(x_2, x_5, x_6)} \\ &= \sum_{x_8} \sum_{x_6} P(x_2)P(x_8|\bar{x}_7) \overbrace{\sum_{x_5} P(x_5|x_2)m_4(x_2, x_5, x_6)} \\ &= \sum_{x_8} \sum_{x_6} P(x_2)P(x_8|\bar{x}_7) \overbrace{m_5(x_2, x_6)} \\ &= \sum_{x_8} P(x_2)P(x_8|\bar{x}_7) \overbrace{\sum_{x_6} m_5(x_2, x_6)} \\ &= \left(\sum_{x_8} P(x_2)P(x_8|\bar{x}_7) \right) \overbrace{m_6(x_2)} = m_8(x_2)m_6(x_2) \end{aligned}$$

Exact inference: variable elimination

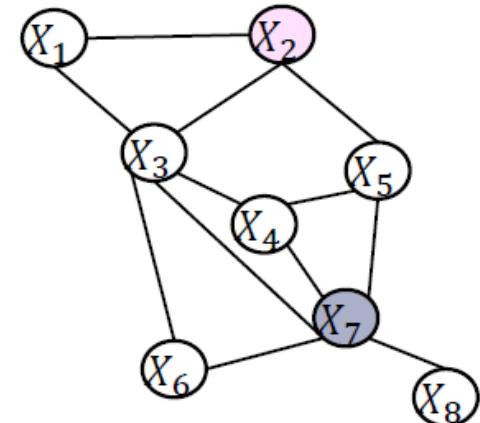
Example

- 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 $X_1, X_3, X_4, X_5, X_6, X_8$

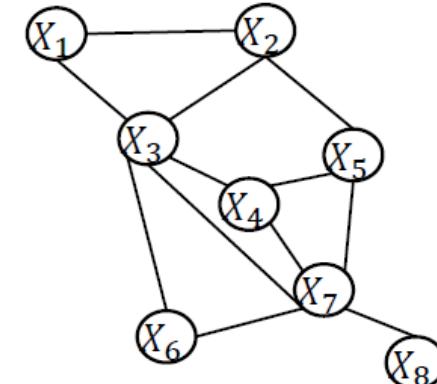
$$P(x_2, \bar{x}_7)$$

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

Exact inference: variable elimination

Example

$$\begin{aligned}
 P(x_2, \bar{x}_7) &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} \sum_{x_3} \phi(x_3, x_4) \phi(x_2, x_5) \phi(x_3, x_6, \bar{x}_7) \phi(x_4, x_5, \bar{x}_7) \phi(\bar{x}_7, x_8) \underbrace{\sum_{x_1} \phi(x_1, x_2, x_3)}_{m_1(x_2, x_3)} \\
 &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} \sum_{x_3} \phi(x_3, x_4) \phi(x_2, x_5) \phi(x_3, x_6, \bar{x}_7) \phi(x_4, x_5, \bar{x}_7) \phi(\bar{x}_7, x_8) m_1(x_2, x_3) \\
 &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} \phi(x_2, x_5) \phi(x_4, x_5, \bar{x}_7) \phi(\bar{x}_7, x_8) \underbrace{\sum_{x_3} \phi(x_3, x_4) \phi(x_3, x_6, \bar{x}_7) m_1(x_2, x_3)}_{m_3(x_2, x_6, x_4)} \\
 &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \sum_{x_4} \phi(x_2, x_5) \phi(x_4, x_5, \bar{x}_7) \phi(\bar{x}_7, x_8) m_3(x_2, x_6, x_4) \\
 &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \phi(x_2, x_5) \phi(\bar{x}_7, x_8) \underbrace{\sum_{x_4} \phi(x_4, x_5, \bar{x}_7) m_3(x_2, x_6, x_4)}_{m_4(x_2, x_5, x_6)} \\
 &= \sum_{x_8} \sum_{x_6} \sum_{x_5} \phi(x_2, x_5) \phi(\bar{x}_7, x_8) m_4(x_2, x_5, x_6) \\
 &= \sum_{x_8} \sum_{x_6} \phi(\bar{x}_7, x_8) \underbrace{\sum_{x_5} \phi(x_2, x_5) m_4(x_2, x_5, x_6)}_{m_5(x_2, x_6)} \\
 &= \sum_{x_8} \sum_{x_6} \phi(\bar{x}_7, x_8) m_5(x_2, x_6) \\
 &= \sum_{x_8} \phi(\bar{x}_7, x_8) \underbrace{\sum_{x_6} m_5(x_2, x_6)}_{m_6(x_2)} \\
 &= \left(\sum_{x_8} \phi(\bar{x}_7, x_8) \right) m_6(x_2)
 \end{aligned}$$



Exact inference: variable elimination

- ▶ In each elimination step, we need $O(k^m)$ computations where m is the number of variables in 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 intractable.

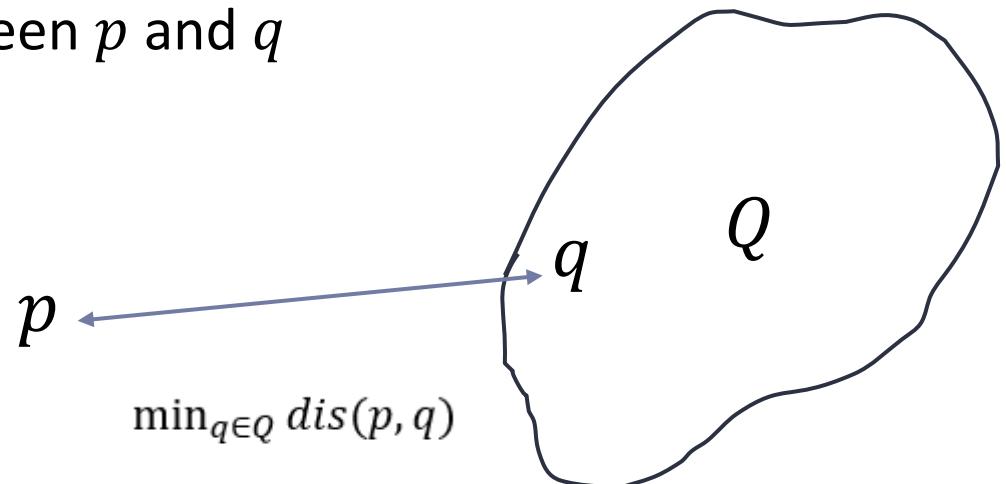
Variational inference

- ▶ 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

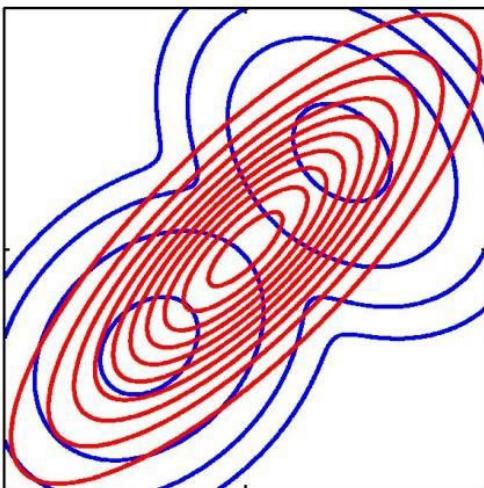
$$\begin{aligned} & \min_q KL(p \parallel q) \\ & \min_q KL(q \parallel p) \end{aligned}$$

KL-divergence

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

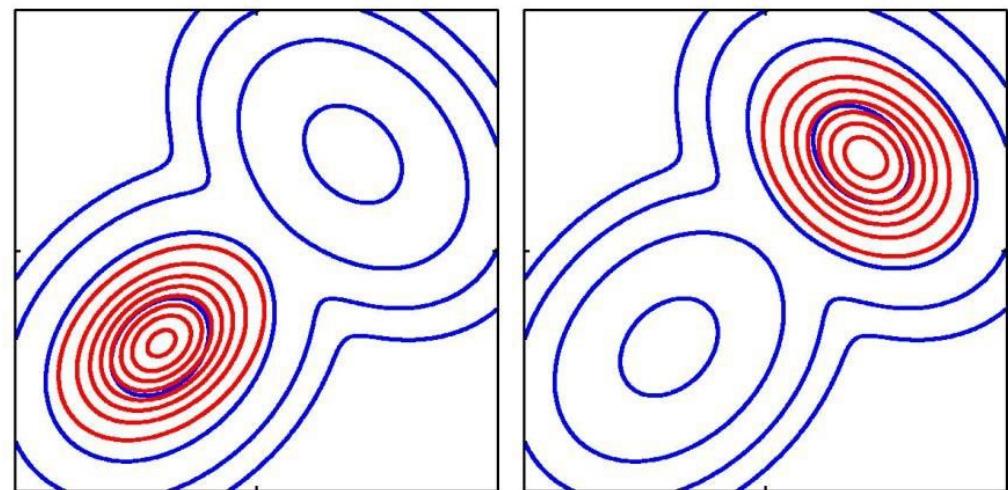
M-projection

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



I-projection

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



Bishop Book

Variational inference

- ▶ In variational inference: I-projection
 - ▶ Because of the computational complexity of p .
- ▶ We should solve the following optimization to find the best q :

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

$$\begin{aligned} \text{KL}(q(Z) \parallel p(Z|X)) &= \int q(Z) \log \frac{q(Z)}{p(Z|X)} dZ = \int q(Z) \log \frac{q(Z)p(X)}{p(Z,X)} dZ \\ &= \int q(Z) \log \frac{q(Z)p(X)}{p(Z,X)} dZ = \int q(Z) \log \frac{q(Z)}{p(Z,X)} dZ + \int q(Z) \log p(X) dZ \\ &= \text{KL}(q(Z) \parallel p(Z,X)) + \log p(x) \end{aligned}$$

Variational inference

- ▶ $KL(q(Z) \parallel p(Z|X)) = KL(q(Z) \parallel p(Z,X)) + \log p(x)$
- ▶ Two facts:
 - ▶ $KL(q(Z) \parallel p(Z|X)) > 0 \rightarrow \log p(x) > -KL(q(Z) \parallel p(Z,X))$

\longleftrightarrow
Evidence lower bound (ELBO)
 - ▶ $\log p(x) < 0 \rightarrow KL(q(Z) \parallel p(Z,X)) > KL(q(Z) \parallel p(Z|X))$

Variational inference

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



The upper bound

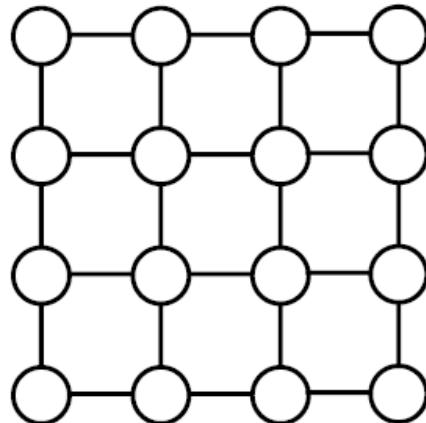
- In variational inference, we minimize the above upper bound

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

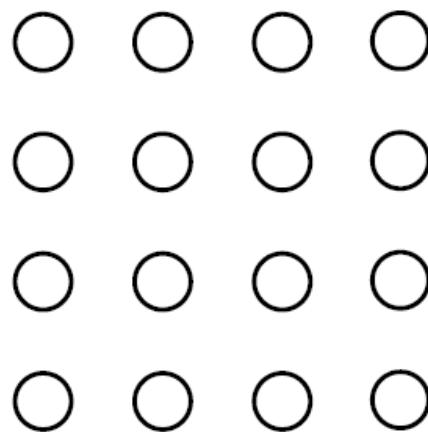
Variational mean filed approximation

- ▶ A common type of variational Bayes

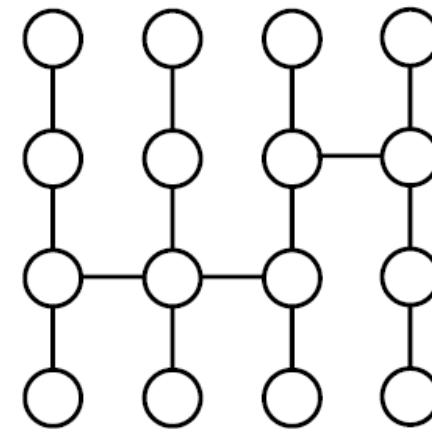
Mean-field assumption: the unknown variables can be partitioned so that each partition is independent of the others



Original Graph



Naïve Mean Field



Structured Mean Field

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:

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

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 :

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

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:

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

► Proof:

$$\begin{aligned} KL(q(Z) \parallel p(Z, X)) &= \int q(Z) \log \frac{q(Z)}{p(Z, X)} dZ \\ &= E_{q(Z)} \left[\log \frac{q(Z)}{p(X, Z)} \right] = E_{q(Z)}[\log q(Z)] - E_{q(Z)}[\log p(X, Z)] \end{aligned}$$

| 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,

1: $E_{q(Z)}[\log q(Z)] = \sum_i E_{q_i(z_i)}[\log q_i(z_i)]$

- ▶ Also,

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

Variational mean filed approximation proof cont.

▶ Therefore,

$$\begin{aligned} & KL(q(Z) \parallel p(Z, X)) \\ &= \sum_i E_{q_i(z_i)}[\log q_i(z_i)] - E_{q_j(z_j)} \left[E_{q_{-j}}[\log p(X, Z)] \right] \end{aligned}$$

▶ and

$$\begin{aligned} & \frac{\partial KL(q(Z) \parallel p(Z, X))}{\partial q_j} \\ &= \frac{\partial \int_{z_j} q_j(z_j) \left(-E_{q_{-j}}[\log p(X, Z)] + \log q_j(z_j) \right) dz_j + const}{\partial q_j} \end{aligned}$$

Variational mean filed approximation proof cont.

- ▶ According to “Euler–Lagrange equation” we can write,

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

- ▶ Remember the goal is:

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

- ▶ Therefore:

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

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

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 $E_p[f]$ as follows (empirical expectation),

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

Sampling based approximation

Monte Carlo method: for an arbitrary function $f(x)$ of random variable x , we can estimate $E_p[f]$ as follows (empirical expectation),

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

- ▶ Marginal probability: $p(x_1 = k) \rightarrow f = I(x_1 = k)$
- ▶ 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, \dots, x_M

For $i = 1$ to N

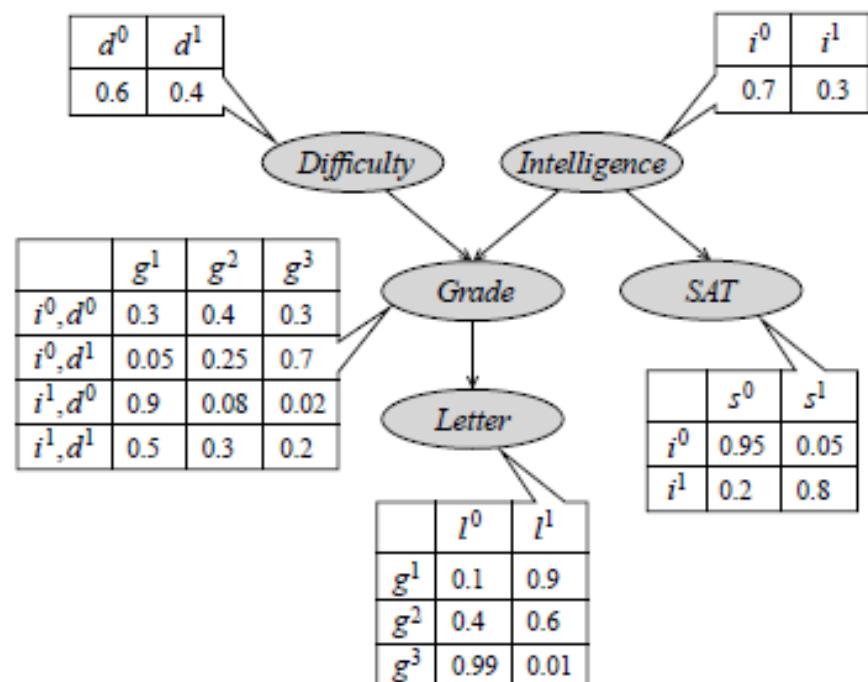
 For $j = 1$ to M

? Sample x_j^i from the distribution $p(x_j | \text{parent}(x_j))$

 Add $\{x_1^i, x_2^i, \dots, x_M^i\}$ 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 $p(L|G)$



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 dominate $p \rightarrow q(x) > 0$ whenever $p(x) > 0$
- ▶ We sample from the proposal distribution q and consider a weight for each sample:

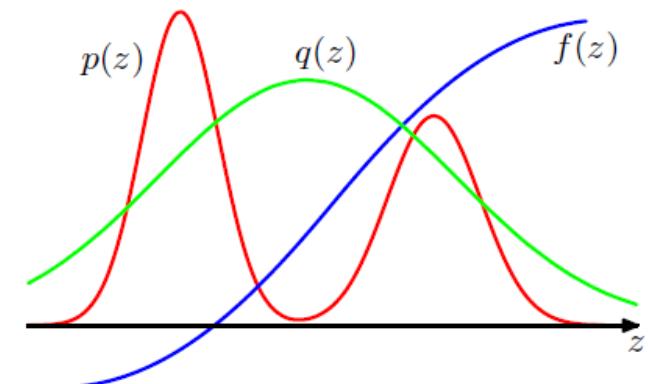
$$E_p[f] = \int f(x) p(x) dx = \int f(x) \frac{p(x)}{q(x)} q(x) dx$$

$$E_p[f] \simeq \frac{1}{n} \sum_{i=1}^n f(x^i) \frac{p(x^i)}{q(x^i)} \quad x^i \sim q(x)$$

$$E_p[f] \simeq \frac{1}{n} \sum_{i=1}^n f(x^i) w(x^i) \quad w(x^i) = \frac{p(x^i)}{q(x^i)}$$

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 $P(x)f(x)$ 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 $P(x)f(x)$ is large.



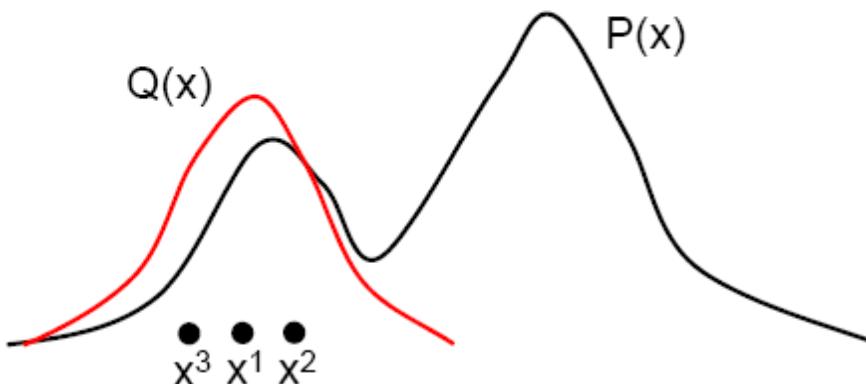
Problems of naïve Monte Carlo method

- ▶ 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

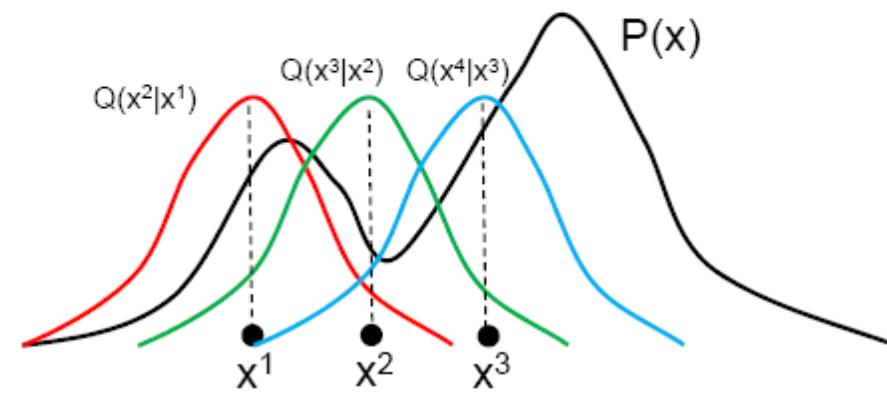
Markov chain Monte Carlo (MCMC)

- ▶ 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 $Q(x'|x)$



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

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

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 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 $x^* \sim q(x^*|x)$

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

Sample $u \sim \text{uniform}(0,1)$

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

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

Else:

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

Discard Burn-in samples

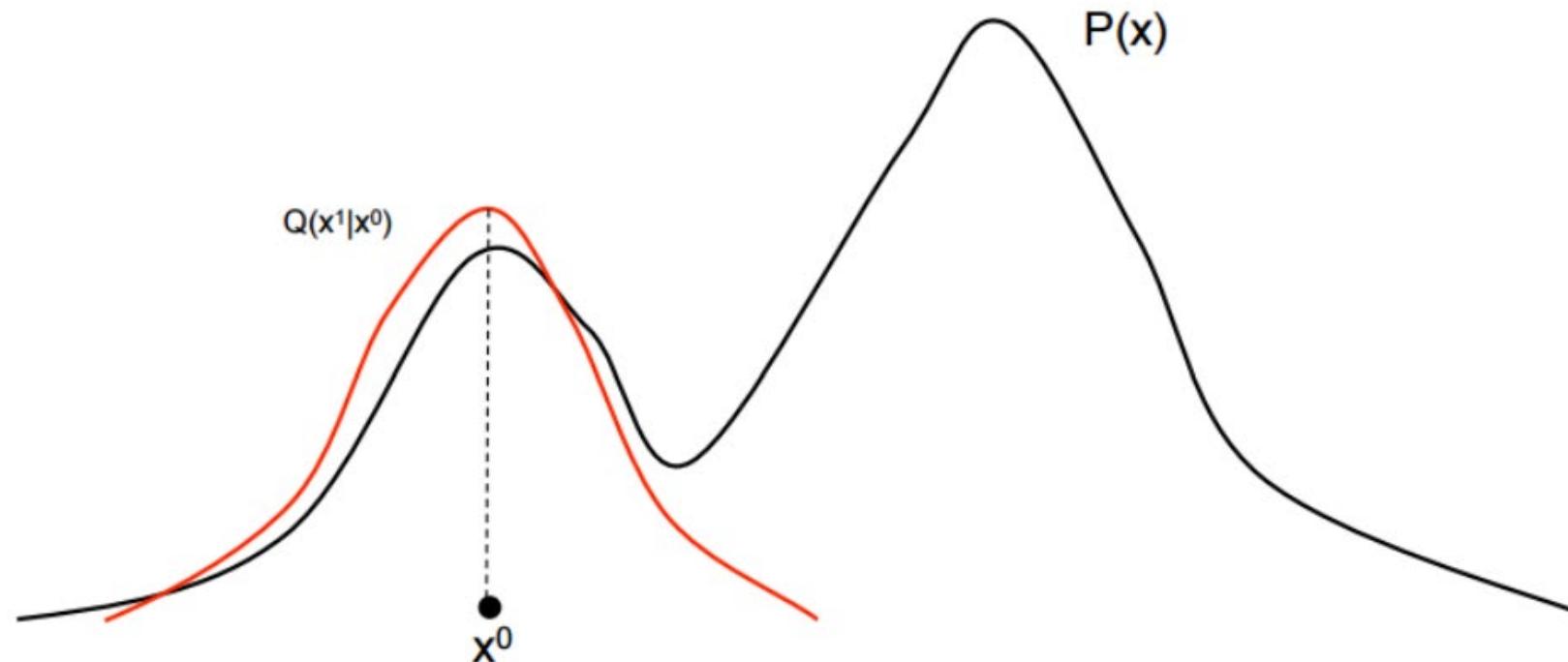


Markov chain Monte Carlo (MCMC)

- ▶ 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 $x^{(0)}$

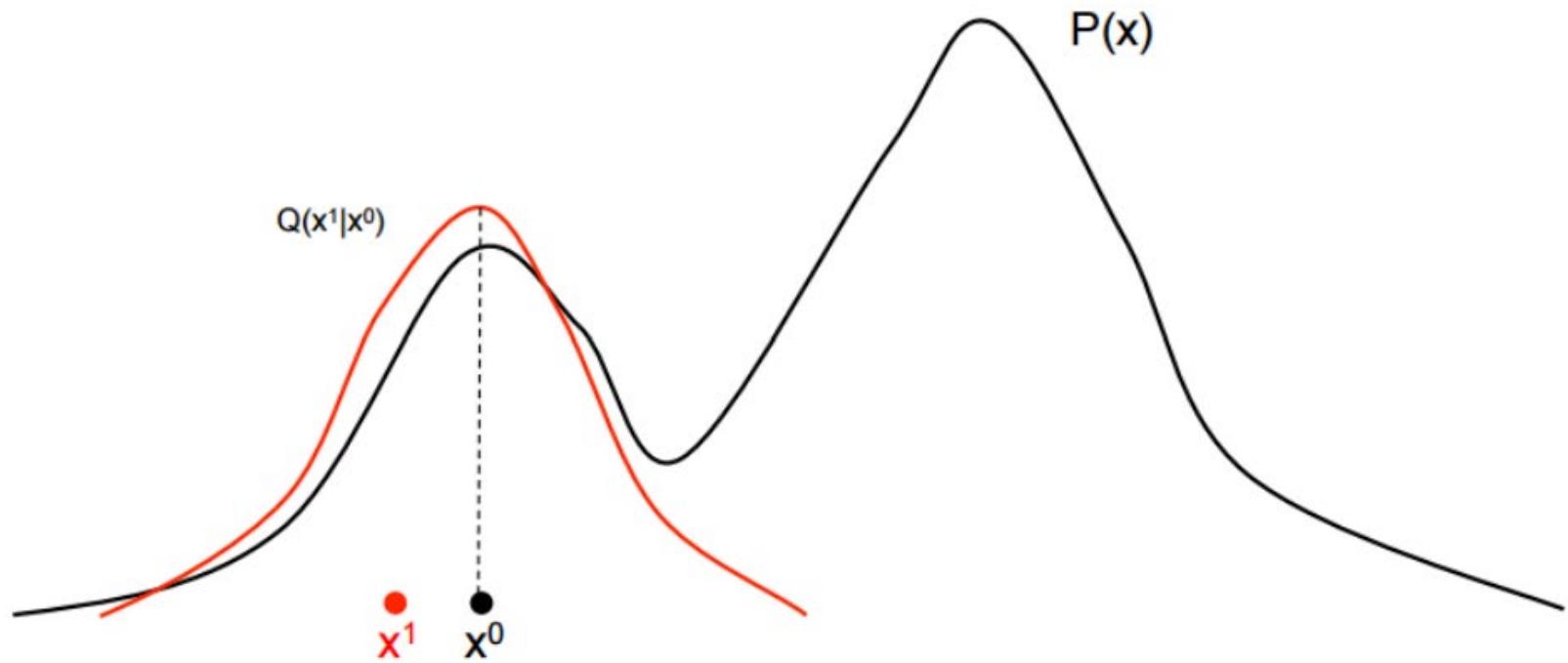
...



Markov chain Monte Carlo (MCMC)

► Metropolis-Hastings example:

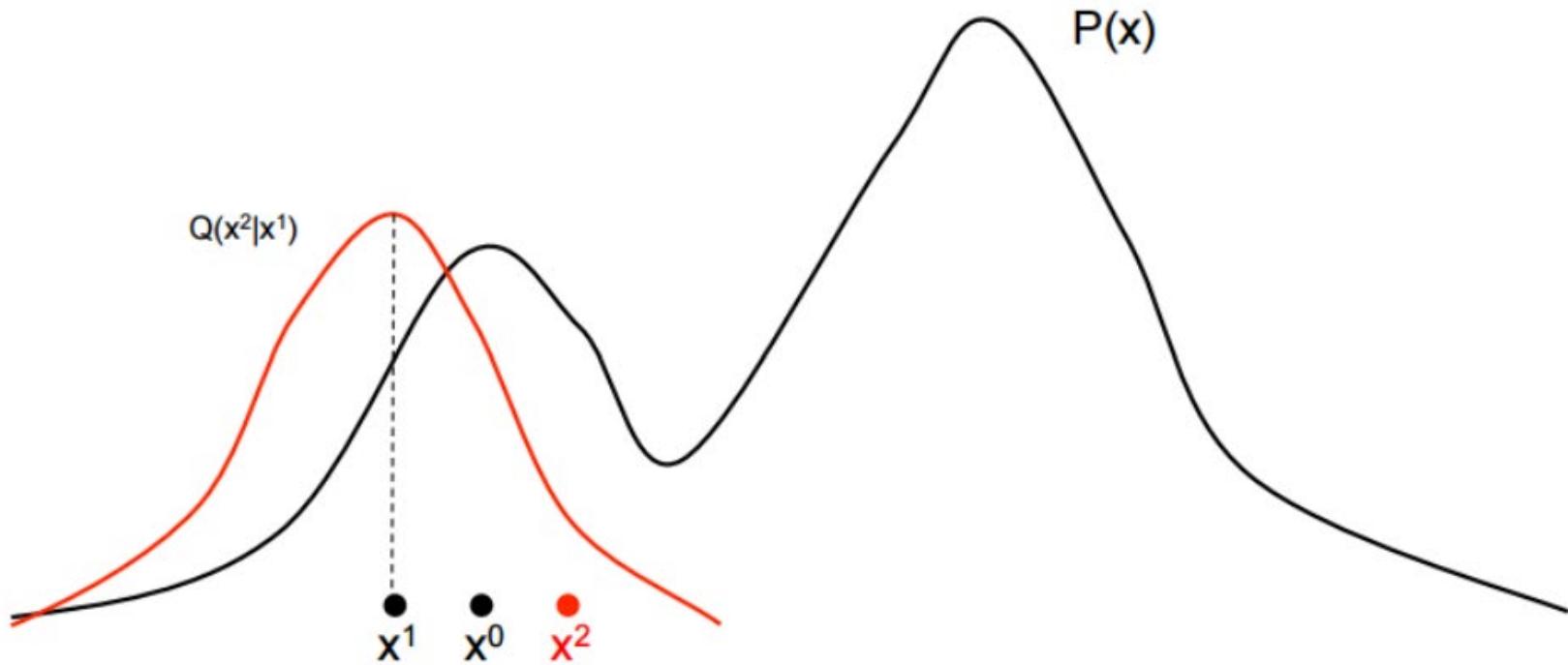
Initialize $x^{(0)}$
Draw, accept x^1



Markov chain Monte Carlo (MCMC)

► Metropolis-Hastings example:

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



Markov chain Monte Carlo (MCMC)

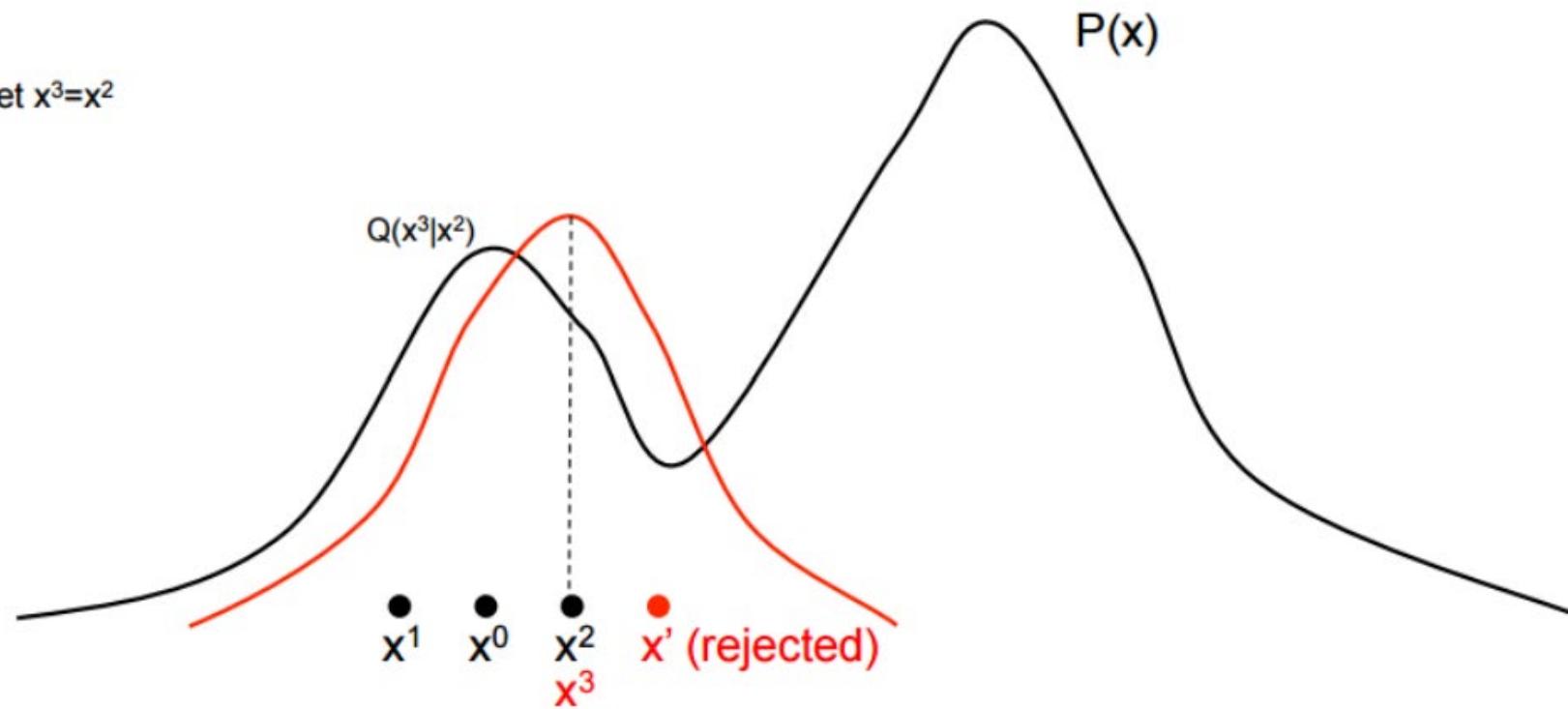
► Metropolis-Hastings example:

Initialize $x^{(0)}$

Draw, accept x^1

Draw, accept x^2

Draw but reject; set $x^3=x^2$

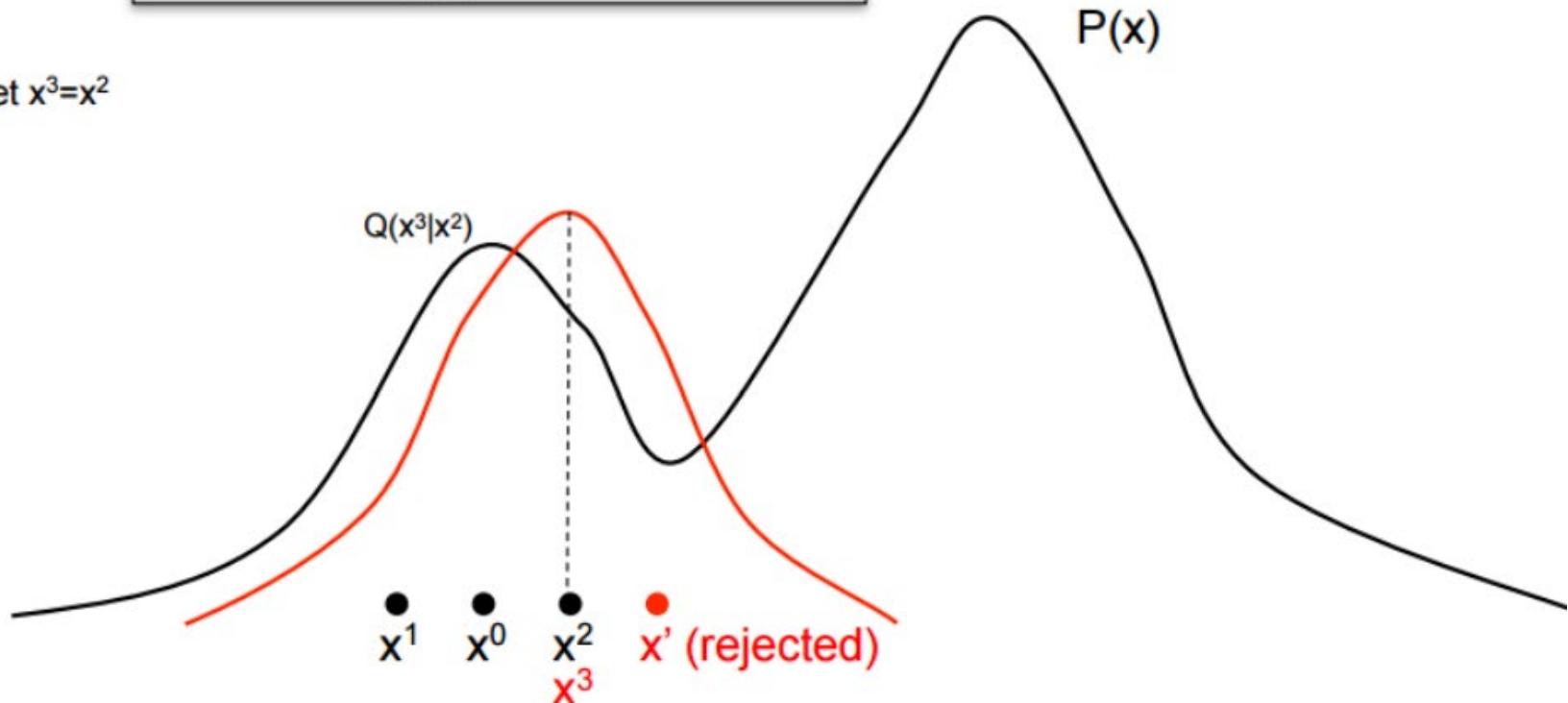


Markov chain Monte Carlo (MCMC)

► Metropolis-Hastings example:

Initialize $x^{(0)}$
Draw, accept x^1
Draw, accept x^2
Draw but reject; set $x^3=x^2$

We reject because $P(x')/P(x^2)$ is very small,
hence $A(x'|x^2)$ is close to zero!

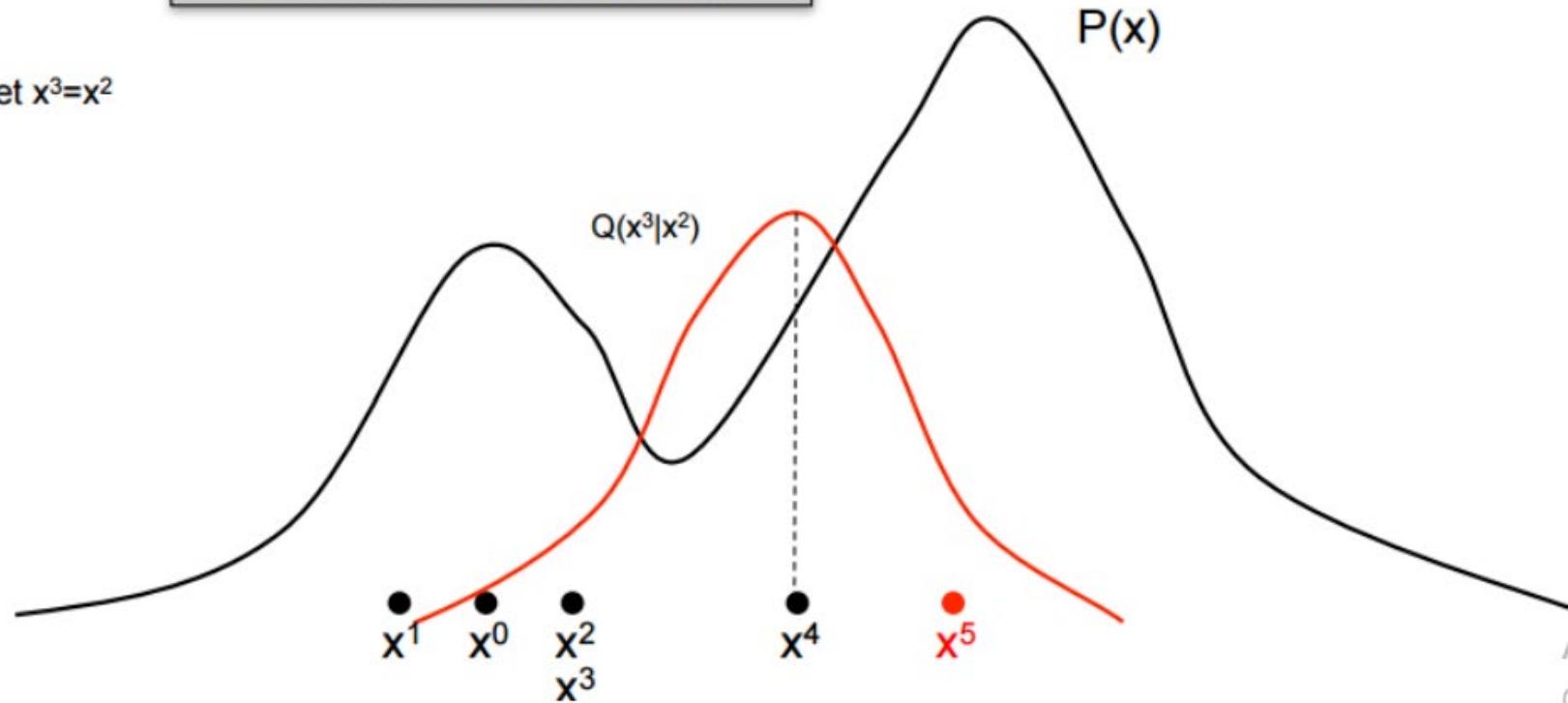


Markov chain Monte Carlo (MCMC)

► Metropolis-Hastings example:

Initialize $x^{(0)}$
Draw, accept x^1
Draw, accept x^2
Draw but reject; set $x^3=x^2$
Draw, accept x^4
Draw, accept x^5

The adaptive proposal $Q(x'|x)$ allows us to sample both modes of $P(x)$!



Next topic

- ▶ Probabilistic graphical models
 - ▶ Learning