CS 3750 Machine Learning
Lecture 6

Approximate probabilistic inference:
- **Markov Chain Monte Carlo (MCMC)**
- **Variational methods**

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Markov chain Monte Carlo

- **Importance sampling:** samples are generated according to Q and every sample from Q is reweighted according to w, but the Q distribution may be very far from the target
- **MCMC** is a strategy for generating samples from the target distribution, including conditional distributions
- **MCMC:**
  - Markov chain defines a sampling process that
  - initially generates samples very different from the target distribution (e.g. posterior)
  - but gradually refines the samples so that they are closer and closer to the posterior.

MCMC

- The construction of a Markov chain requires two basic ingredients
  - a transition matrix P
  - an initial distribution π_0
- Assume a finite set S={1,…m} of states, then **a transition matrix** is

$$P = \begin{pmatrix} p_{11} & p_{12} & \cdots & p_{1m} \\ p_{21} & p_{22} & \cdots & p_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ p_{m1} & p_{m2} & \cdots & p_{mm} \end{pmatrix}$$

Where $p_{ij} \geq 0 \quad \forall (i,j) \in S^2$ and $\sum_{j \in S} p_{ij} = 1 \quad \forall i \in S$

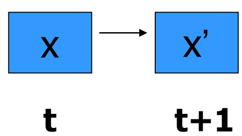
Markov Chain

- Markov chain defines a random process of selecting states

$x^{(0)}, x^{(1)}, \ldots x^{(m)}, \ldots$

Initial state selected based on π_0

Subsequent states selected based on the previous state and the transition matrix



- **Chain Dynamics**

$$P^{(t+1)}(X^{(t+1)} = x') = \sum_{x \in Dom(X)} P^{(t)}(X^{(t)} = x) T(x \rightarrow x')$$

Probability of a state x' being selected at time t+1

transition matrix

MCMC

- **Markov chain** satisfies

$$P(X_{n+1}=j \mid X_0=i_0, X_1=i_1, \dots X_n=i_n) = P(X_{n+1}=j \mid X_n=i_n)$$

- **Irreducibility:** A MC is called irreducible (or un-decomposable) if there is a positive transition probability for all pairs of states within a limited number of steps
- In irreducible chains there may still exist a periodic structure such that for each state $i \in S$, the set of possible return times to *i* when starting in *i* is a subset of the set $p\mathbb{N} = \{p, 2p, 3p, \dots\}$ containing all but a finite set of these elements. The smallest number *p* with this property is the so-called **period of the chain**

$$p = \gcd\{n \in N : p_{ii}^{(n)} > 0\}$$

MCMC

- **Aperiodicity:** An irreducible chain is called aperiodic (or acyclic) if the period *p* equals 1 or, equivalently, if for all pairs of states there is an integer n_{ij} such that for all $n \geq n_{ij}$, the probability $p^{(n)}_{ij}>0$.
- If a Markov chain satisfies both **irreducibility and aperiodicity**, then it **converges to an invariant distribution *q(x)***
- A Markov chain with transition matrix *P* will have an **equilibrium distribution** q **iff** $q = qP$.
- A sufficient, but not necessary, condition to ensure a particular q(x) is the invariant distribution of transition matrix P is the following **reversibility (detailed balance) condition**

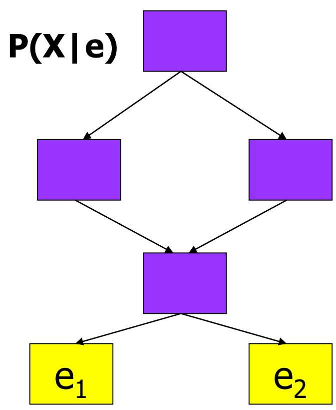
$$q(x^i)P(x^{i-1} \mid x^i) = q(x^{i-1})P(x^i \mid x^{i-1})$$

Markov Chain Monte Carlo

Objective: generate samples from the posterior distribution

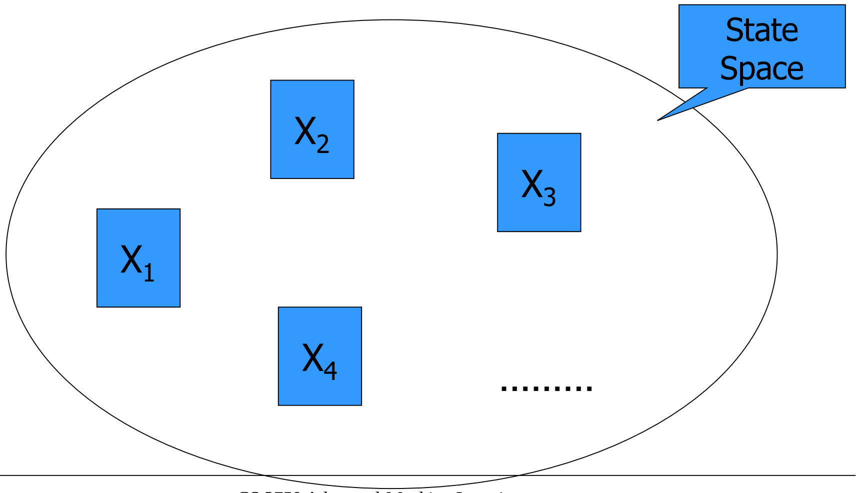
- **Idea:**
  - Markov chain defines a sampling process that
  - initially generates samples very different from the target posterior
  - but gradually refines the samples so that they are closer and closer to the posterior.

MCMC



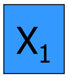
- P(X|e)— the query we want to compute
- e_1 & e_2 are known evidence
- Sampling from the distribution P(X) is very different from the desired posterior P(X|e)

Markov Chain Monte Carlo (MCMC)



MCMC (Cont.)

- **Goal:** a sample from P(X|e)
- Start from some P(X) and generate a sample x1



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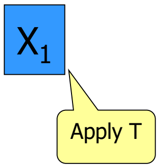
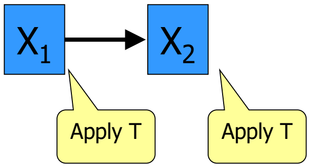


MCMC (Cont.)

- **Goal:** a sample from P(X|e)
- Start from some P(X) and generate a sample x1
- From x1 and transition generate x2



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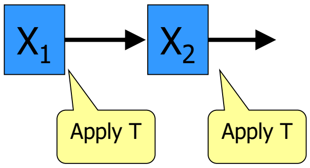
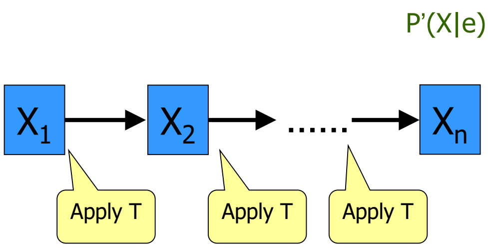


MCMC (Cont.)

- **Goal:** a sample from P(X|e)
- Start from some P(X) and generate a sample x1
- From x1 and transition generate x2
- Repeat for n steps



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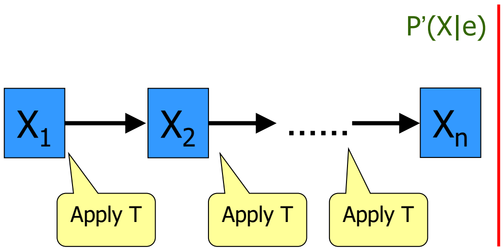

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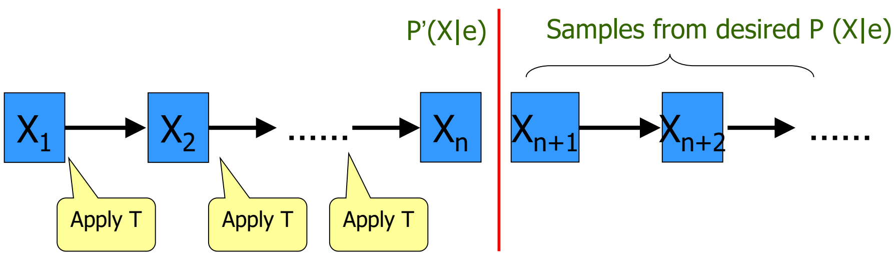


MCMC

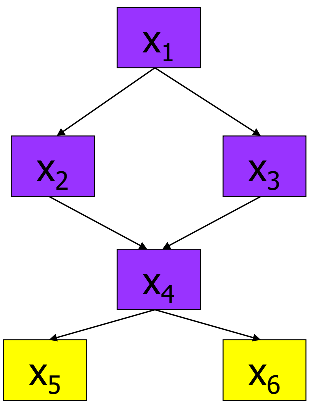
- In general, an MCMC sampling process doesn't have to converge **to a stationary distribution**
- A finite state Markov Chain has a unique stationary distribution **iff** the markov chain is regular
  - regular: exist some k, for each pair of states x and x', the probability of getting from x to x' in exactly k steps is greater than 0
- We want Markov chains that converge to a unique target distribution from any initial state

Big question:

- How to build such Markov chains?

Gibbs Sampling

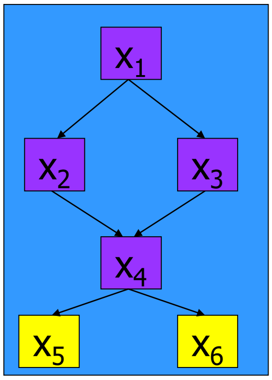
- A simple method to define MC for BBN
can benefit from the structure (independences) in the network



- **Evidence:**
  - x_5 =T
  - x_6 =T
- all variables have binary values T or F

Gibbs Sampling

Initial state



$\mathbf{X_0}$

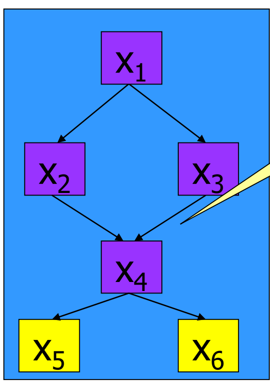
x_1=F, x_2=T
x_3=T, x_4=T

x_5=x_6=T (Fixed)

Gibbs Sampling

Initial state

Update Value of x_4

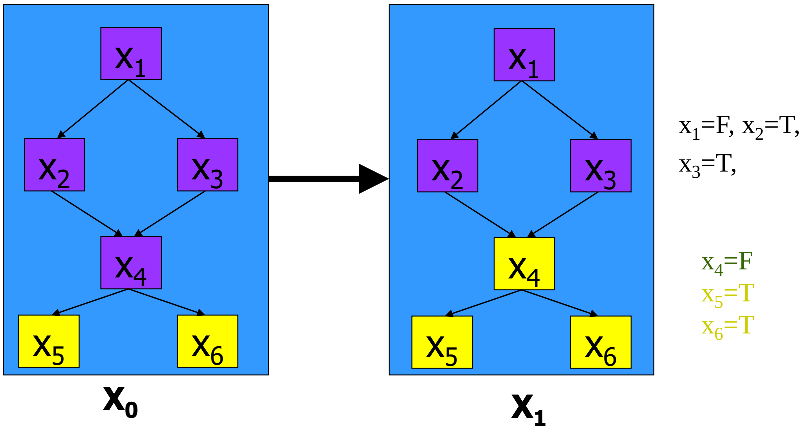


$\mathbf{X_0}$

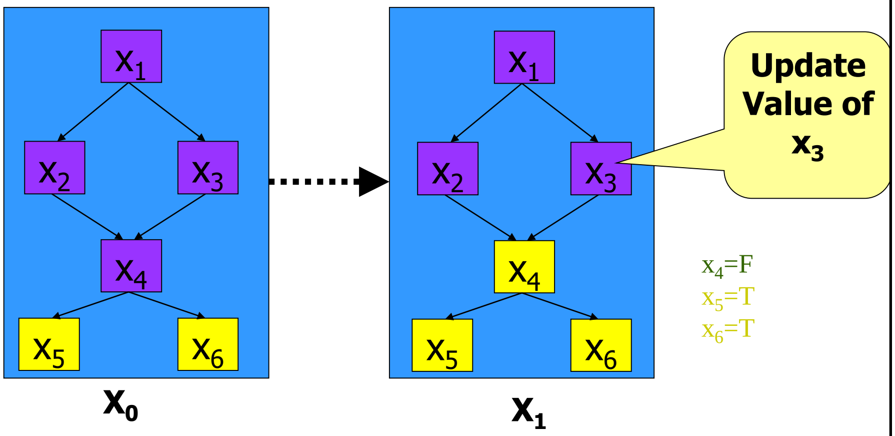
x_1=F, x_2=T
x_3=T, x_4=T

x_5=x_6=T (Fixed)

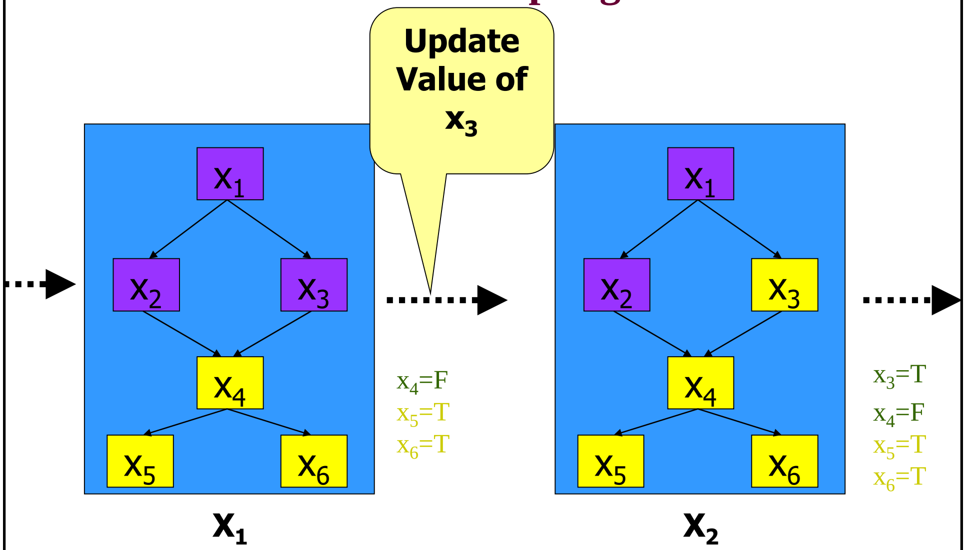
Gibbs Sampling



Gibbs Sampling

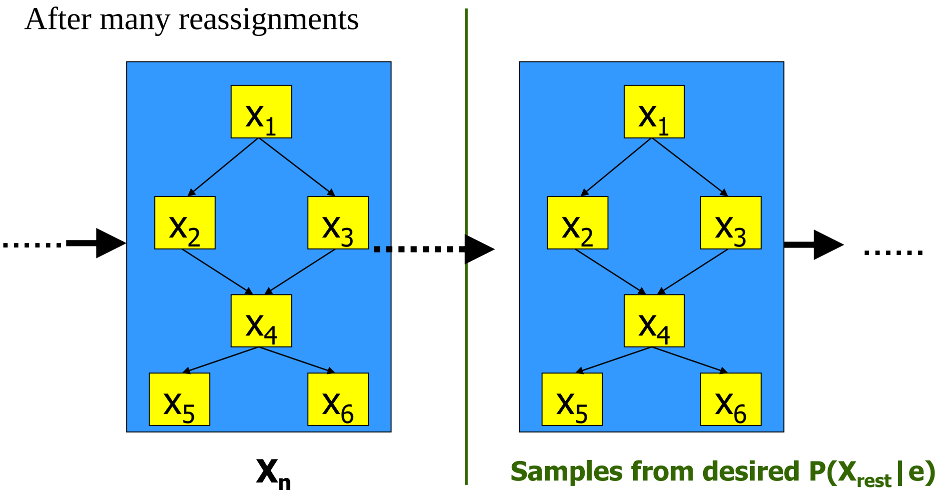


Gibbs Sampling



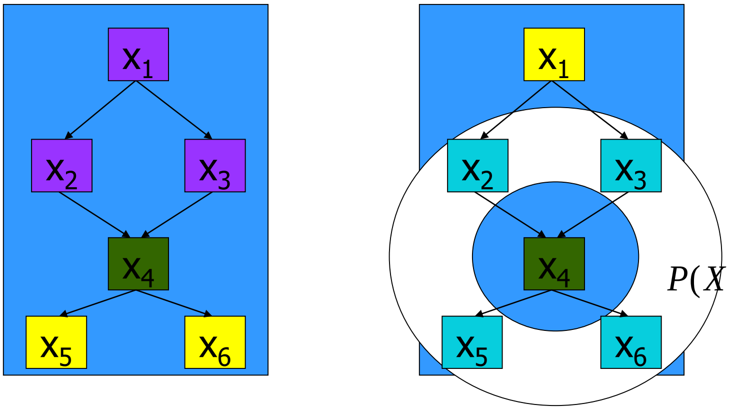
Gibbs Sampling

After many reassignments



Gibbs Sampling

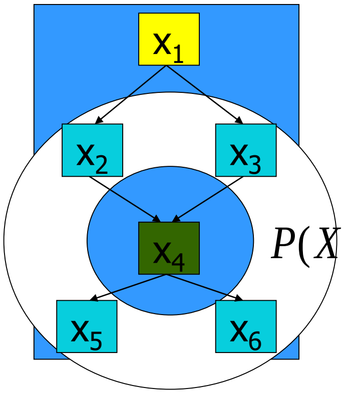
Keep resampling each variable using the value of variables in its local neighborhood (Markov blanket)



$$P(X_4 \mid x_2, x_3, x_5, x_6)$$

Gibbs Sampling

- Gibbs sampling takes advantage of the graphical model structure
- Markov blanket makes the variable independent from the rest of the network



$$P(X_4 \mid x_2, x_3, x_5, x_6)$$

Building a Markov Chain

- **A reversible Markov chain:**
- A sufficient, but not necessary, condition to ensure a particular q(x) is the invariant distribution of transition matrix P is the following reversibility (detailed balance) condition

$$q(x^i)P(x^{i-1} \mid x^i) = q(x^{i-1})P(x^i \mid x^{i-1})$$

- **Metropolis-Hastings algorithm**
  - builds a reversible Markov Chain
  - Uses a proposal distribution to generate candidate states
    - Either accept it and take a transition to state x'
    - Or reject it and stay at current state x

Building a Markov Chain

- **Metropolis-Hastings algorithm**
  - builds a reversible Markov Chain
  - uses the **proposal distribution** (similar to proposal the distribution in importance sampling) to generate candidates for x'
    - A proposal distribution Q: $T^{Q}(x \rightarrow x')$
    - Example: Uniform over the values of variables
  - Either accept a proposal and take a transition to state x'
  - Or reject it and stay at current state x
    - Acceptance probability

$$A(x \rightarrow x')$$

Building a Markov Chain

- **Transition for the MH:**

$$T(x \to x') = T^Q(x \to x') A(x \to x') \quad if \;\; x \neq x'$$

$$T(x \to x) = T^Q(x \to x) + \sum_{x' \neq x} T^Q(x \to x')(1 - A(x \to x'))$$

otherwise

- **From reversibility condition:**

$$q(x) T(x \to x') = q(x') T(x' \to x)$$

- **We get**

$$A(x \to x') = \min[1, \frac{q(x') T^Q(x' \to x)}{q(x) T^Q(x \to x')}]$$

Building a Markov Chain

- **Comparing Metropolis Hastings with Gibbs sampling**
  - For Gibbs

$$A(u_i, x_i \to u_i, x'_i)$$
$$= \min[1, \frac{P(x'_i \mid u_i) T^Q(u_i, x'_i \to u_i, x_i)}{P(x_i \mid u_i) T^Q(u_i, x_i \to u_i, x_i^{'})}]$$
$$= \min[1, \frac{P(x'_i \mid u_i) P(x_i \mid u_i)}{P(x_i \mid u_i) P(x'_i \mid u_i)}]$$
$$= \min[1, 1] = 1$$

  - Special MH, for which acceptance probability is 1.

Metropolis Hastings algorithm

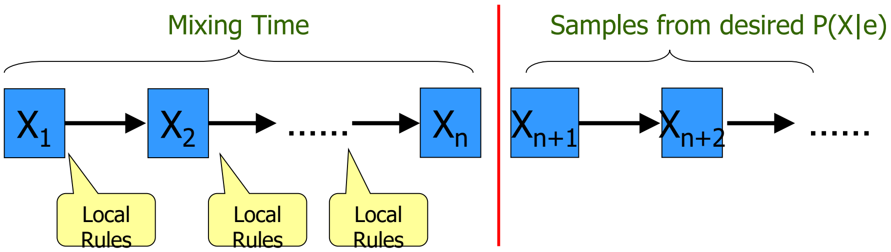
- **Assumptions:**
  - We can't draw the samples from q(x)
  - We can evaluate q(x) for any x
- We use a Markov chain that moves towards x* with acceptance probability

$$A(x, x^*) = \min\left[1, \frac{q(x^*)\,p(x \mid x^*)}{q(x)\,p(x^* \mid x)}\right]$$

- The transition kernel defined by this process satisfies the detailed balance condition

Mixing Time in Using Markov Chain

- **Mixing Time**
  - The number of steps we take until we collect a sample from the target distribution. (# = n)



Summary

- **Markov Chain Monte Carlo method** attempts to generate samples from posterior distribution
- **Metropolis Hastings algorithm** is a general scheme for specifying a Markov chain.
- **Gibbs sampling** is a special case that takes advantage of the network structure (Markov Blanket)

Variational approximations

Variational approximation

Assume we have a function $f(Z)$ that is hard to calculate

Example: *posterior probability in a complex BBNs*

$$P(Z \mid X)$$

- *this inference can be very hard*

Idea: replace calculations of $f(Z)$ **with an optimization over a simpler parametric function** $q(Z \mid \lambda)$

$$f(Z) \sim \max_{\lambda} q(Z \mid \lambda)$$

Variational lower bound

Let *X denote observed variables and*
Z denote target variables

$$P(Z \mid X) = \frac{P(X, Z)}{P(X)}$$

$$\log P(Z \mid X) = \log P(X, Z) - \log P(X)$$

$$\log P(X) = \log P(X, Z) - \log P(Z \mid X)$$

Assume some distribution: $\boxed{Q_\theta(Z \mid X)}$ *defined by parameters* θ

Average both sides with E_{Q_θ}

$$\sum_Z Q_\theta(Z \mid X) \log P(X) = \sum_Z Q_\theta(Z \mid X) \log P(X, Z) - \sum_Z Q_\theta(Z \mid X) \log P(Z \mid X)$$

$$\log P(X) = E_{Q_\theta}\left(\log P(X, Z)\right) - E_{Q_\theta}\left(\log P(Z \mid X)\right)$$

Variational lower bound

$$\log P(X) = E_{Q_\theta}(\log P(X,Z)) - E_{Q_\theta}(\log P(Z \mid X))$$

$$\log P(X) = \sum_Z Q_\theta(Z \mid X) \log P(X,Z) - \sum_Z Q_\theta(Z \mid X) \log P(Z \mid X)$$

$$\log P(X) = \sum_Z Q_\theta(Z \mid X) \log P(X,Z) - \sum_Z Q_\theta(Z \mid X) \log P(Z \mid X)$$
$$+ \sum_Z Q_\theta(Z \mid X) \log Q_\theta(Z \mid X) - \sum_Z Q_\theta(Z \mid X) \log Q_\theta(Z \mid X)$$

Kullback-Leibler divergence: distance between 2 distributions

$$KL(Q \mid P) = \sum_Z Q_\theta(Z \mid X) \log Q_\theta(Z \mid X) - \sum_Z Q_\theta(Z \mid X) \log P(Z \mid X)$$

Functional (Evidence lower bound or ELBO):

$$F(Q,P) = \sum_Z Q_\theta(Z \mid X) \log P(X,Z) - \sum_Z Q_\theta(Z \mid X) \log Q_\theta(Z \mid X)$$

$$\log P(X) = F(Q,P) + KL(Q \mid P)$$

Variational lower bound

$$\log P(X) = F(Q,P) + KL(Q \mid P)$$

distance between $Q_\theta(Z \mid X), P(Z \mid X)$

Always ≥ 0

Equals 0 if $Q_\theta(Z \mid X) = P(Z \mid X)$

We can optimize the approximation $Q_\theta(Z \mid X)$ by minimizing

$$\min_\theta KL(Q_\theta \mid P)$$

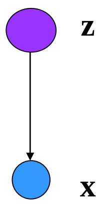
We can also do this by maximizing $F(Q_\theta, P)$

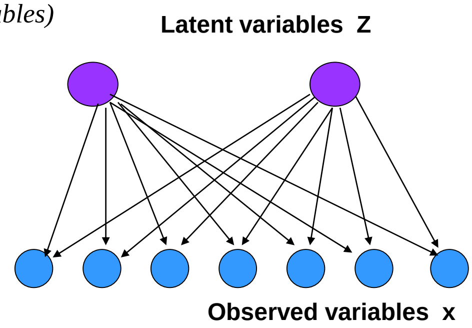
$$\max_\theta F(Q_\theta, P) \longleftarrow \text{Often much easier}$$

$$F(Q,P) = \sum_Z Q_\theta(Z \mid X) \log P(X,Z) - \sum_Z Q_\theta(Z \mid X) \log Q_\theta(Z \mid X)$$

Latent variable models

Let *X denote observed variables and*
Z denote hidden (latent variables)





Inference opposite the links is hard: $P(\mathrm{Z} \mid \mathrm{X})$

Solution: Define a simpler distribution : $Q_\theta(Z \mid X)$ to approximate $P(\mathrm{Z} \mid \mathrm{X})$

Optimize: $\max_\theta F(Q_\theta, P)$

$$F(Q,P) = \sum_Z Q_\theta(Z \mid X) \log P(X \mid Z) + \sum_Z Q_\theta(Z \mid X) \log P(Z) - \sum_Z Q_\theta(Z \mid X) \log Q_\theta(Z \mid X)$$

Mean field approximation

How to construct approximation of $Q_\theta(Z \mid X)$

Mean field approximation: ?

$$Q_\theta(Z \mid X) = \prod_i Q_i(Z_i \mid \theta_i)$$

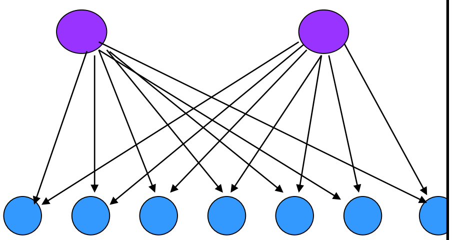
$$\max_\theta F(Q_\theta, P)$$

$$\max_\theta \sum_{Z_1, Z_2, \ldots Z_i} Q_\theta(Z \mid X) \log P(X, Z) - \sum_{Z_1, Z_2, \ldots Z_i} Q_\theta(Z \mid X) \log Q_\theta(Z \mid X)$$

$$\max_{\theta_1, \theta_2, \ldots \theta_i} \sum_{Z_1, Z_2, \ldots Z_i} \prod_i Q_i(Z_i \mid \theta_i) \log P(X, Z) - \sum_{Z_1, Z_2, \ldots Z_i} \prod_i Q_i(Z_i \mid \theta_i) \log \prod_i Q_i(Z_i \mid \theta_i)$$

Latent variable models

Let *X denote observed variables and Z denote hidden (latent variables)*



$$Q_\theta(Z \mid X) = \prod_i Q_i(Z_i \mid \theta_i)$$

$$\max_\theta F(Q_\theta, P)$$

$$\max_{\theta_1,\theta_2,\ldots\theta_i} \sum_{Z_1,Z_2,..Z_i} \prod_i Q_i(Z_i \mid \theta_i) \log P(X \mid Z) + \sum_{Z_1,Z_2,..Z_i} \prod_i Q_i(Z_i \mid \theta_i) \log P(Z_i) - \sum_{Z_1,Z_2,..Z_i} \prod_i Q_i(Z_i \mid \theta_i) \log \prod_i Q_i(Z_i \mid \theta_i)$$

Latent variable models

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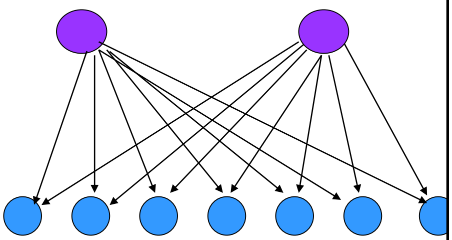

$$Q_\theta(Z \mid X) = \prod_i Q_i(Z_i \mid \theta_i)$$

$$\max_\theta F(Q_\theta, P)$$

$$\max_{\theta_1,\theta_2,\ldots\theta_i} \sum_{Z_1,Z_2,..Z_i} \prod_i Q_i(Z_i \mid \theta_i) \log P(X \mid Z) + \sum_i \sum_{Z_i} Q_i(Z_i \mid \theta_i) \log P(Z_i) - \sum_i \sum_{Z_i} Q_i(Z_i \mid \theta_i) \log Q_i(Z_i \mid \theta_i)$$

Express analytically F, differentiate wrt parameters and set to 0
→ Mean field equations that can be used to get optimal set θ