# Variational Inference

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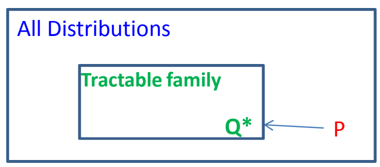
Nov. 6th 2008

## Outline

- Approximate Inference
- Variational inference formulation
  - Mean Field
    - Examples
  - Structured VI
    - Examples

# Approximate Inference

- Exact inference is exponential in clique size
- Posterior is **highly peaked**
  - Can be approximated by a **simpler** distribution
- Formulate inference as an optimization problem
  - Define an objective: how good is **Q**
  - Define a family of simpler distributions to search over
  - Find **Q*** that best approximate **P**

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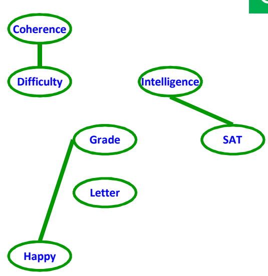
  - Find **Q*** that best approximate **P**
- Today we will cover **variational Inference**
  - Just a possible way of such a formulation
- There are many other ways
  - Variants of **loopy BP** (later in the semester)

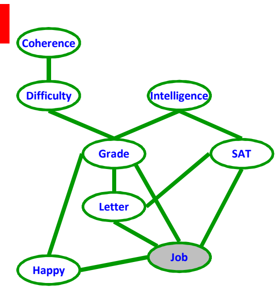
# What is Variational Inference?

Q




•Tractable Posterior **Family**
- **Set CPT (factors)**
- **Get distribution, Q**

P




- Posterior "hard" to compute
- We know the CPTs (factors)

$$Q^* = \min_{Q \in \mathcal{Q}} KL(Q \| P)$$

- Fully instantiated distribution Q*
- Enables exact Inference
  - Has low tree-width
  - Clique tree, variable elimination , etc.

# VI Questions

- Which family to choose
  - Basically we want to **remove some** edges
    - Mean field: fully factorized
    - Structured : Keep **tractable** sub-graphs
- How to carry the optimization

$$Q^* = \min_{Q \in \mathcal{Q}} KL(Q \| P)$$

- Assume P is a Markov network
  - Product of factors (that is all)

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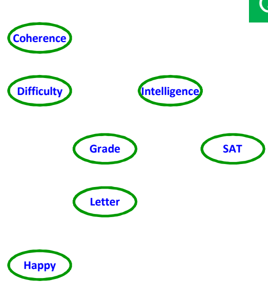
# Mean-field Variational Inference

Q

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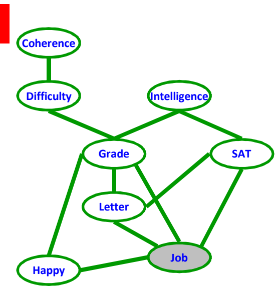


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$$Q^* = \operatorname*{Min}_{Q\in\mathcal{Q}} KL(Q\|P)$$

- Fully instantiated distribution Q*
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## D(q||p) for mean field – KL the reverse direction: cross-entropy term

- p: $\frac{1}{Z}\prod_i \phi_i(C_i)$
- q: $\prod_j Q_j(x_j)$

$$D(q||p) = \sum_{x} q(x)\log q(x) - \sum_{x} q(x)\log p(x)$$

(– cross entropy)

$$\sum_x q(x)\log p(x) = \sum_x q(x)\log \frac{1}{Z}\prod_i \phi_i(C_i) = \sum_i\sum_x q(x)\log\phi_i(C_i) - \sum_x q(x)\log Z$$

($\log Z \leftarrow$ constant wrt $q$)

$$\sum_x q(x)\log\phi_i(C_i) = \sum_{c_i} q(c_i)\log\phi_i(c_i) = E_q[\log\phi_i]$$

easy to compute!! :) (as long as $C_i$ not too large)

for mean fields $q(c_i) = \prod_{x_j\in C_i} Q_j(x_j)$



## The Energy Functional

$P = \frac{1}{Z}\prod_i \phi_i(C_i)$ $\quad Q = \prod_j q_j(x_j)$

- **Theorem** : $\ln Z = F[P_{\mathcal{F}}, Q] + D(Q||P_{\mathcal{F}})$

  Maximize ≡ Minimize

- Where energy functional:

$$F[P_{\mathcal{F}}, Q] = \sum_{\phi\in\mathcal{F}} E_Q[\ln\phi] + H_Q(\mathcal{X})$$

Tractable By construction

- Our problem now is

$$Q^* = \max_{\substack{Q\in\mathcal{Q}\\ \sum_{x_i} Q(X_i)=1}} F[P_F, Q]$$

You get →

Lower bound on lnZ

$$\ln Z \le F[P_F, Q] \quad \forall Q$$

Maximizing F[P,Q] tighten the bound
And gives better prob. estimates

$P = \frac{1}{Z} \prod_i \phi_i(C_i)$

## The Energy Functional

$Q = \prod_j q_j(x_j)$

- Our problem now is

$$F[P_{\mathcal{F}}, Q] = \sum_{\phi \in \mathcal{F}} E_Q[\ln \phi] + H_Q(\mathcal{X})$$

Tractable
By **construction**

$$Q^* = \underset{\substack{Q \in \mathcal{Q} \\ \sum_{x_i} Q(X_i) = 1}}{\text{Max}} F[P_F, Q]$$

- **Theorem**: Q is a stationary point of mean field approximation iff for each *j*:

$$Q_i(x_i) = \frac{1}{Z_i} \exp\left\{ \sum_{\phi \in \mathcal{F}} E_Q[\ln \phi \mid x_i] \right\}$$

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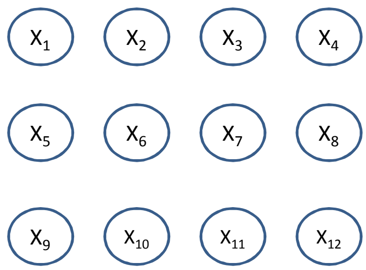
$$Q_i(x_i) = \frac{1}{Z_i} \exp\left\{ \sum_{\phi \in \mathcal{F}} E_Q[\ln \phi \mid x_i] \right\}$$

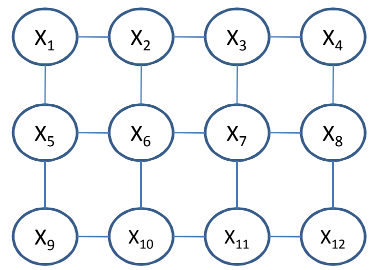
# Example

Q : fully factorized MN




$$Q(X) = \prod_i q_i(X_i)$$

P: Pairwise MN




$$P(X) \propto \prod_{i,j \in E} \phi(X_i, X_j)$$

- Given the factors in P, we want to get the factors for Q.
- Iterative procedure. Fix all $q_{-i}$ , compute $q_i$ via the above equation
- Iterate until you reach a fixed point

$$Q_i(x_i) = \frac{1}{Z_i} \exp\left\{ \sum_{\phi \in \mathcal{F}} E_Q[\ln \phi \mid x_i] \right\}$$

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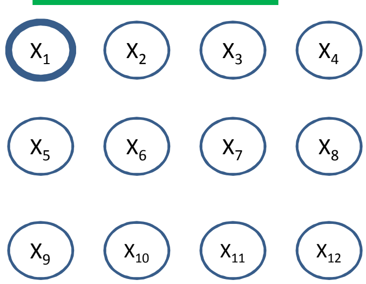


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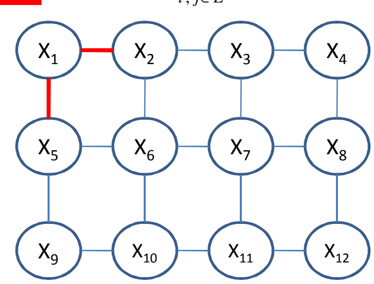


$$q_i(x_i) \propto \exp\left\{ \sum_{\phi_i : X_i \in scope[\phi_i]} E_{Q(U_\phi - \{X_i\})}[\ln \phi_i(x_i, U_\phi)]_i \right\}$$

$$q_i(x_1) \propto \exp\left\{ \begin{matrix} E_{Q(\{X_1, X_2\} - \{X_i\})}[\ln \phi\ (x_1, x_2)] + \\ E_{Q(\{X_1, X_5\} - \{X_i\})}[\ln \phi\ (x_1, x_5)] \end{matrix} \right\}$$

$$Q_i(x_i) = \frac{1}{Z_i}\exp\left\{\sum_{\phi\in\mathcal{F}} E_Q[\ln\phi \mid x_i]\right\}$$

# Example

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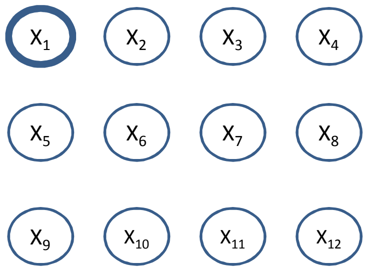


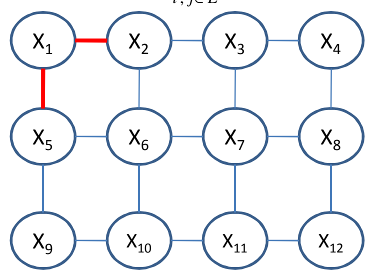


$$q_i(x_i) \propto \exp\left\{\sum_{\phi_i : X_i\in scope[\phi_i]} E_{Q(U_\phi - \{X_i\})}\left[\ln\phi_i(x_i, U_{\phi_i})\right]\right\}$$

$$q_i(x_1) \propto \exp\left\{E_{q(X_2)}\left[\ln\phi(x_1, x_2)\right] + E_{q(X_5)}\left[\ln\phi(x_1, x_5)\right]\right\}$$

$$\propto \exp\left\{\sum_{x_2} q_2(x_2)\ln\phi(x_1, x_2) + \sum_{x_5} q_5(x_5)\ln\phi(x_1, x_5)\right\}$$

$$Q_i(x_i) = \frac{1}{Z_i}\exp\left\{\sum_{\phi\in\mathcal{F}} E_Q[\ln\phi \mid x_i]\right\}$$

# Example

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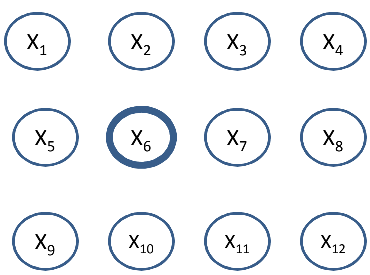


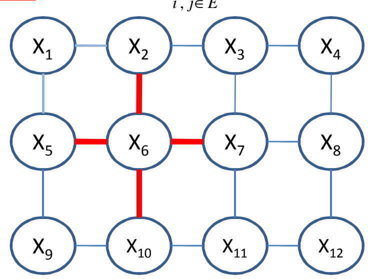


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In your homework

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# Example

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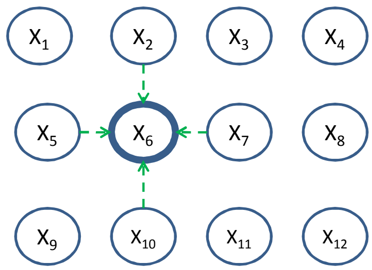


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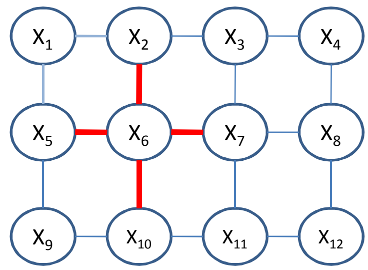


Intuitively

- $q(X_6)$ get to be tied with $q(x_i)$ for all xi that **appear in a factor with it in P**
  - **i.e. fixed point equations are tied according to P**
- What $q(x_6)$ gets is **expectations under these $q(x_i)$** of how **the factor looks like**
- can be somehow interpreted as **message passing** as well (**but we won't cover this**)

$$q_i(x_i) \propto \exp\left\{ \sum_{\phi_i : X_i \in scope[\phi_i]} E_{Q(U_\phi - \{X_i\})}\left[\ln \phi_i(x_i, U_\phi)\right]_i \right\}$$

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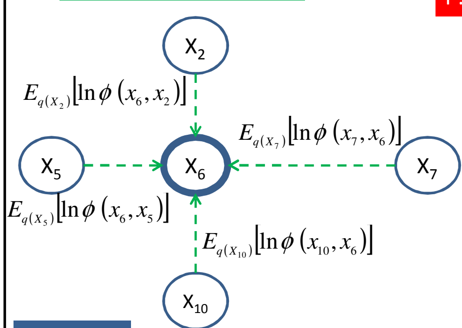


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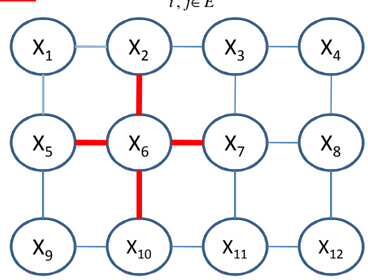


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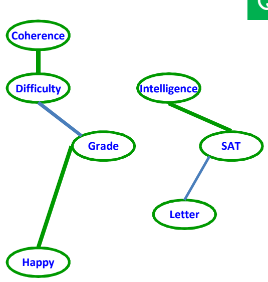
- Inference in LDA (time permits)

# Structured Variational Inference

Q

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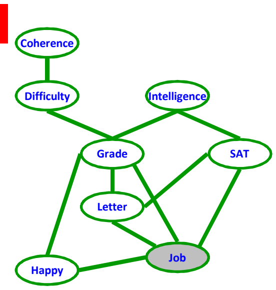


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- Fully instantiated distribution Q*
- **Enables exact Inference**
  - **Has low tree-width**
  - You don't have to remove all edges
  - Just keep tractable sub graphs: **trees, chain**

# Structured Variational Inference

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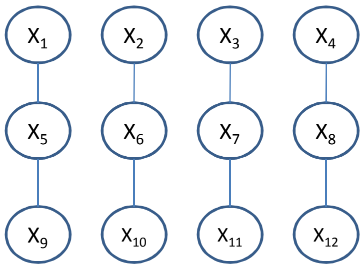
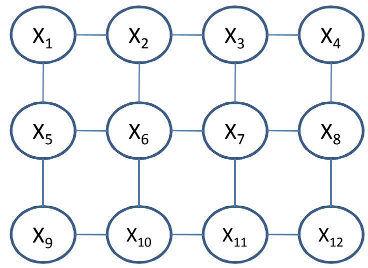



$$Q(X) \propto \prod_{i,j \in E_q} \psi_{i,j}(X_i, X_j)$$

$$P(X) \propto \prod_{i,j \in E} \phi(X_i, X_j)$$

**Goal**

Given factors in P, get factors in Q that minimize energy functional

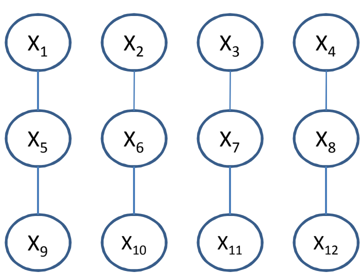
$$F[P_{\mathcal{F}}, Q] = \sum_{\phi \in \mathcal{F}} E_Q[\ln \phi] + H_Q(\mathcal{X})$$

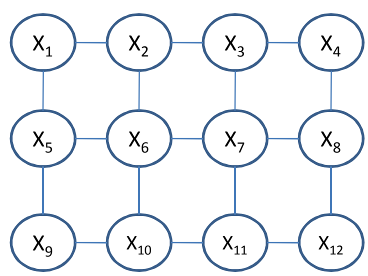
**Still** tractable
By **construction**

# Fixed point Equations

Q : **tractably** factorized MN

P: Pairwise MN

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$$\psi_j(\mathbf{c}_j) \propto \exp\left[\sum_{\phi \in A_j} E_Q[\ln \phi | \mathbf{c}_j] - \sum_{\psi_k \in B_j} E_Q[\ln \psi_k | \mathbf{c}_j]\right]$$

Factors that scope() is not independent of $C_j$ in Q

# Fixed point Equations

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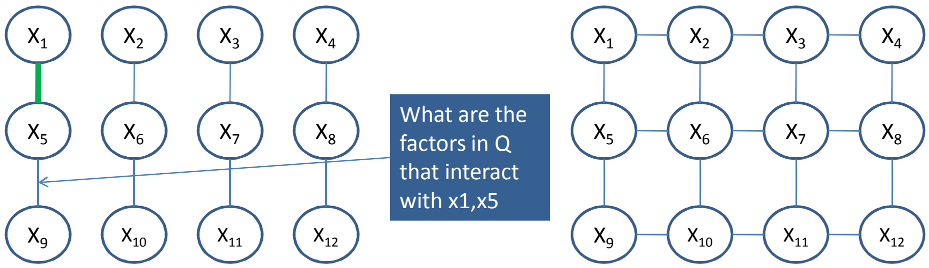


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Factors that scope() is not independent of $C_j$ in Q

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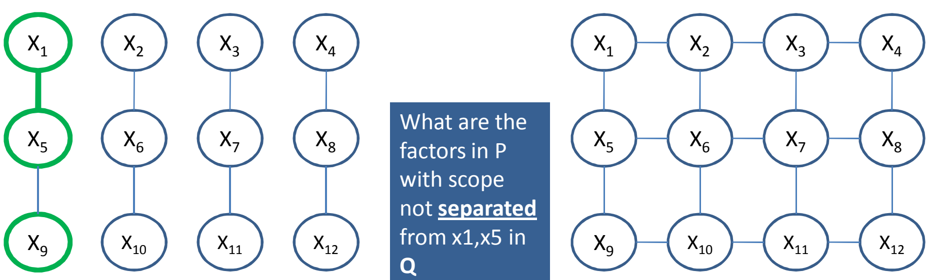


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- First, get variables that can not be separated form $x_1$ and $x_5$ in **Q**
- Second collect the factors they appear in in P

$$\psi_j(\mathbf{c}_j) \propto \exp\left[\sum_{\phi\in A_j} E_Q[\ln\phi|\mathbf{c}_j] - \sum_{\psi_k\in B_j} E_Q[\ln\psi_k|\mathbf{c}_j]\right]$$

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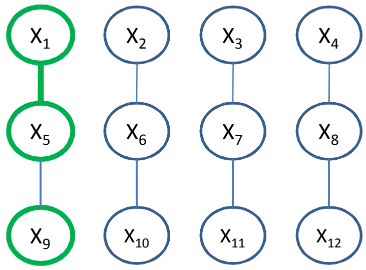
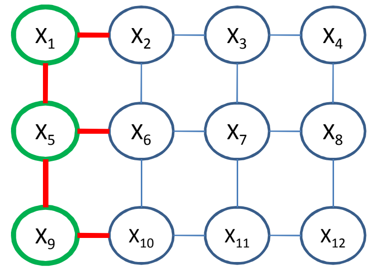



$$Q(X) \propto \prod_{i,j\in E_q} \psi_{i,j}(X_i, X_j)$$

What are the factors in P with scope not **separated** from x1,x5 in **Q**

P: Pairwise MN




$$P(X) \propto \prod_{i,j\in E} \phi(X_i, X_j)$$

- First, get variables that can not be separated form $x_1$ and $x_5$ in **Q**
-Second collect the factors they appear in in P
- Expectation is taken over **Q(scope[factor] | $c_j$)**

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# Fixed point Equations

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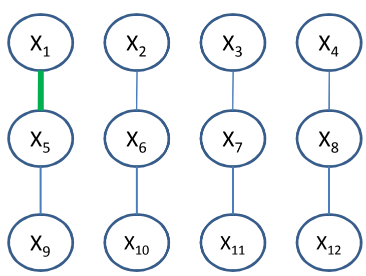


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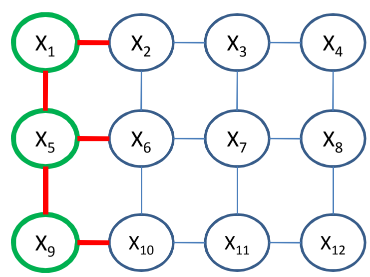


$$P(X) \propto \prod_{i,j\in E} \phi(X_i, X_j)$$

B = $\psi_{59}$

A = $\phi_{15}\ \phi_{59}\ \phi_{12}\ \phi_{56}\ \phi_{9,10}$

$$\psi_j(\mathbf{c}_j) \propto \exp\left[\sum_{\phi\in A_j} E_Q[\ln\phi|\mathbf{c}_j] - \sum_{\psi_k\in B_j} E_Q[\ln\psi_k|\mathbf{c}_j]\right]$$

$$E_Q[\ln\phi(x_5,x_9) \mid x_1,x_5] = E_{Q(x_9|x_1,x_5)}[\ln\phi(x_5,x_9)]$$

$\psi_j(\mathbf{c}_j) \propto \exp\left[\sum_{\phi \in A_j} E_Q[\ln \phi | \mathbf{c}_j] - \sum_{\psi_k \in B_j} E_Q[\ln \psi_k | \mathbf{c}_j]\right]$

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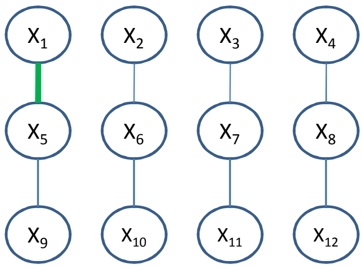


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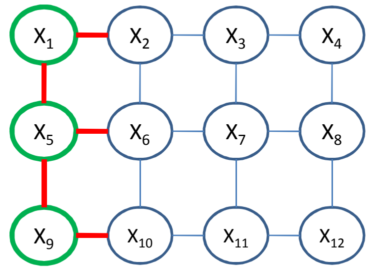


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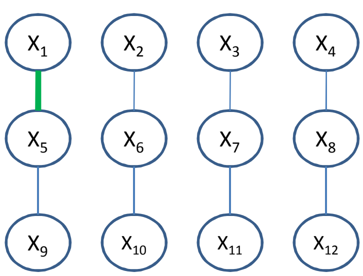
$\psi_j(\mathbf{c}_j) \propto \exp\left[\sum_{\phi \in A_j} E_Q[\ln \phi | \mathbf{c}_j] - \sum_{\psi_k \in B_j} E_Q[\ln \psi_k | \mathbf{c}_j]\right]$

$$E_Q\left[\ln \psi_{5,9}(x_5, x_9) \mid x_1, x_5\right] = E_{Q(x_9 \mid x_1, x_5)}\left[\ln \psi(x_5, x_9)\right]$$

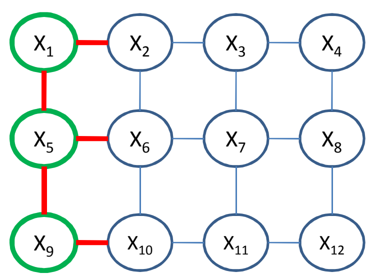
$\psi_j(\mathbf{c}_j) \propto \exp\left[\sum_{\phi \in A_j} E_Q[\ln \phi | \mathbf{c}_j] - \sum_{\psi_k \in B_j} E_Q[\ln \psi_k | \mathbf{c}_j]\right]$

# Fixed point Equations

Q : **tractably** factorized MN




P: Pairwise MN




$$\mathrm{Q}(\mathrm{X}) \propto \prod_{i,j \in E_q} \psi_{i,j}(X_i, X_j)$$

$$\mathrm{P}(\mathrm{X}) \propto \prod_{i,j \in E} \phi(X_i, X_j)$$

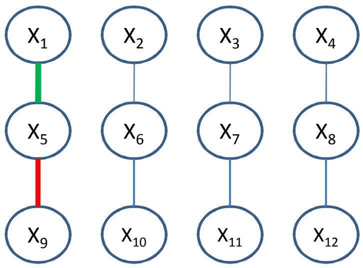
$$E_Q\left[\ln \phi_{9,10}(x_9, x_{10}) \mid x_1, x_5\right] = E_{Q(x_9, x_{10} \mid x_1, x_5)}\left[\ln \phi_{9,10}(x_9, x_{10})\right]$$

$$Q(x_9, x_{10} \mid x_1, x_5) = Q(x_9 \mid x_1, x_5) Q(x_{10})$$

$$\psi_j(\mathbf{c}_j) \propto \exp\left[\sum_{\phi\in A_j} E_Q[\ln\phi|\mathbf{c}_j] - \sum_{\psi_k\in B_j} E_Q[\ln\psi_k|\mathbf{c}_j]\right]$$

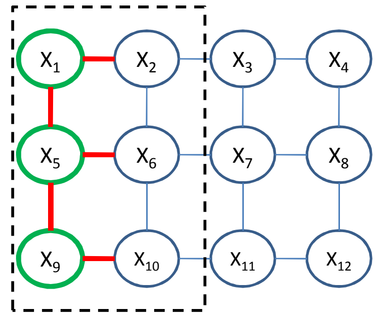
## Some intuition

Q : **tractably** factorized MN




$$Q(X) \propto \prod_{i,j\in E_q} \psi_{i,j}(X_i, X_j)$$

P: Pairwise MN




$$P(X) \propto \prod_{i,j\in E} \phi(X_i, X_j)$$

-What have we picked from P when dealing with the first factor (X1,x5)?
 -Factors that interact with (x1,x5) in both P and Q
 - Fixed point equations are tied in the same way these variables are tied in P and Q
- can be also interpreted as passing message over Q of expectations on these factors
- Q: how to compute these madrigals in Q efficiently? Homework!

# Variational Inference in Practice

- Highly used
  - Fast and efficient
  - Approximation quality might be not that good
    - Always peaked answers (we are using the wrong KL)
    - Always captures modes of P
    - Spread of P is usually lost
  - Famous applications of VI
    - VI for topic models (LDA)
      - You can derive LDA equations in few lines using the fully factorized update equations (**exercise**)
      - We might go over it in a special recitations but try it if you are doing a project in topic models
    - Involved temporal models
    - Many more…