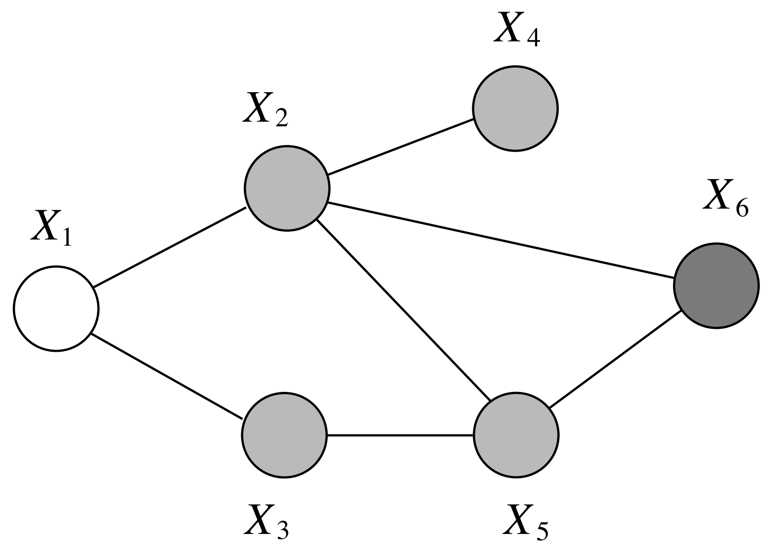
Probabilistic Graphical Models

Brown University CSCI 2950-P, Spring 2013
Prof. Erik Sudderth

Lecture 10: Triangulation and Junction Tree Algorithms

Some figures courtesy Michael Jordan's draft textbook,
An Introduction to Probabilistic Graphical Models

Inference in Undirected Graphs



$$\begin{aligned}
p(x_1, \bar{x}_6) &= \frac{1}{Z} \sum_{x_2} \sum_{x_3} \sum_{x_4} \sum_{x_5} \sum_{x_6} \psi(x_1, x_2)\psi(x_1, x_3)\psi(x_2, x_4)\psi(x_3, x_5)\psi(x_2, x_5, x_6)\delta(x_6, \bar{x}_6) \\
&= \frac{1}{Z} \sum_{x_2} \psi(x_1, x_2) \sum_{x_3} \psi(x_1, x_3) \sum_{x_4} \psi(x_2, x_4) \sum_{x_5} \psi(x_3, x_5) \sum_{x_6} \psi(x_2, x_5, x_6)\delta(x_6, \bar{x}_6) \\
&= \frac{1}{Z} \sum_{x_2} \psi(x_1, x_2) \sum_{x_3} \psi(x_1, x_3) \sum_{x_4} \psi(x_2, x_4) \sum_{x_5} \psi(x_3, x_5) m_6(x_2, x_5) \\
&= \frac{1}{Z} \sum_{x_2} \psi(x_1, x_2) \sum_{x_3} \psi(x_1, x_3) m_5(x_2, x_3) \sum_{x_4} \psi(x_2, x_4) \\
&= \frac{1}{Z} \sum_{x_2} \psi(x_1, x_2) m_4(x_2) \sum_{x_3} \psi(x_1, x_3) m_5(x_2, x_3) \\
&= \frac{1}{Z} \sum_{x_2} \psi(x_1, x_2) m_4(x_2) m_3(x_1, x_2) \;=\; \frac{1}{Z} m_2(x_1)
\end{aligned}$$

A Graph Elimination Algorithm

Algebraic Marginalization Operations

- Marginalize out the variable associated with sum node
- Compute a new potential table involving all other variables which depend on the just-marginalized variable

Graph Manipulation Operations

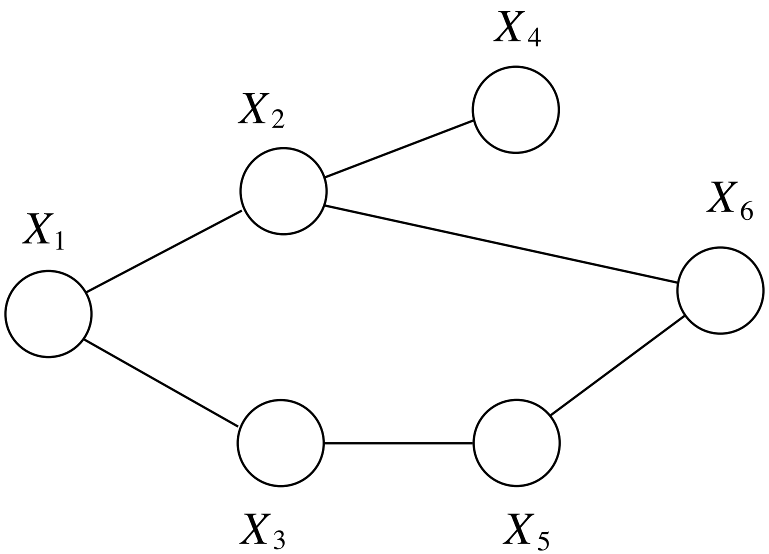
- Remove, or *eliminate*, a single node from the graph
- Add edges (if they don't already exist) between all pairs of nodes who were neighbors of the just-removed node

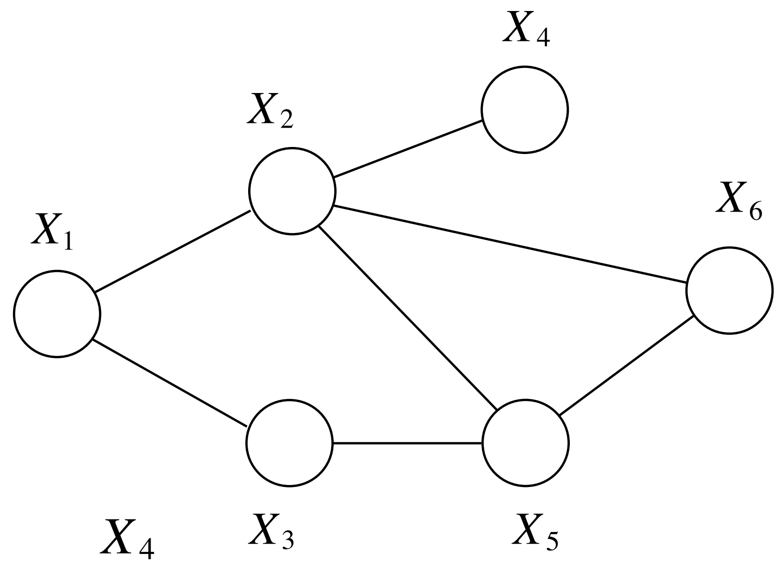
A Graph Elimination Algorithm

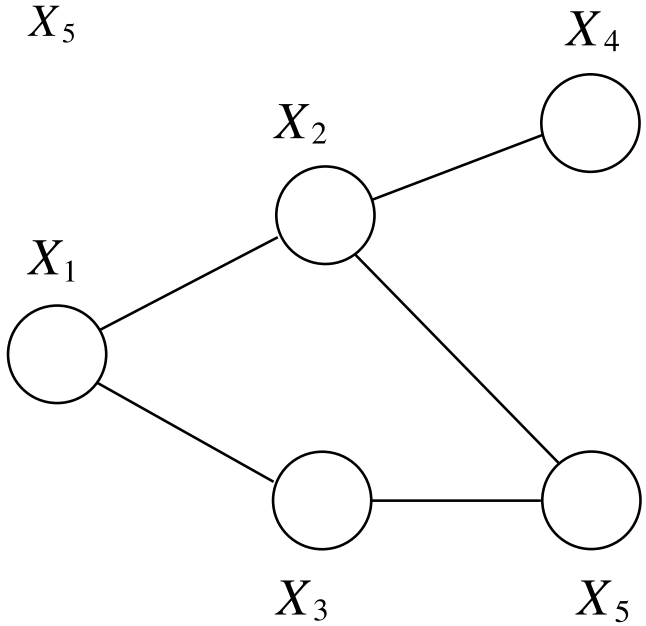
- Choose an elimination ordering (query nodes should be last)
- Eliminate a node, remove its incoming edges, add edges between all pairs of its neighbors
- Iterate until all non-query nodes are eliminated

Graph Elimination Example

Elimination Order: (6,5,4,3,2,1)







Graph Elimination Example

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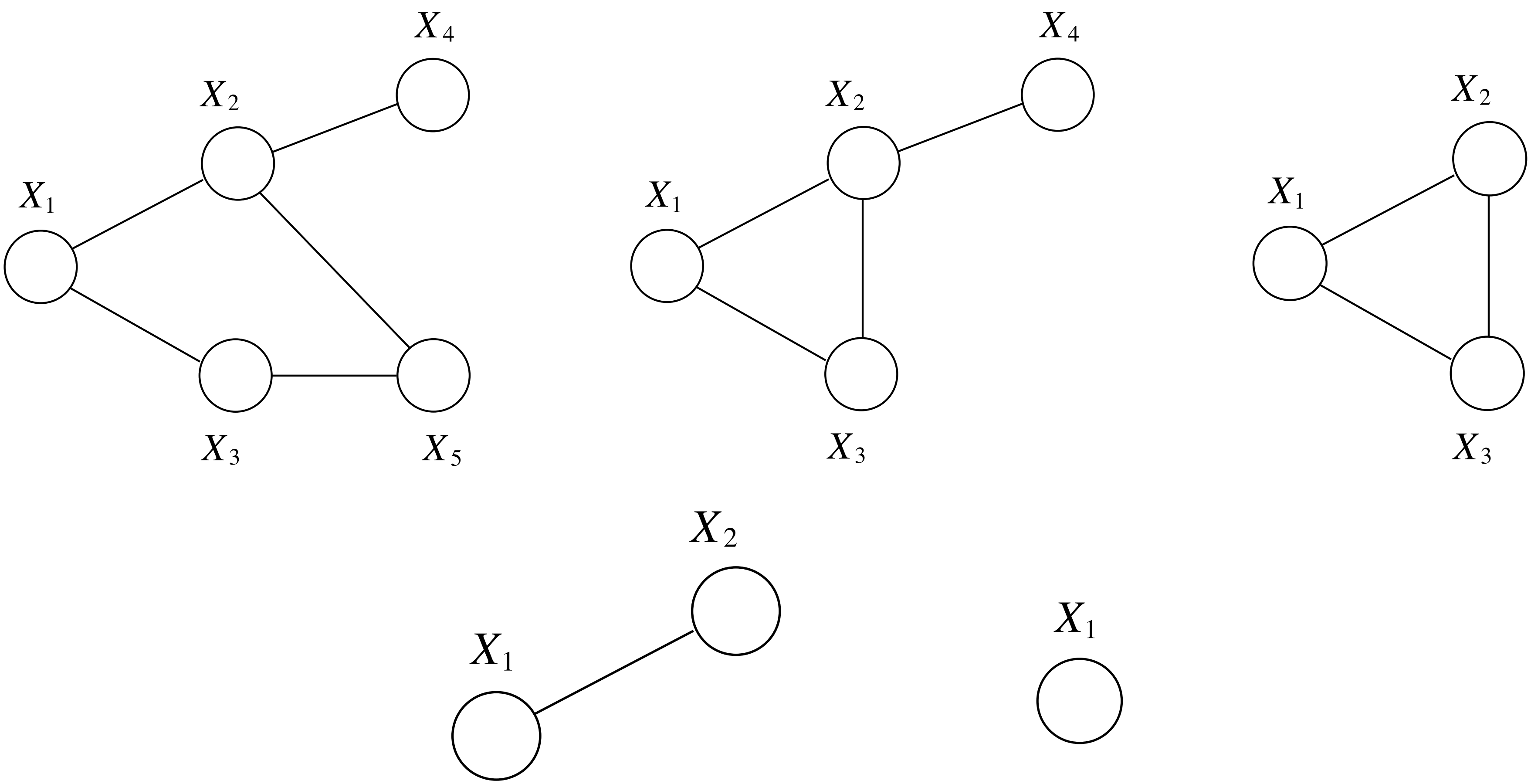
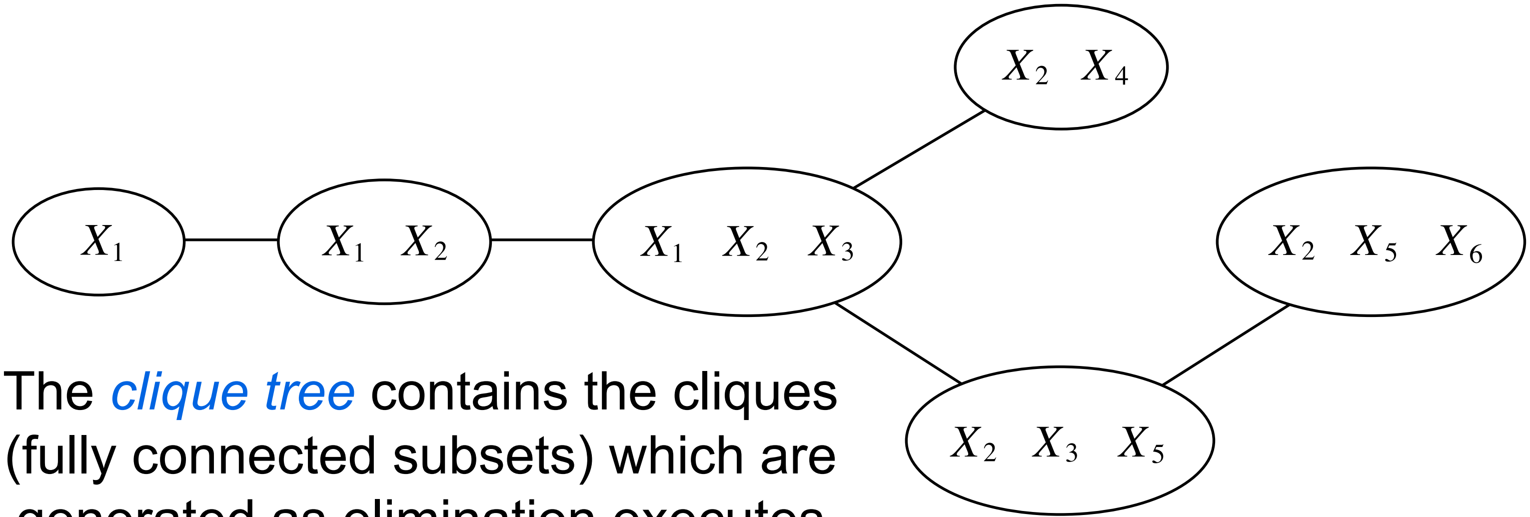
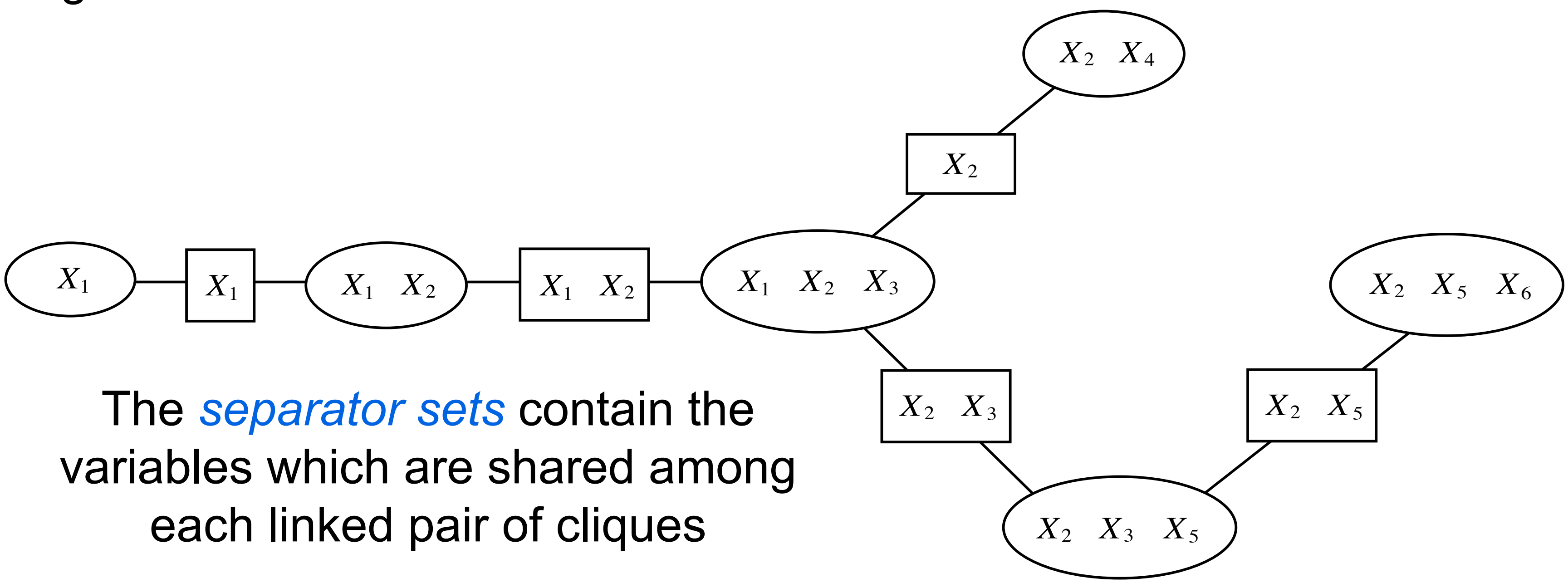


Elimination Clique Tree

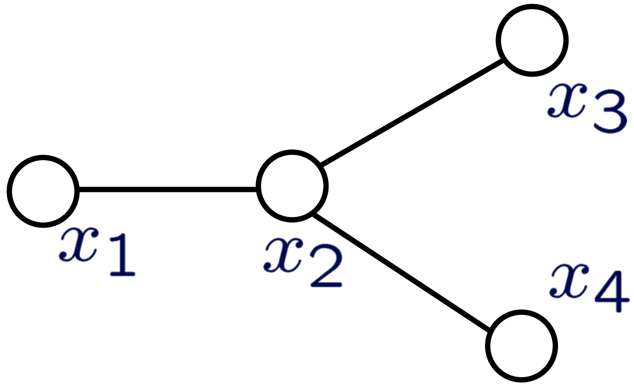


The *clique tree* contains the cliques (fully connected subsets) which are generated as elimination executes



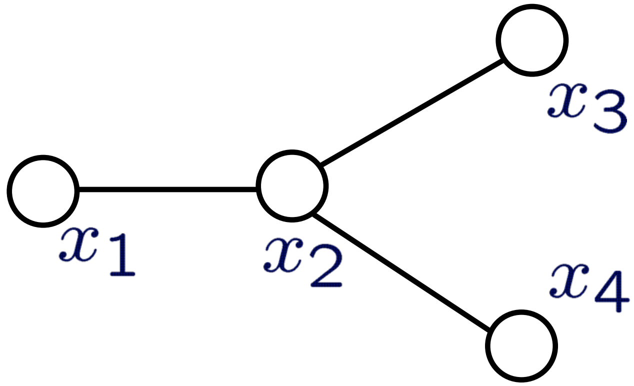
The *separator sets* contain the variables which are shared among each linked pair of cliques

Elimination for Trees



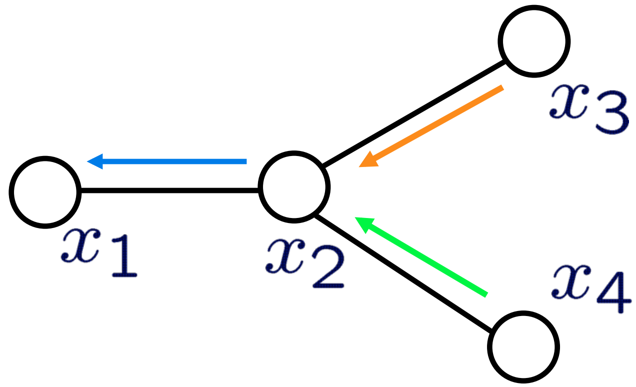
$$\begin{aligned} p_1(x_1) &= \sum_{x_2,x_3,x_4} \psi_1(x_1)\psi_{12}(x_1,x_2)\psi_2(x_2)\psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4) \\ &= \psi_1(x_1) \sum_{x_2,x_3,x_4} \psi_{12}(x_1,x_2)\psi_2(x_2)\psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4) \end{aligned}$$

Elimination for Trees



$$p_1(x_1) = \sum_{x_2,x_3,x_4} \psi_1(x_1)\psi_{12}(x_1,x_2)\psi_2(x_2)\psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4)$$
$$= \psi_1(x_1) \sum_{x_2,x_3,x_4} \psi_{12}(x_1,x_2)\psi_2(x_2)\psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4)$$
$$= \psi_1(x_1) \sum_{x_2} \psi_{12}(x_1,x_2)\psi_2(x_2) \sum_{x_3,x_4} \psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4)$$

Elimination for Trees

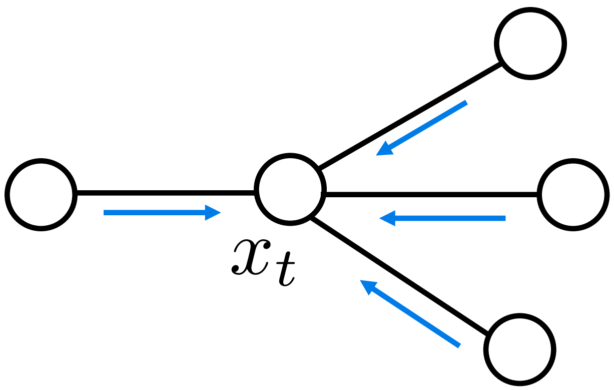


$$
\begin{aligned}
p_1(x_1) &= \sum_{x_2,x_3,x_4} \psi_1(x_1)\psi_{12}(x_1,x_2)\psi_2(x_2)\psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4) \\
&= \psi_1(x_1) \sum_{x_2,x_3,x_4} \psi_{12}(x_1,x_2)\psi_2(x_2)\psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4) \\
&= \psi_1(x_1) \sum_{x_2} \psi_{12}(x_1,x_2)\psi_2(x_2) \sum_{x_3,x_4} \psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4) \\
&= \psi_1(x_1) \underbrace{\sum_{x_2} \psi_{12}(x_1,x_2)\psi_2(x_2) \underbrace{\left[\sum_{x_3} \psi_{23}(x_2,x_3)\psi_3(x_3)\right]}_{m_{32}(x_2)} \cdot \underbrace{\left[\sum_{x_4} \psi_{24}(x_2,x_4)\psi_4(x_4)\right]}_{m_{42}(x_2)}}_{m_{21}(x_1)}
\end{aligned}
$$

$$
m_{21}(x_1) = \sum_{x_2} \psi_{12}(x_1,x_2)\psi_2(x_2)m_{32}(x_2)m_{42}(x_2)
$$

Belief Propagation (Sum-Product)

BELIEFS: Posterior marginals

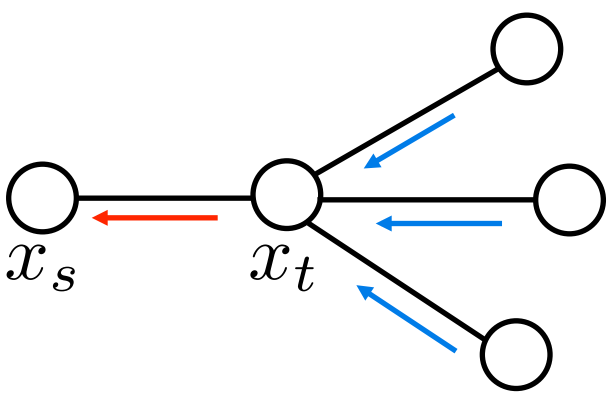


$$\hat{p}_t(x_t) \propto \psi_t(x_t) \prod_{u \in \Gamma(t)} m_{ut}(x_t)$$

$\Gamma(t) \longrightarrow$ neighborhood of node t
(adjacent nodes)

MESSAGES: Sufficient statistics

$$m_{ts}(x_s) \propto \sum_{x_t} \psi_{st}(x_s, x_t)\psi_t(x_t) \prod_{u \in \Gamma(t) \setminus s} m_{ut}(x_t)$$



I) Message Product
II) Message Propagation

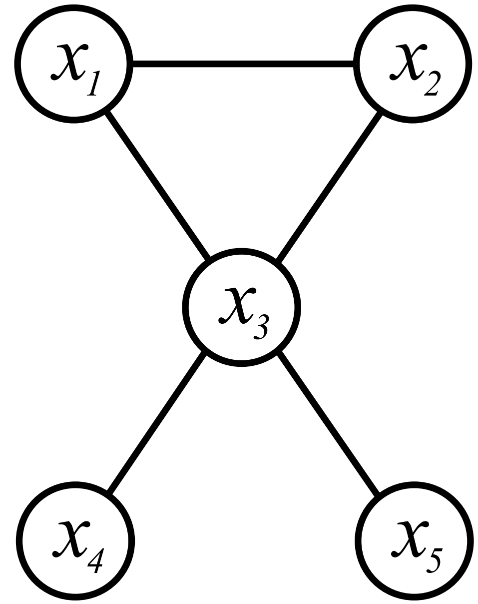
Undirected Inference Algorithms

	One Marginal	***All Marginals***
Tree	elimination applied to leaves of tree	belief propagation or sum-product algorithm
Graph	elimination algorithm	junction tree algorithm: belief propagation on a junction tree

- For directed models, first convert to undirected factor graph form (moralization)
- A *junction tree* is a clique tree with special properties

Undirected Graphical Models

$$p(x) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \psi_c(x_c)$$



- Parameterization exactly captures those non-degenerate distributions which are Markov with respect to this graph
- For now, we *will* assume that potentials are restricted to maximal cliques

$\mathcal{C} \longrightarrow$ set of maximal cliques (fully connected subsets) of nodes

$\mathcal{E} \longrightarrow$ set of undirected edges (s,t) linking pairs of nodes

$\mathcal{V} \longrightarrow$ set of N nodes or vertices, $\{1, 2, \ldots, N\}$

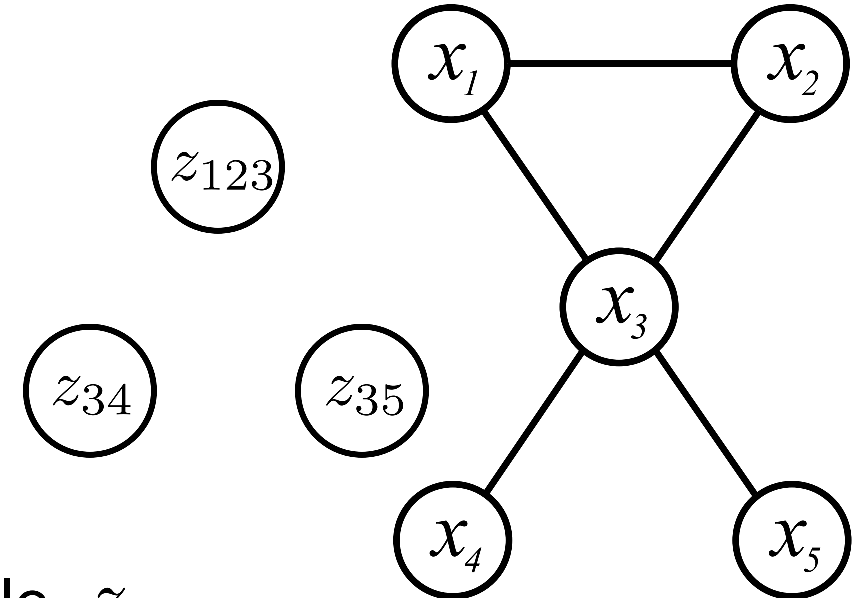
$Z \longrightarrow$ normalization constant (partition function)

Clique-Based Inference Algorithms

$$p(x) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \psi_c(x_c)$$

$$z_c = \{x_s \mid s \in c\}, \; c \in \mathcal{C}$$

$$p(z) \propto \prod_{c \in \mathcal{C}} \psi_c(z_c)$$



- For each clique c, define a variable z_c which enumerates *joint* configurations of dependent variables
- Does this define an equivalent joint distribution?

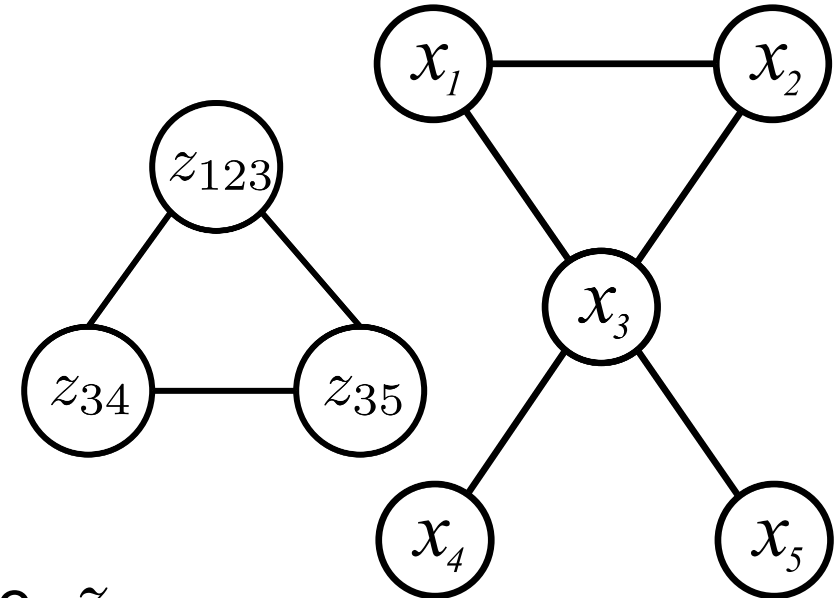
PROBLEM: We have defined multiple copies of the variables in the true model, but not enforced any relationships among them

Clique-Based Inference Algorithms

$$p(x) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \psi_c(x_c)$$

$$z_c = \{x_s \mid s \in c\}, \;\; c \in \mathcal{C}$$

$$p(z) \propto \prod_{c \in \mathcal{C}} \psi_c(z_c) \prod_{d \neq c} \psi_{cd}(z_c, z_d)$$



- For each clique c, define a variable z_c which enumerates *joint* configurations of dependent variables
- Add potentials enforcing consistency between all pairs of clique variables which share one of the original variables:

$$\psi_{cd}(z_c, z_d) = \begin{cases} 1 & z_c = z_d \text{ for all } x_s, s \in c \cap d \\ 0 & \text{otherwise} \end{cases}$$

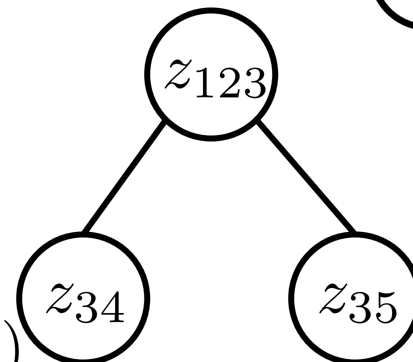
PROBLEM: The graph may have a large number of pairwise consistency constraints, and inference will be difficult

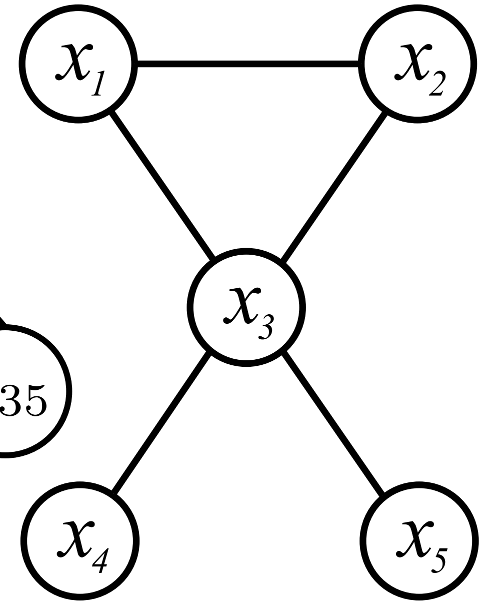
Clique-Based Inference Algorithms

$$p(x) = \frac{1}{Z} \prod_{c \in \mathcal{C}} \psi_c(x_c)$$

$$z_c = \{x_s \mid s \in c\}, \; c \in \mathcal{C}$$

$$p(z) \propto \prod_{c \in \mathcal{C}} \psi_c(z_c) \prod_{(c,d) \in \mathcal{E}(\mathcal{C})} \psi_{cd}(z_c, z_d)$$



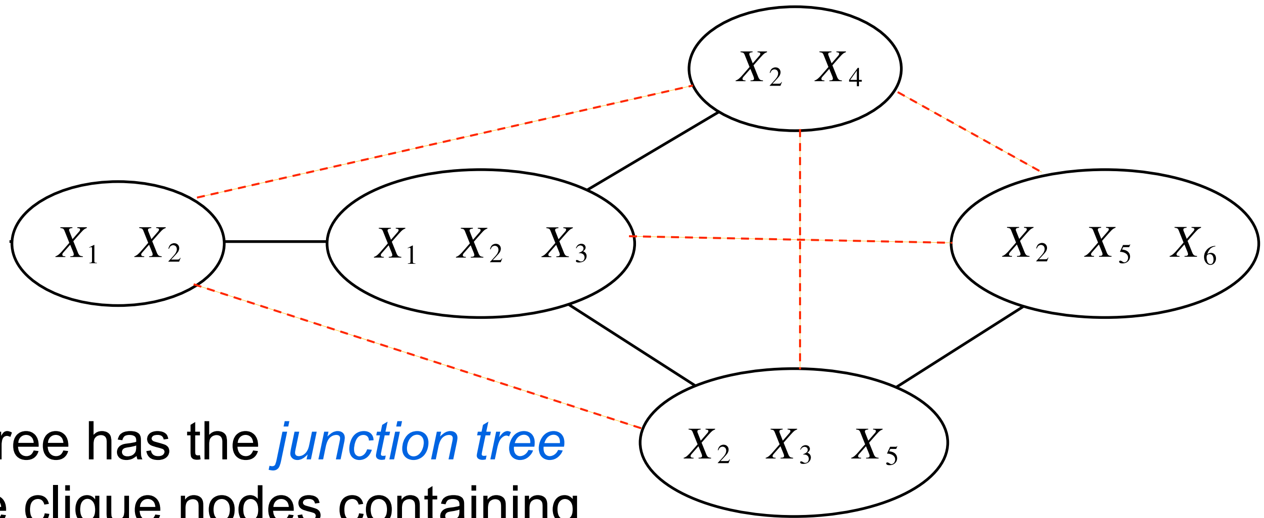


- For each clique c, define a variable z_c which enumerates *joint* configurations of dependent variables
- Add potentials enforcing consistency between some subset of pairs of cliques, taking advantage of transitivity of equality:

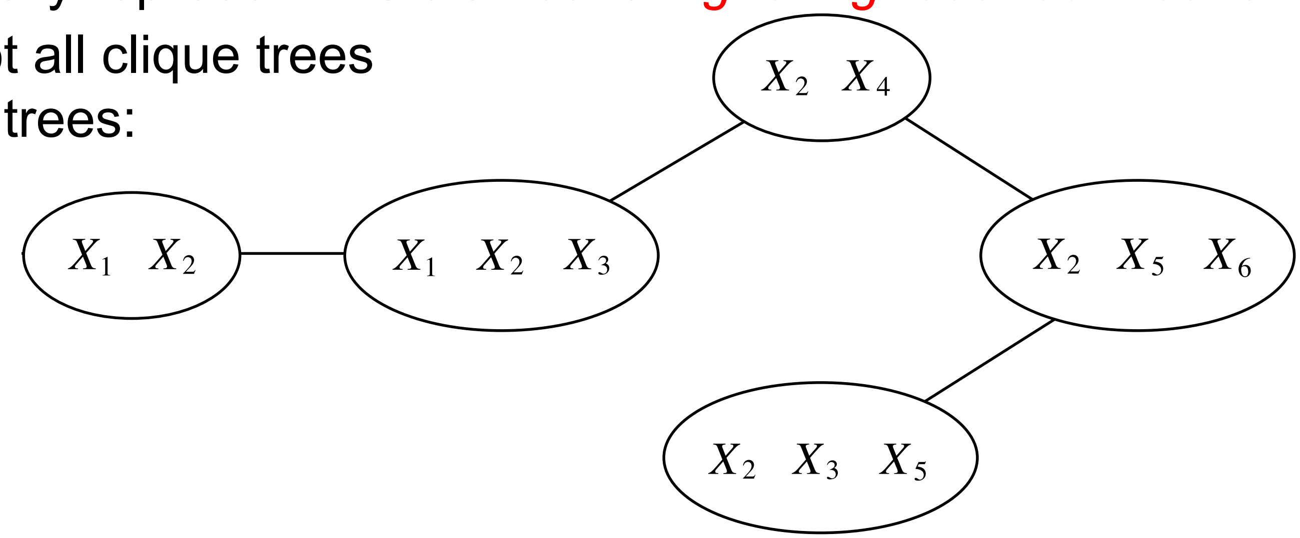
$$x_a = x_b, x_b = x_c \rightarrow x_a = x_c$$

Question: How many edges are needed for global consistency? When can we build a tree-structured clique graph?

Clique Trees and Junction Trees

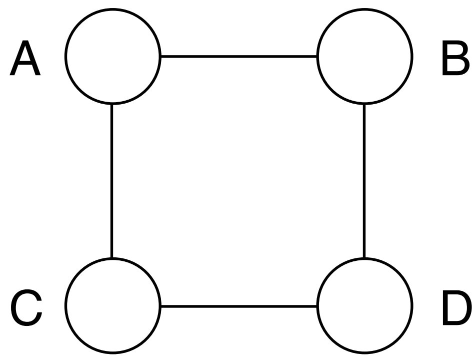


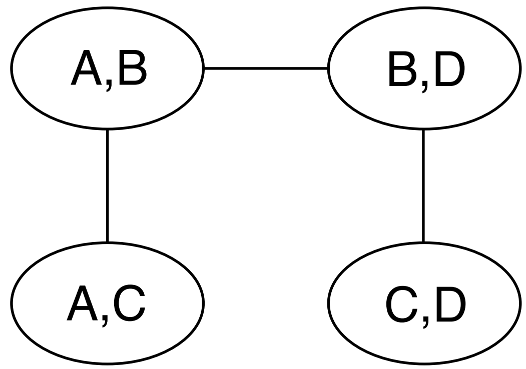
- This clique tree has the *junction tree* property: the clique nodes containing any variable from the original model form a *connected* subtree
- We can exactly represent the distribution *ignoring redundant constraints*
- Note that not all clique trees are junction trees:

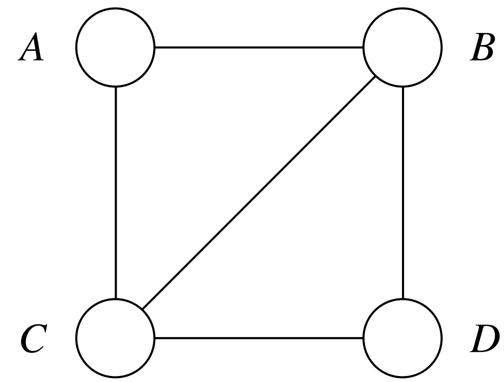


Finding a Junction Tree

The junction tree property. A clique tree possesses the *junction tree property* if for every pair of cliques V and W, all cliques on the (unique) path between V and W contain $V \cap W$.







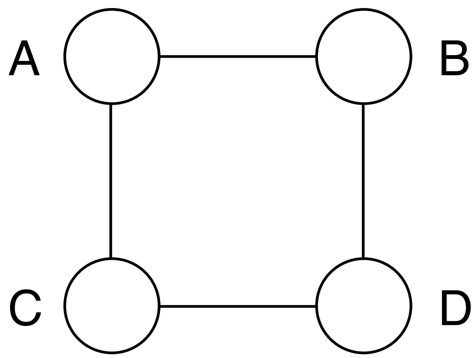
- Given a set of cliques, how can we efficiently find a clique tree with the junction tree (running intersection) property?
- How can we be sure that at least one junction tree exists?

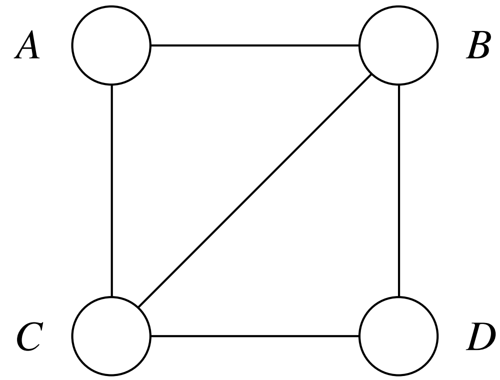
- Strategy: Augment the graph with additional edges
  - ➢ Cliques of original graph are always subsets of cliques of the augmented graph, so original distribution still factorizes appropriately
  - ➢ As cliques grow, will eventually be able to construct a junction tree

Question: Which undirected graphs have junction trees?

Junction Trees and Triangulation

The junction tree property. A clique tree possesses the *junction tree property* if for every pair of cliques V and W, all cliques on the (unique) path between V and W contain $V \cap W$.





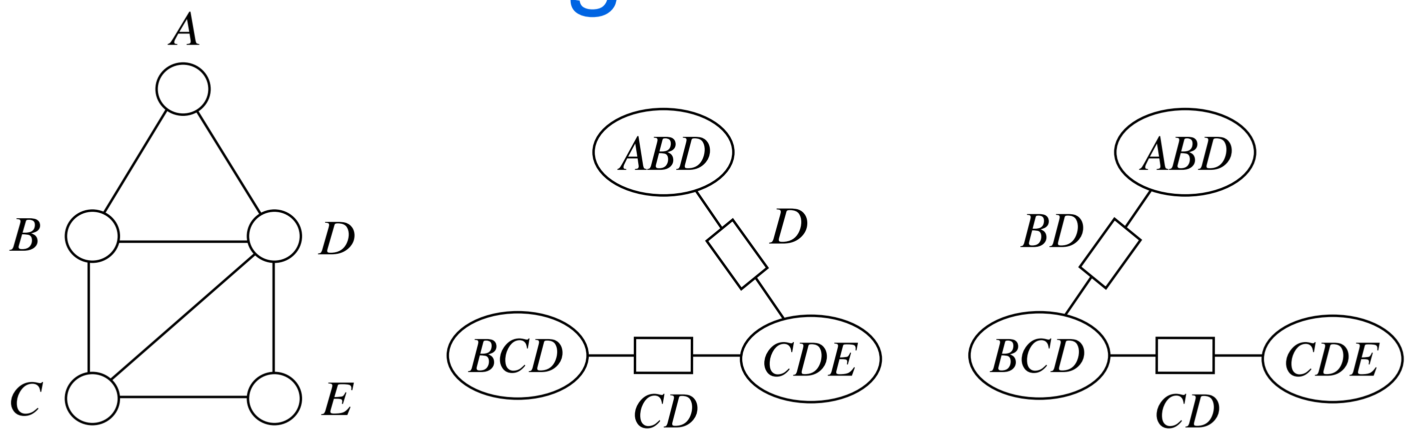
- A *chord* is an edge connecting two non-adjacent nodes in some *cycle*
- A cycle is *chordless* if it contains no chords
- A graph is *triangulated* if it contains no chordless cycles

Theorem: The maximal cliques of a graph have a corresponding junction tree *if and only if* that undirected graph is triangulated

Lemma 2 *Let $\mathcal{G} = (V, E)$ be a noncomplete triangulated graph with at least three nodes. Then there exists a decomposition of V into disjoint sets A, B and S such that S separates A and B and S is complete.*

- Key induction argument in constructing junction tree from triangulation
- Implies existence of *elimination ordering which introduces no new edges*

Constructing a Junction Tree



Theorem: A clique tree is a junction tree *if and only if* it is a maximal spanning tree of the weighted clique intersection graph

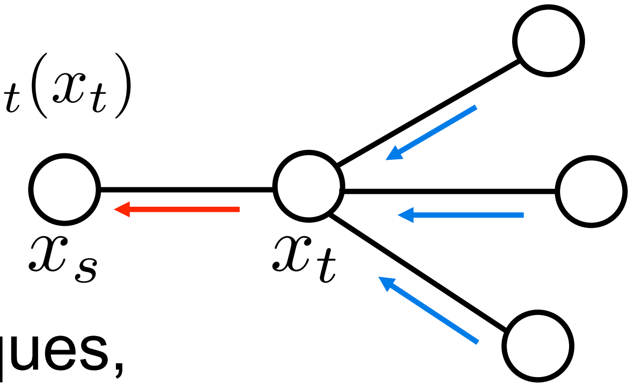
- **Graph**: Fully connected with nodes corresponding to maximal cliques
- **Edge weights:** Cardinality of *separator set* (intersection) of cliques
- **Computational complexity:** Quadratic in number of maximal cliques

Junction Tree Algorithms for General-Purpose Inference

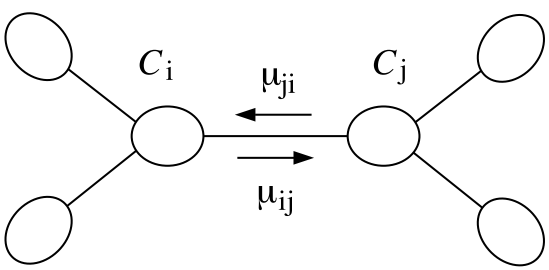
1. Triangulate the target undirected graphical model
   - Any elimination ordering generates a valid triangulation
   - Optimal triangulation is NP-hard (in multiple ways)
2. Arrange triangulated cliques into a junction tree
3. Execute variant of sum-product algorithm on junction tree

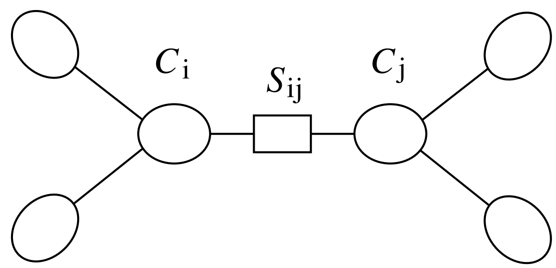
Sum-Product for Junction Trees

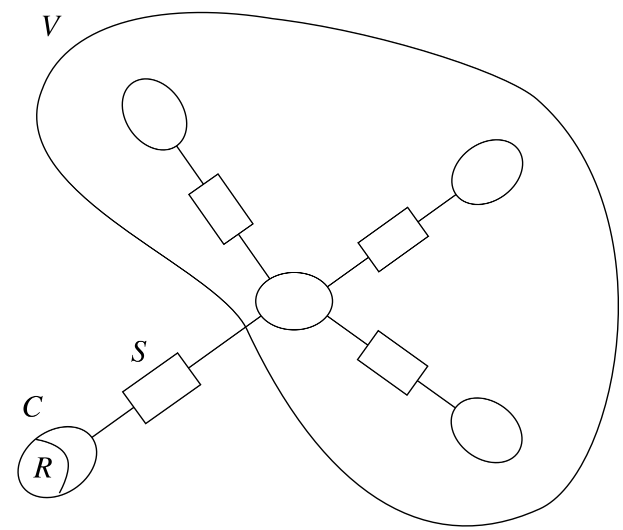
$$m_{ts}(x_s) \propto \sum_{x_t} \psi_{st}(x_s, x_t)\psi_t(x_t) \prod_{u \in \Gamma(t) \setminus s} m_{ut}(x_t)$$



Consider a junction tree linking a set of cliques, with pairwise equality constraints among intersections:







Messages are functions of the separating sets (variables shared among cliques):

$$\mu_{ji}(x_{S_{ji}}) \propto \sum_{x_{R_j}} \psi_{C_j}(x_{C_j}) \prod_{k \neq j} \mu_{kj}(x_{S_{kj}})$$

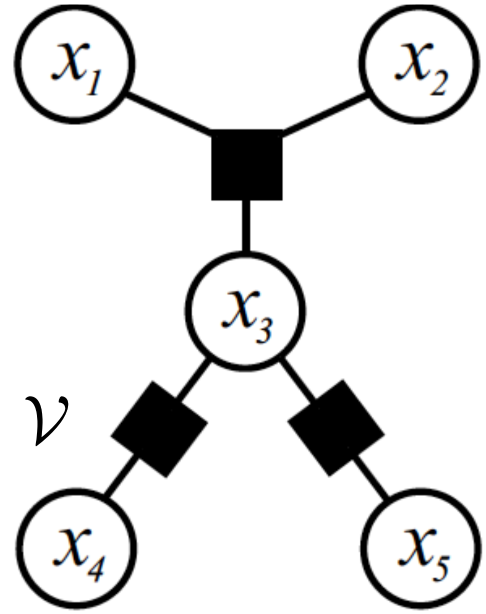
$$R_j = C_j \setminus S_{ij}$$

Shafer-Shenoy Junction Tree Algorithm

Undirected Graphical Models

$$p(x \mid \theta) = \frac{1}{Z(\theta)} \prod_{f \in \mathcal{F}} \psi_f(x_f \mid \theta_f)$$

$$Z(\theta) = \sum_x \prod_{f \in \mathcal{F}} \psi_f(x_f \mid \theta_f)$$



$\mathcal{F} \longrightarrow$ set of hyperedges linking subsets of nodes $f \subseteq \mathcal{V}$

$\mathcal{V} \longrightarrow$ set of N nodes or vertices, $\{1, 2, \ldots, N\}$

- Assume an exponential family representation of each factor:

$$p(x \mid \theta) = \exp\left\{ \sum_{f \in \mathcal{F}} \theta_f^T \phi_f(x_f) - A(\theta) \right\}$$

$$\psi_f(x_f \mid \theta_f) = \exp\{\theta_f^T \phi_f(x_f)\} \qquad A(\theta) = \log Z(\theta)$$

- Partition function *globally* couples the local factor parameters

Learning for Undirected Models

- Undirected graph encodes dependencies within a single training example:

$$p(\mathcal{D} \mid \theta) = \prod_{n=1}^{N} \frac{1}{Z(\theta)} \prod_{f \in \mathcal{F}} \psi_f(x_{f,n} \mid \theta_f) \qquad \mathcal{D} = \{x_{\mathcal{V},1}, \ldots, x_{\mathcal{V},N}\}$$

- Given N independent, identically distributed, completely observed samples:

$$\log p(\mathcal{D} \mid \theta) = \left[\sum_{n=1}^{N} \sum_{f \in \mathcal{F}} \theta_f^T \phi_f(x_{f,n}) \right] - N A(\theta)$$

$$p(x \mid \theta) = \exp\left\{ \sum_{f \in \mathcal{F}} \theta_f^T \phi_f(x_f) - A(\theta) \right\}$$

$$\psi_f(x_f \mid \theta_f) = \exp\{\theta_f^T \phi_f(x_f)\} \qquad A(\theta) = \log Z(\theta)$$

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- Given N independent, identically distributed, completely observed samples:

$$\log p(\mathcal{D} \mid \theta) = \left[\sum_{n=1}^{N} \sum_{f \in \mathcal{F}} \theta_f^T \phi_f(x_{f,n}) \right] - N A(\theta)$$

- Take gradient with respect to parameters for a single factor:

$$\nabla_{\theta_f} \log p(\mathcal{D} \mid \theta) = \left[\sum_{n=1}^{N} \phi_f(x_{f,n}) \right] - N \mathbb{E}_\theta[\phi_f(x_f)]$$

- Must be able to compute *marginal distributions* for factors in current model:
  - Tractable for tree-structured factor graphs via sum-product
  - For general graphs, use the junction tree algorithm to compute