# CMPUT463/563 Probabilistic Graphical Models

#### Exact Inference: Message Passing

Lili Mou

Dept. Computing Science, University of Alberta

lmou@ualberta.ca



#### Outline

- Variable elimination (last lecture)
  - Dynamic programming: pulling sum/max inside
  - Sum-product, max-product identical, due to semirings
  - To eliminate a node X: consider all potentials involving  $X\Rightarrow$  marginalize/max X out  $\Rightarrow$  Put resulting potential back, with scope N(X)
- Message passing
  - VE two passes => answer all queries of a variable
  - Belief propagation: Sum-product message passing
- Message passing on factor trees
- Message passing on junction trees

#### Variable Elimination

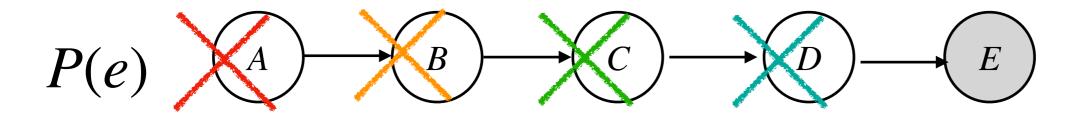
Input: Variables Y, Z, X = x, set of factors  $\Phi$ 

Elimination order (assuming  $Z_1, Z_2, \dots, Z_k$  wlog)

- 1.  $\Phi \leftarrow \Phi$  with evidence potentials
- 2. For  $i = 1, \dots, k$
- 2.1  $\Phi' \leftarrow \{ \phi \in \Phi' : Z_i \in \text{scope}(\phi) \}$
- 2.2.  $\varphi \leftarrow \sum_{z_i} \prod_{\phi \in \Phi'} \phi$
- 2.3  $\Phi = \Phi \setminus \Phi' \cup \{\varphi\}$

Return  $\prod_{\phi \in \Phi} \phi$  as a factor on Y given X

### Examples



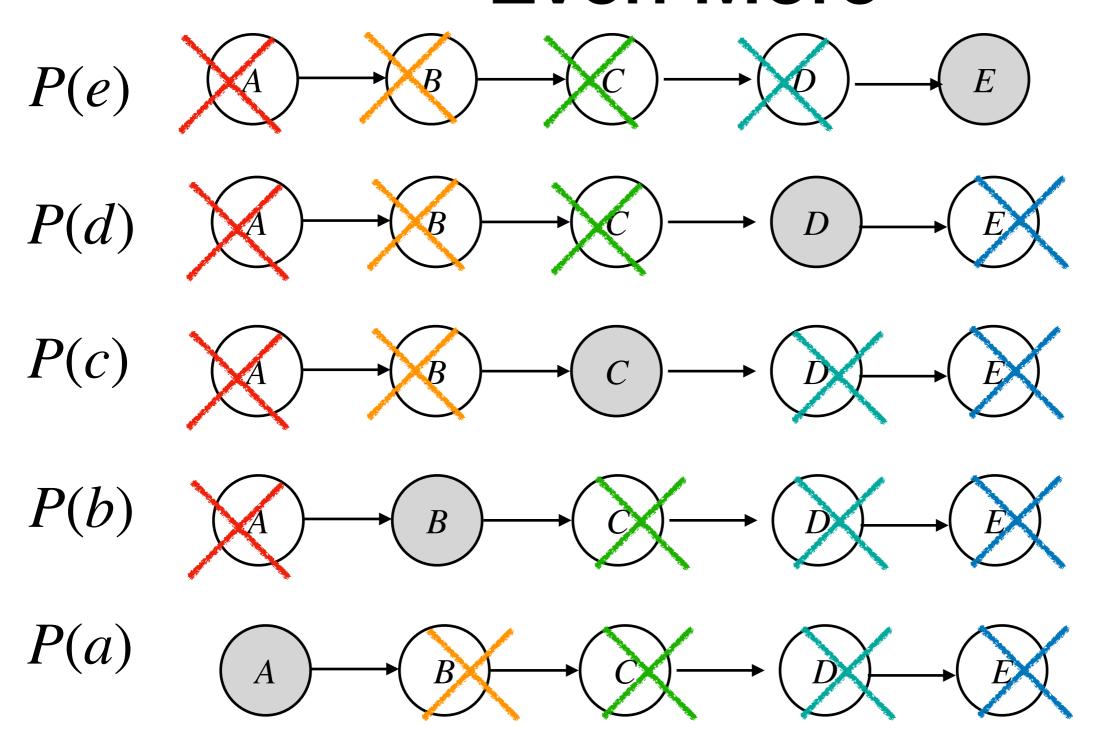
$$P(e) = \sum_{d} \sum_{c} \sum_{b} \sum_{a} P(a)P(b|a)P(c|b)P(d|c)P(e|d)$$

$$P(d) \longrightarrow B \longrightarrow C \longrightarrow D \longrightarrow E$$

$$P(d) = \sum_{a} \sum_{b} \sum_{a} \sum_{b} P(a)P(b|a)P(c|b)P(d|c)P(e|d)$$

Observation: If we have multiple queries for a graph, some DP results are reusable

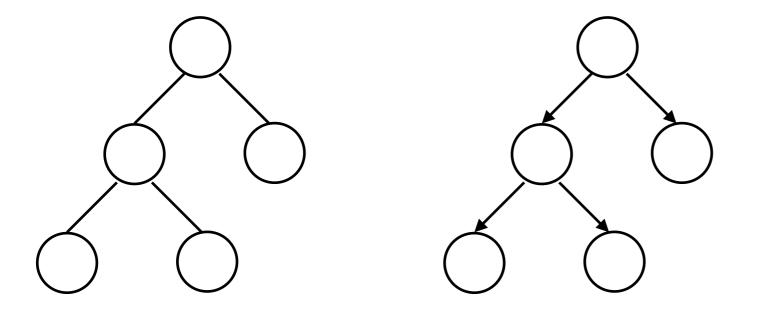
#### **Even More**

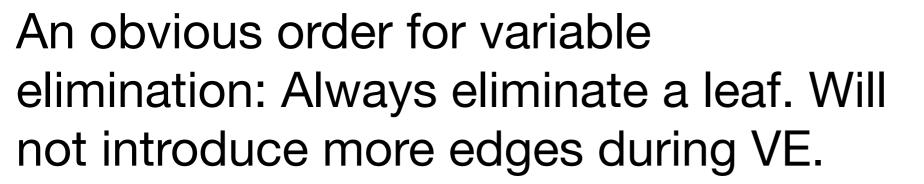


Observation: DP twice (from left and from right), all marginals are obtained. Congratulations! You are inventing the belief propagation algorithm

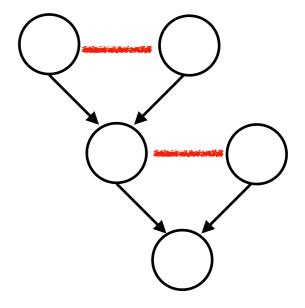
#### **Trees**

For certain graphs (namely, trees) DP results are reusable for different queries. A chain is a special case of trees.





Any node separates a tree into two parts. VE needed for both sides, but is reusable

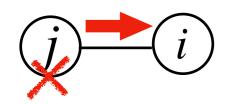


Work with factor graphs. Later

# Message Passing

Without loss of generality, we assume having **one singleton** potential for each node and **one pairwise** potential for two connected nodes.

#### **Initialization**



Consider a leaf node j. If j does not have a neighbor, it's done. Otherwise, j can only have one neighbor, which we call i.

$$m_{ji}(x_i) = \sum_{x_j} \phi(x_j) \phi(x_i, x_j)$$

 $m_{ii}$  is called the message from j to i, a potential when j is eliminated.

Sum-product message passing is also called belief propagation; such a message is also called a belief.

# Message Passing

#### Recursion

Suppose node j is now a leaf and can have at most one neighbor, which we call i. Other neighbors of j are already eliminated.

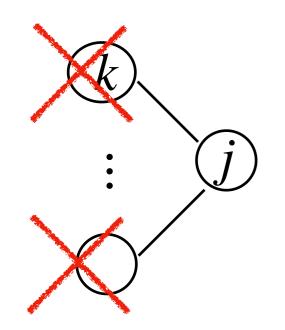
$$\vdots \qquad j \qquad i \qquad m_{ji}(x_i) = \sum_{x_j} \left( \phi(x_j) \phi(x_i, x_j) \prod_{k \in N(j) \setminus \{i\}} m_{kj}(x_j) \right)$$

 $m_{ji}$  is called the *message* from j to i, the potential after eliminating variables up to j before i, with a scope of i only.

Who can pass message? j can pass message to i if j has received messages from all its neighbors except i.

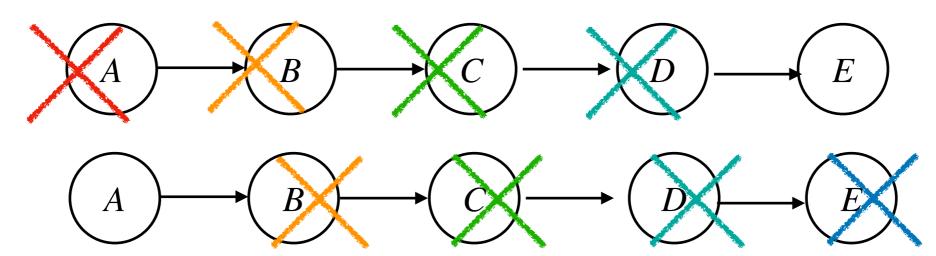
# Message Passing

#### **Termination**



Suppose node j is now a leaf and it does not have other neighbors. Done!

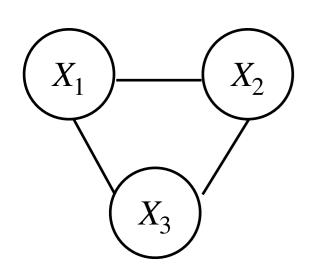
But note: this is half of the story



We need message passing the other way around. It's also true for trees.

### Non-Tree Structures

Assuming singleton and pairwise potentials



Suppose the query is  $P(X_3)$ . If we start sending messages from a node, say  $X_1$ , we have

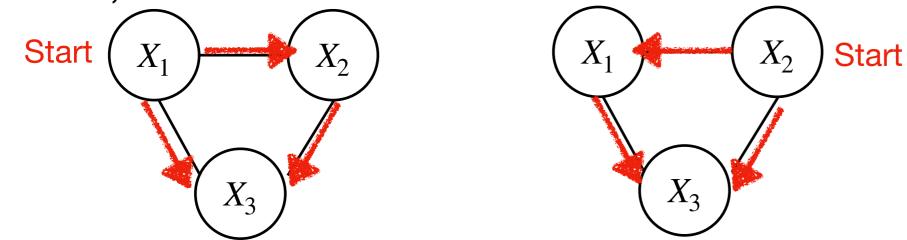
$$m_{12} = \sum_{X_1} \phi(X_1)\phi(X_1, X_2)$$
  $m_{13} = \sum_{X_1} \phi(X_1)\phi(X_1, X_3)$ 

$$P(X_3) = \sum_{X_2} \sum_{X_1} \phi(X_1)\phi(X_2)\phi(X_3)\phi(X_1, X_2)\phi(X_2, X_3)\phi(X_1, X_3)$$

Factorization in such a style is fundamentally wrong

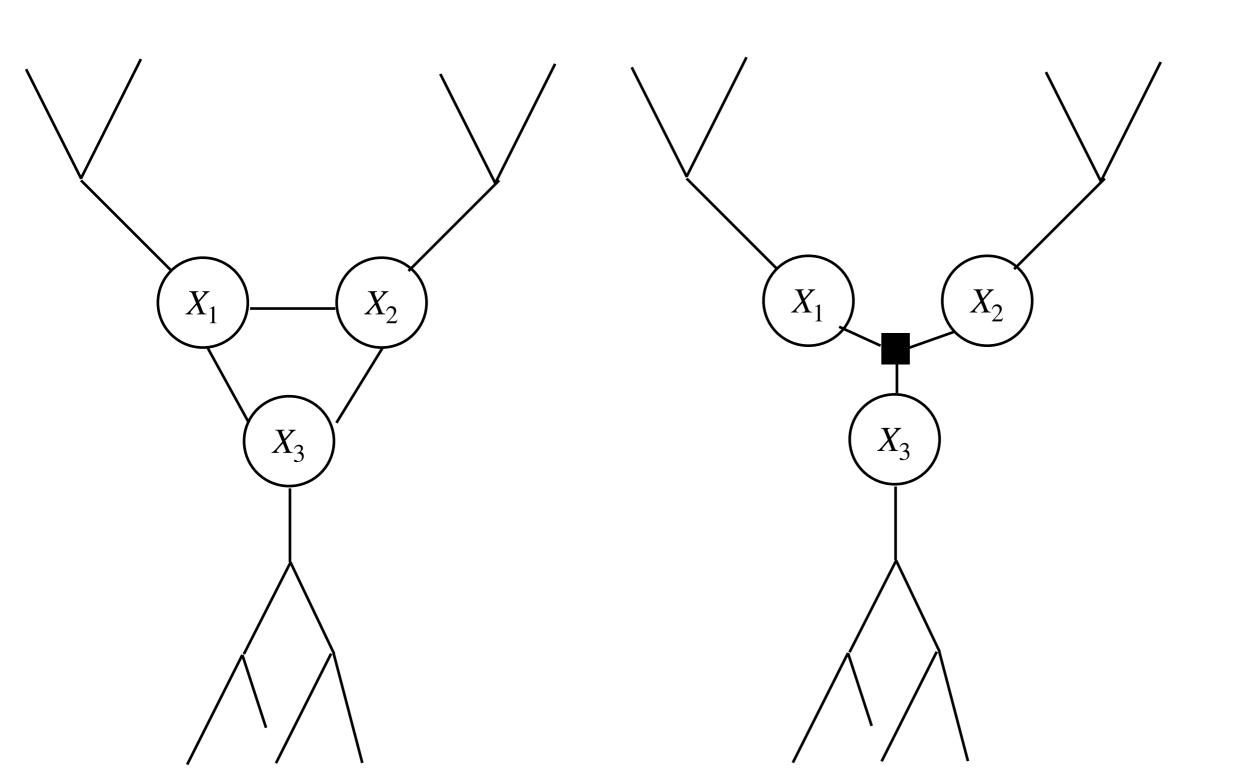
$$\sum_{x} xyz = \left(\sum_{x} xz\right) \left(\sum_{x} xy\right)$$

In fact, you can show that two message passings yield different results, which is also the evidence that such factorization is wrong

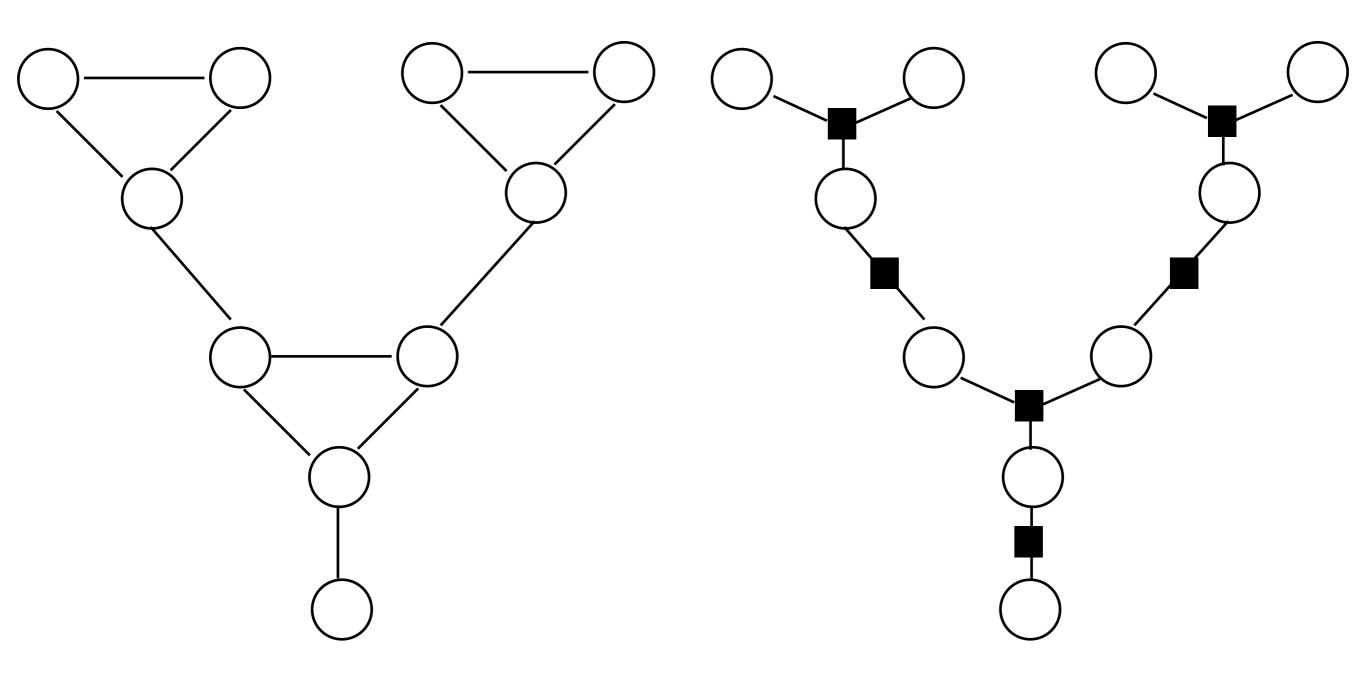


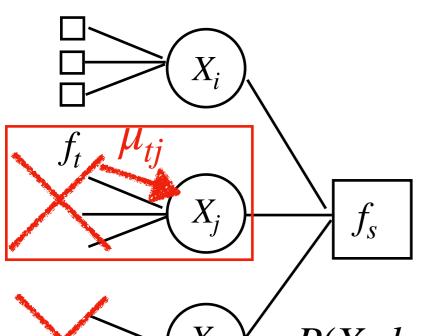
#### Non-Tree Structures

But suppose the remaining structures are tree-like, message passing can treat  $X_1, X_2, X_3$  as a whole, as a factor



Factor graph is a bipartite graph between variables and factors. We consider such graphs that are trees.

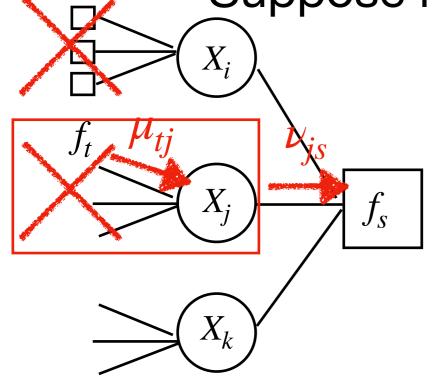




Suppose we would like to eliminate  $X_j$  and  $X_k$ , whose left nodes are already eliminated with potentials  $\mu_{tj}$  from factor t to node j

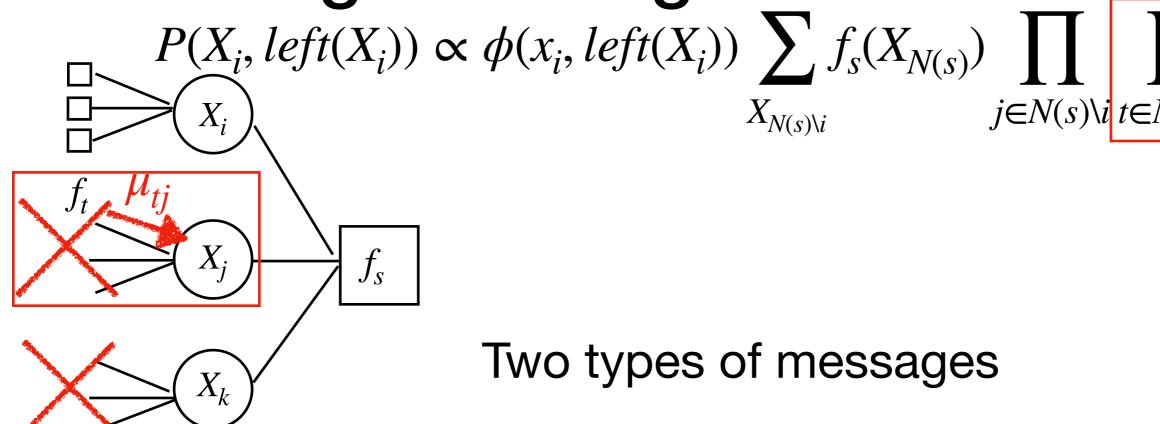
$$P(X_i, left(X_i)) \propto \phi(x_i, left(X_i)) \sum_{X_{N(s) \setminus i}} f_s(X_{N(s)}) \prod_{j \in N(s) \setminus i} \prod_{t \in N(j) \setminus s} \mu_{tj}(x_j)$$

Suppose now we would like to eliminate  $X_i$  and  $X_k$ 



Reusable! DP is possible

$$\nu_{js} = \prod_{t \in N(j) \setminus s} \mu_{tj}(x_j)$$



Two types of messages

 $X_{N(s)\setminus i}$ 

 $\nu_{is}$ : variables j to factor s

$$\nu_{js}(x_i) = \prod_{t \in N(j) \setminus s} \mu_{tj}(x_j)$$

 $j \in N(s) \setminus i t \in N(j) \setminus s$ 

(marginalization is deferred with the factor  $f_s$ )

 $\mu_{si}$ : factor s to variable i

$$\mu_{si}(x_i) = \sum_{X_{N(s)\setminus i}} f_s(X_{N(s)}) \prod_{j \in N(s)\setminus i} \nu_{js}(x_j)$$

(potential on  $X_i$  by eliminating other variables in the factor)

$$P(X_i, left(X_i)) \propto \phi(x_i, left(X_i)) \sum_{X_{N(s) \setminus i}} f_s(X_{N(s)}) \prod_{j \in N(s) \setminus i} \prod_{t \in N(j) \setminus s} \mu_{tj}(x_j)$$

$$\nu_{js}(x_i) = \prod_{t \in N(j) \setminus s} \mu_{tj}(x_j)$$

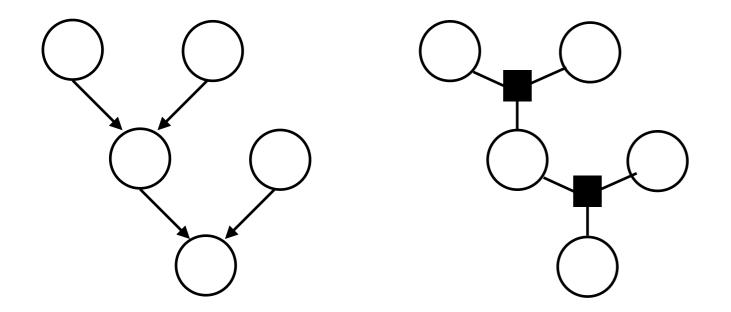
$$\mu_{si}(x_i) = \sum_{X_{N(s)\backslash i}} f_s(X_{N(s)}) \prod_{j \in N(s)\backslash i} \nu_{js}(x_j)$$

Message passing on factor trees is indeed an exact inference algorithm, as it's reusing VE intermediate results

# Complexity

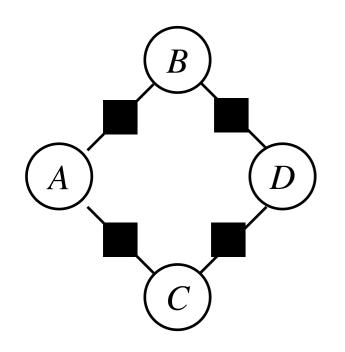
Complexity: exponential wrt largest factor

For ancestor trees, as efficient as representation the conditional probability

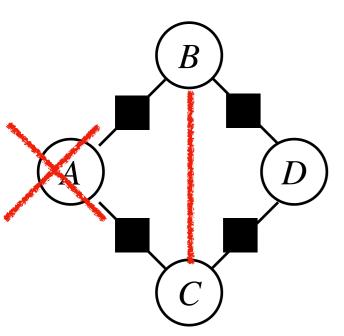


If the factor graph is cyclic, then we need to consider more variables at a time

# What if factor graph is cyclic?



- The factor graph is cyclic. We cannot start message passing on the factor graph.
- However, we don't have to consider all variables either

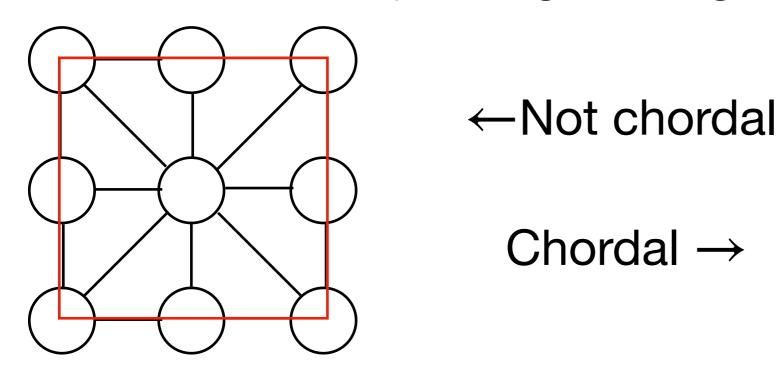


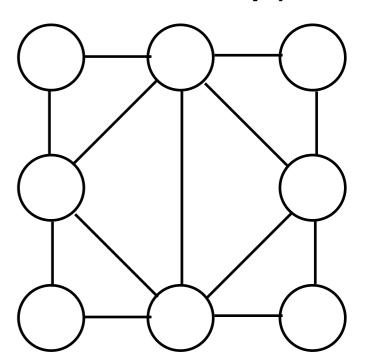
For example, when we eliminate A, we connect B, C without involving D

A special type of graphs: chordal graphs

### Chordal Graphs

Def: A graph is *chordal* (aka *triangulated*) if any loop of length >=4 has a chord (a straight line going across the loop)





Many graph-theoretical results:

- For a chordal graph, there exists a VE order that does not introduce new edges
- The graph induced by VE is chordal

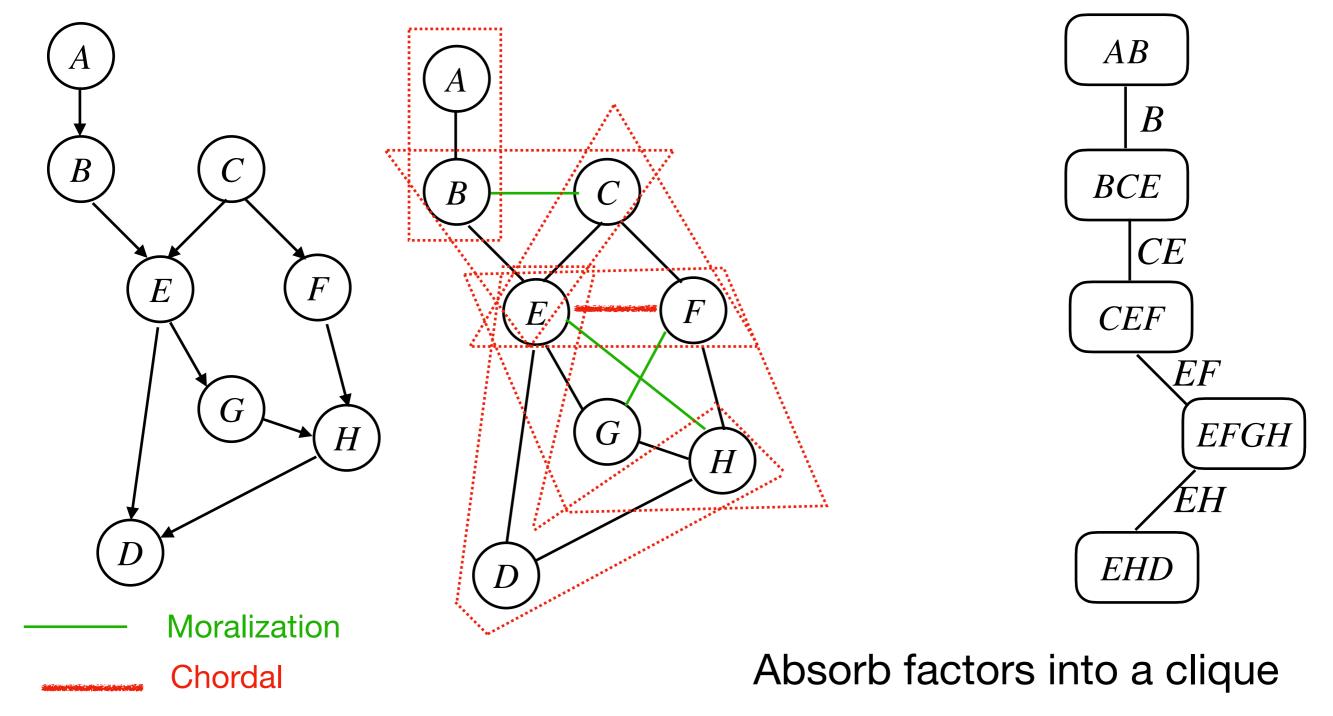
#### **Junction Tree**

For a chordal graph, define a vertex  $C_i$  in the junction tree as a max clique. Connect the nodes by spanning tree algorithms (e.g., max spanning tree with intersecting variables)

This will correspond to VE with some order such that  $C_i - C_j$  if the message of i is used in computing the message of j.

Running intersection property: If a variable occurs in  $C_i$  and  $C_j$ , then it must occur on every nodes in the trail  $C_i - \cdots - C_j$ . VE satisfies running intersection property because a variable eliminated will not recur.

Elimination order: *ABCDEFGH* 

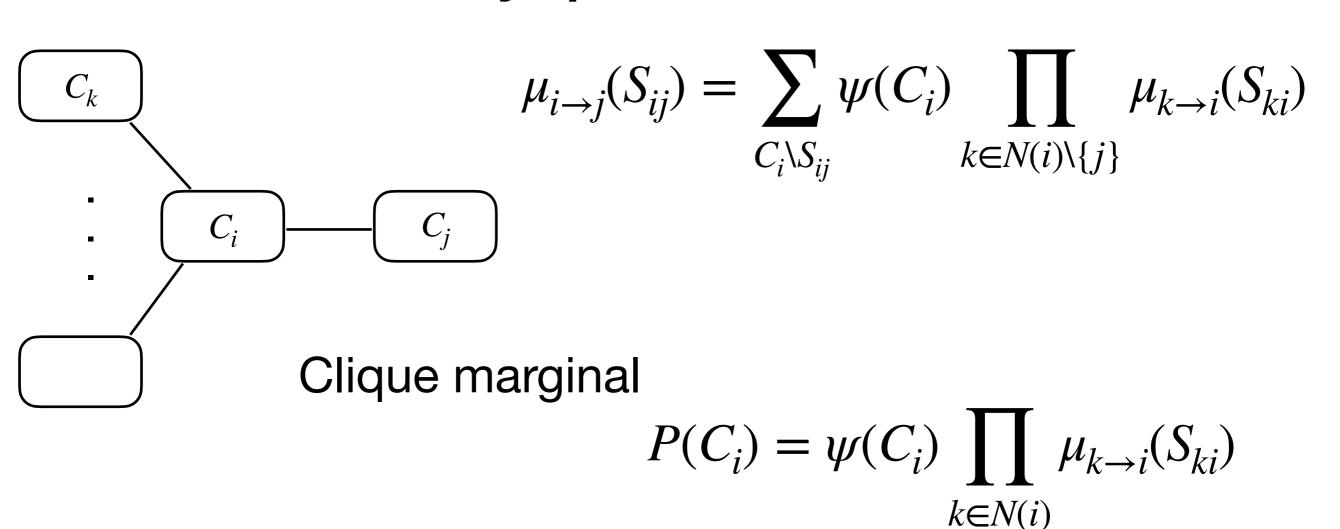


Now we can design a MP-like algorithm to eliminate variables Results will be clique marginals

Let the variables of *i*th clique be  $C_i$ . Let  $S_{ij} = C_i \cap C_j$ 

Sending message from  $C_i$  to  $C_j$  is to eliminate variables  $C_i \backslash S_{ij}$ 

#### **Shafer-Shenoy update:**



Shafer-Shenoy update: 
$$\mu_{i \to j}(S_{ij}) = \sum_{C_i \setminus S_{ij}} \psi(C_i) \prod_{k \in N(i) \setminus \{j\}} \mu_{k \to i}(S_{ki})$$

Clique marginal

$$P(C_i) = \psi(C_i) \prod_{k \in N(i)} \mu_{k \to i}(S_{ki})$$

#### **Hugin update**

- Store the product in the potential. Store previous message on the edge and discount it during MP back.
- More time efficient

#### <u>Initialization</u>

$$\phi_i(C_i) = \psi(C_i)$$

$$\phi_{ij}(S_{ij}) = 1$$

 $\underline{\mathsf{Update}} \; \mathsf{from} \; C_i \; \mathsf{to} \; C_j \; \mathsf{over} \; S_{ij}$ 

$$\phi_{ij}(S_{ij})^{(\text{new})} = \sum_{C_i \setminus S_{ij}} \phi_i(C_i)$$

$$\phi_j(C_j)^{\text{(new)}} = \phi_j(C_j) \frac{\phi_{ij}(C_{ij})^{\text{(new)}}}{\phi_{ij}(C_{ij})}$$

Denominator = 1 if first time passing an edge from i to j; or = message from i to j, if second time passing from j to i

#### Summary

- 1. Moralize (easy)
- 2. Triangulate the graph (NP-hard) Can be
- 3. Build the junction tree
- 4. Shafer-Shenoy update or Hugin update

Two-pass message passing => marginals of all potentials