

# CS5340 Uncertainty Modeling in Al

Lecture 6: Factor Graph and the Junction Tree Algorithm

Asst. Prof. Lee Gim Hee
AY 2018/19
Semester 1

## Course Schedule

Week	Date	Торіс	Remarks
1	15 Aug	Introduction to probabilities and probability distributions	
2	22 Aug	Fitting probability models	Hari Raya Haji*
3	29 Aug	Bayesian networks (Directed graphical models)	
4	05 Sep	Markov random Fields (Undirected graphical models)	
5	<b>12</b> Sep	I will be traveling	No Lecture
6	19 Sep	Variable elimination and belief propagation	
-	26 Sep	Recess week	No lecture
7	03 Oct	Factor graph and the junction tree algorithm	
8	10 Oct	Parameter learning with complete data	
9	17 Oct	Mixture models and the EM algorithm	
10	24 Oct	Hidden Markov Models (HMM)	
11	31 Oct	Monte Carlo inference (Sampling)	
12	07 Nov	Variational inference	
13	14 Nov	Graph-cut and alpha expansion	

<sup>\*</sup> Make-up lecture: 25 Aug (Sat), 9.30am-12.30pm, LT 15



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# Acknowledgements

- A lot of slides and content of this lecture are adopted from:
- Michael I. Jordan "An introduction to probabilistic graphical models", 2002. Chapters 4.2, 4.3 and 17 <a href="http://people.eecs.berkeley.edu/~jordan/prelims/chapter4.pdf">http://people.eecs.berkeley.edu/~jordan/prelims/chapter17.pdf</a>
- Daphne Koller and Nir Friedman, "Probabilistic graphical models" Chapter 10
- 3. David Barber, "Bayesian reasoning and machine learning" Chapter 6
- 4. Kevin Murphy, "Machine learning: a probabilistic approach" Chapter 20.4
- 5. Christopher Bishop "Machine learning and pattern recognition" Chapter 8.4.3



## Learning Outcomes

- Students should be able to:
- Represent a joint distribution with a factor graph, and use it to compute the marginal/conditional probabilities.
- 2. Use the max-product algorithm to find the maximal probability and its configurations.
- 3. Convert a DGM/UGM into the junction tree and use it to compute the marginal/conditional probabilities.



# Factor Graphs

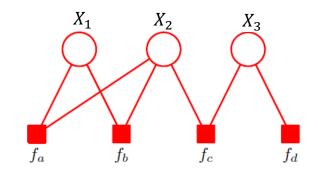
- DGMs and UGMs: allow a global function of several variables to be expressed as a product of factors over subsets of those variables.
- Factor graphs make this decomposition explicit by introducing additional nodes for the factors in addition to the nodes representing the variables.
- Unlike DGMs and UGMs, factor graphs are NOT designed for conditional independence, but for more explicit details of the factorization.



## Factor Graphs: Graphical Representation

• A factor graph is a bipartite graph:

$$\mathcal{G}(\mathcal{V},\mathcal{F},\mathcal{E})$$



#### where

- vertices  $\mathcal{V} \in \{X_1, \dots, X_n\}$ : index the random variables,
- vertices  $\mathcal{F} \in \{..., f_s, ...\}$ : index the factors and
- undirected edges  $\mathcal{E}$ : link each factor node  $f_S$  to all variable nodes  $X_S$  that  $f_S$  depends.
- We use round nodes to represent random variables and square nodes to represent factors.



# Factor Graphs: Joint Distribution

 We write the joint distribution over a set of variables in the form of a product of factors:

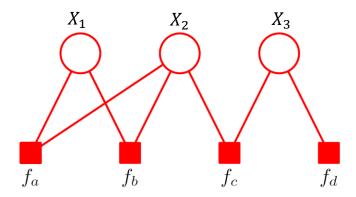
$$p(\mathbf{x}) = \prod_{s} f_s(\mathbf{x}_s)$$

- Where  $X_S$  denotes a subset of the variables  $X \in \{X_1, ..., X_n\}$ .
- Each factor  $f_s$  is a function of a corresponding set of variables  $X_s$ .



# Factor Graphs

#### **Example:**



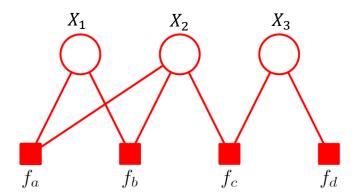
$$p(\mathbf{x}) = f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$$

- Note that there are two factors  $f_a(x_1, x_2)$  and  $f_b(x_1, x_2)$  that are defined over the same set of variables.
- In an undirected graph, product of two such factors would simply be lumped together into the same clique potential.



# Factor Graphs

#### **Example:**



$$p(\mathbf{x}) = f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$$

- Similarly,  $f_c(x_2, x_3)$  and  $f_d(x_3)$  could be combined into a single potential over  $X_2$  and  $X_3$ .
- The factor graph keeps such factors explicit, so is able to convey more detailed information about the underlying factorization.



# Convert DGM to Factor Graph

Recall the factorization of DGMs is defined as:

$$p(x_1, ..., x_N) = \prod_{i=1}^N p(x_i | x_{\pi_i})$$

• Convert a DGM into a factor graph by representing the local conditional distributions  $p(x_i|x_{\pi_i})$  as factors  $f_s(\mathbf{x}_s)$ .



# Convert UGM to Factor Graph

Recall the factorization of UGMs is defined as:

$$p(\mathbf{y}|\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \prod_{c \in \mathcal{C}} \psi_c(\mathbf{y}_c|\boldsymbol{\theta}_c)$$

- Convert a UGM into a factor graph by representing the potential functions over the maximal cliques as factors  $f_s(\mathbf{x}_s)$ .
- Normalizing coefficient 1/Z can be viewed as a factor defined over the empty set of variables.

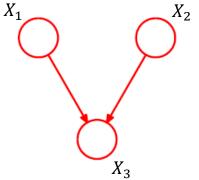


# DGM/UGM to Factor Graph

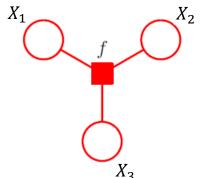
 Note that there may be several different factor graphs that correspond to the same DGM / UGM.

 Factor graphs to be more specific about the precise form of the factorization.  $f_a(x_1) = p(x_1)$ 

#### **Example: Directed Graph**

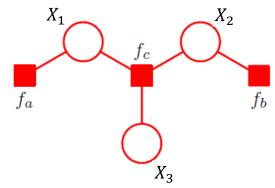


$$p(x_1)p(x_2)p(x_3|x_1,x_2)$$



$$\int_{X_3} f(x_1, x_2, x_3) = n(x_1)n(x_2, x_3)$$

$$p(x_1)p(x_2)p(x_3|x_1,x_2)$$
  $f(x_1,x_2,x_3) = p(x_1)p(x_2)p(x_3|x_1,x_2)$ 



 $f_c(x_1, x_2, x_3) = p(x_3 | x_2, x_1)$ 

Two factor graphs representing the same distribution

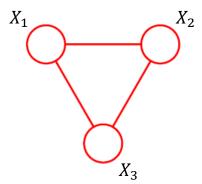
 $f_b(x_2) = p(x_2)$ 

# DGM/UGM to Factor Graph

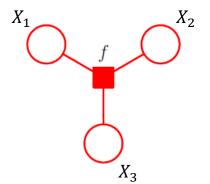
- Note that there may be several different factor graphs that correspond to the same DGM / UGM.
- Factor graphs to be more specific about the precise form of the factorization.

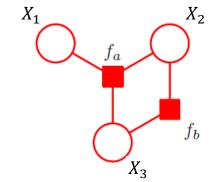
#### **Example: Undirected Graph**

$$f_a(x_1, x_2, x_3) f_b(x_1, x_2) = \psi(x_1, x_2, x_3)$$



Single clique potential  $\psi(x_1, x_2, x_3)$ 





$$f(x_1, x_2, x_3) = \psi(x_1, x_2, x_3)$$

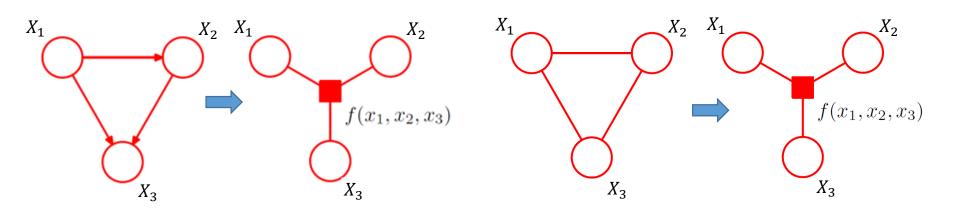
Two factor graphs representing the same distribution



## Factor Graphs: Sum-Product Algorithm

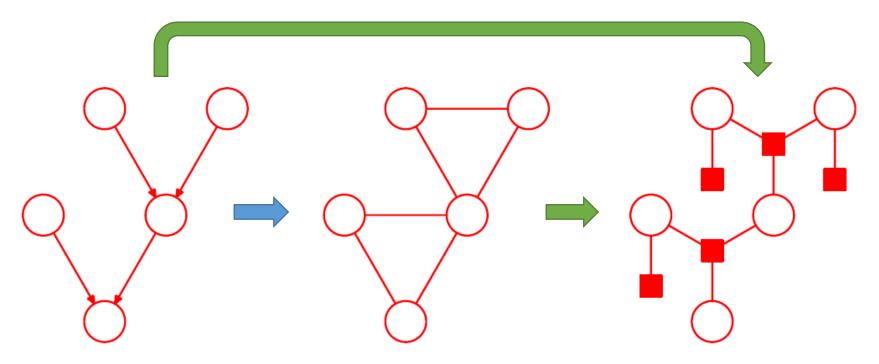
- Alternative representation for the sum-product algorithm for "tree-like" graphs.
- More importantly, some DGMs/UGMs with local cycles become a tree when converted to factor graphs.

**Example:** Turning local cycle into a tree





# Polytrees



- Cycles appear after directed to undirected graph conversion.
- Local cycles disappeared after factor graph conversion.
- Note the factor graph conversion can be directly from a DGM.



Image source: "Pattern recognition and machine learning", Christopher Bishop

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## Factor Graphs: Sum-Product Algorithm

 Our goal: Compute all singleton marginal probabilities under the factorized representation of the joint probability.

- As in the earlier Sum-Product algorithm, we define two kinds of messages:
  - 1. Messages v: flow from variable to factor nodes.
  - 2. Messages  $\mu$ : flow from factor to variable nodes.



## Neighborhood Sets of a Node

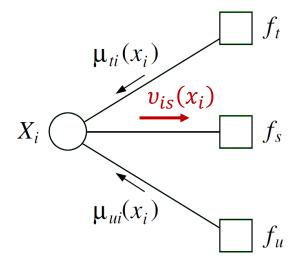
- $N(s) \subset \mathcal{V}$ : Set of neighbors of a factor node  $s \in \mathcal{F}$ .
- N(s) refers to the indices of all variables referenced by the factor  $f_s$ .
- $N(i) \subset \mathcal{F}$ : Set of neighbors of a variable node  $i \in \mathcal{V}$ .
- N(i) for a variable node  $X_i$  refers to the set of all factors that referenced  $X_i$ .



## Messages from Variable to Factor Nodes

• Message  $v_{is}(x_i)$  flows from the variable node  $X_i$  to the factor node  $f_s$ :

$$\nu_{is}(x_i) = \prod_{t \in \mathcal{N}(i) \setminus s} \mu_{ti}(x_i)$$



• The product is taken over all incoming messages to the variable node  $X_i$ , other than the factor node  $f_s$ .



## Messages from Factor to Variable Nodes

• Message  $\mu_{si}(x_i)$  flows from the factor node  $f_s$  to the variable node  $X_i$ :

• The product is taken over all incoming messages to the factor node  $f_s$ , other than the variable node  $X_i$ .



# Messages From The Leaf Nodes

Message from a leaf variable node to factor node:

$$v_{is}(x_i) = 1$$

$$X_i \qquad f_s$$

Message from a leaf factor node to variable node:

$$\mu_{si}(x_i) = f_s(x_i)$$

$$f_s \qquad X_i$$



# Message-Passing Protocol

A node can send a message to a neighboring node when (and only when) it has received messages from all of its other neighbors.

Applies to both variable and factor nodes.

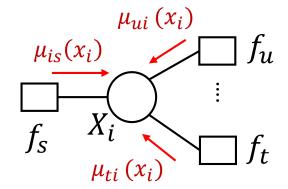


# Marginal Probability of a Node

• Once a node  $X_i$  has received the messages from all its neighbors, the marginal probability is given by:

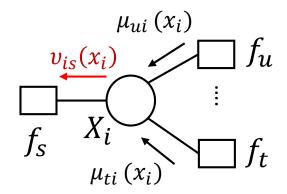
$$p(x_i) \propto \prod_{s \in \mathcal{N}(i)} \mu_{si}(x_i)$$

$$= \nu_{is}(x_i) \mu_{si}(x_i)$$



since

$$\nu_{is}(x_i) = \prod_{t \in \mathcal{N}(i) \setminus s} \mu_{ti}(x_i)$$





```
Sum-Product (\mathcal{T}, E) // main steps of Sum-Product algorithm

1. EVIDENCE(E)
f = \text{CHOOSEROOT}(\mathcal{V})

2. for s \in \mathcal{N}(f)
\mu\text{-COLLECT}(f, s)

3. for s \in \mathcal{N}(f)
\nu\text{-DISTRIBUTE}(f, s)

4. for i \in \mathcal{V}
\text{COMPUTEMARGINAL}(i)
```

```
1. \text{EVIDENCE}(E) // add evidence potentials (convert conditioning into marginalization) 

for i \in E \psi^E(x_i) = \psi(x_i)\delta(x_i, \bar{x}_i) 

for i \notin E \psi^E(x_i) = \psi(x_i)
```



Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002. CS5340 :: G.H. Lee

```
Sum-Product (\mathcal{T}, E) // main steps of Sum-Product algorithm

1. EVIDENCE(E)
f = \text{ChooseRoot}(\mathcal{V})
2. for s \in \mathcal{N}(f)
\mu\text{-Collect}(f, s)
3. for s \in \mathcal{N}(f)
\nu\text{-Distribute}(f, s)
4. for i \in \mathcal{V}
\text{ComputeMarginal}(i)
```

```
1. \text{EVIDENCE}(E) // add evidence potentials (convert conditioning into marginalization) for i \in E \psi^E(x_i) = \psi(x_i)\delta(x_i, \bar{x}_i) for i \notin E \psi^E(x_i) = \psi(x_i)
```

```
// recursively collect messages from leaves to root
\mu-Collect(i, s)
      for j \in \mathcal{N}(s) \setminus i
                                       Message from factor node f_s to the variable node X_i:
            \nu-Collect(s, j)
                                       \mu-SENDMESSAGE(s, i)
                                                                                              \mu_{si}(x_i) = \sum_{x_i \in \mathcal{N}(s)} \left( f_s(x_{\mathcal{N}(s)}) \prod_{i \in \mathcal{N}(s) \setminus i} \nu_{js}(x_j) \right)
      \mu-SENDMESSAGE(s, i)
\nu-Collect(s, i)
                                       Message from variable node X_i to the factor node f_s:
      for t \in \mathcal{N}(i) \backslash s
                                        \nu-SENDMESSAGE(i, s)
                                                                                                                     \nu_{is}(x_i) = \prod \mu_{ti}(x_i)
            \mu-Collect(i, t)
      \nu-SENDMESSAGE(i, s)
                                                                                                                                    t \in \mathcal{N}(i) \setminus s
```



Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002. CS5340 :: G.H. Lee

```
SUM-PRODUCT(\mathcal{T}, E) // main steps of Sum-Product algorithm

1. EVIDENCE(E)
f = \text{CHOOSEROOT}(\mathcal{V})
2. for s \in \mathcal{N}(f)
\mu\text{-COLLECT}(f, s)
3. for s \in \mathcal{N}(f)
\nu\text{-DISTRIBUTE}(f, s)
4. for i \in \mathcal{V}
\text{COMPUTEMARGINAL}(i)
```

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4. Compute Marginal (i) // compute marginal probability  $p(x_i) \propto \nu_{is}(x_i)\mu_{si}(x_i)$ 

 $\nu$ -DISTRIBUTE(i, t)



Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

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```
Sum-Product (\mathcal{T}, E) // main steps of Sum-Product algorithm

1. Evidence (E)
f = \text{ChooseRoot}(\mathcal{V})

2. for s \in \mathcal{N}(f)
\mu\text{-Collect}(f, s)

3. for s \in \mathcal{N}(f)
\nu\text{-Distribute}(f, s)

4. for i \in \mathcal{V}
COMPUTEMARGINAL(i)
```

```
3. \nu-Distribute(i, s)
\nu-SendMessage(i, s)
for j \in \mathcal{N}(s) \setminus i
\mu-Distribute(s, j)
```

```
\mu	ext{-Distribute}(s,i) \ \mu	ext{-SendMessage}(s,i) \ \mathbf{for}\ t \in \mathcal{N}(i) ackslash s \ 
u	ext{-Distribute}(i,t)
```

```
// distribute messages from root to leaves
```

Message from variable node  $X_i$  to the factor node  $f_s$ :  $\nu\text{-SENDMESSAGE}(i,s) \qquad \qquad \nu_{is}(x_i) = \prod_{t \in \mathcal{N}(i) \setminus s} \mu_{ti}(x_i)$  Message from factor node  $f_s$  to the variable node  $X_i$ :

```
\mu\text{-SENDMESSAGE}(s,i) \qquad \qquad \mu_{si}(x_i) = \sum_{x_{\mathcal{N}(s) \setminus i}} \left( f_s(x_{\mathcal{N}(s)}) \prod_{j \in \mathcal{N}(s) \setminus i} \nu_{js}(x_j) \right)
```

4. ComputeMarginal(i) 
$$p(x_i) \propto \nu_{is}(x_i)\mu_{si}(x_i)$$

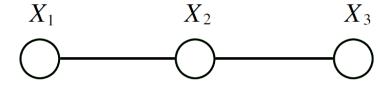
// compute marginal probability



Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002. CS5340 :: G.H. Lee

#### **Example:**

$$p(x|\bar{x}_E) = \frac{1}{Z^E} \left( \psi^E(x_1) \psi^E(x_2) \psi^E(x_3) \psi(x_1, x_2) \psi(x_2, x_3) \right)$$





Convert UGM into a factor graph

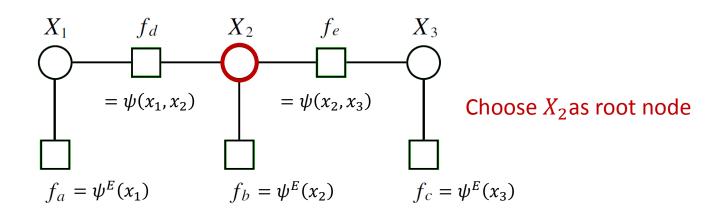
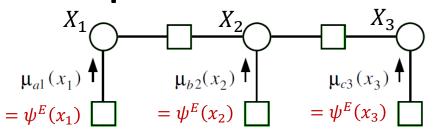


Image Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

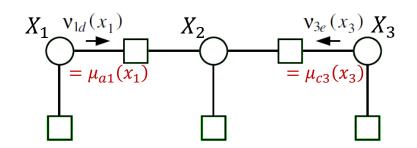


#### **Example:**



Collect messages from leaf nodes:

$$\mu_{si}(x_i) = f_s(x_i) = \psi^E(x_i)$$



**Collect** variable to factor messages:

$$\nu_{is}(x_i) = \prod_{t \in \mathcal{N}(i) \setminus s} \mu_{ti}(x_i)$$

$$\mu_{d2}(x_{2}) = \sum_{x_{1}} \psi(x_{1}, x_{2}) \mu_{a1}(x_{1}) \qquad \mu_{e2}(x_{2}) = \sum_{x_{3}} \psi(x_{2}, x_{3}) \mu_{c3}(x_{3})$$

$$X_{1} \qquad \qquad X_{2} \qquad \qquad X_{3} \qquad \qquad Collection$$

$$\mu_{si}(x_{1}) \qquad \mu_{si}(x_{2}) \qquad \mu_{si}(x_{2}) \qquad \mu_{si}(x_{3}) \qquad \mu_{si}(x_{2}) \qquad \mu_{si}(x_{3}) \qquad \mu_{si}(x_{3}$$

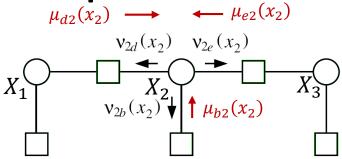
**Collect** factor to variable messages:

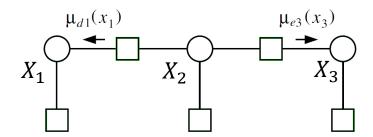
$$\mu_{si}(x_i) = \sum_{x_{\mathcal{N}(s)\setminus i}} \left( f_s(x_{\mathcal{N}(s)}) \prod_{j \in \mathcal{N}(s)\setminus i} \nu_{js}(x_j) \right)$$

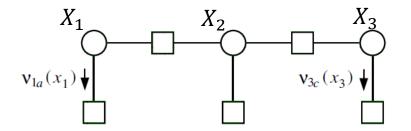
Image Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.



**Example:** 







#### **Distribute** variable to factor messages:

$$\nu_{is}(x_i) = \prod_{t \in \mathcal{N}(i) \setminus s} \mu_{ti}(x_i)$$

$$\nu_{2b}(x_2) = \mu_{d2}(x_2)\mu_{e2}(x_2)$$

$$\nu_{2d}(x_2) = \mu_{b2}(x_2)\mu_{e2}(x_2)$$

$$\nu_{2e}(x_2) = \mu_{b2}(x_2)\mu_{d2}(x_2)$$

#### **Distribute** factor to variable messages:

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

$$\mu_{d1}(x_1) = \sum_{x_2} \psi(x_1, x_2) \nu_{2d}(x_2)$$

$$\mu_{e3}(x_3) = \sum_{x_2} \psi(x_2, x_3) \nu_{2e}(x_2)$$

#### **Distribute** variable to factor messages:

$$\nu_{is}(x_i) = \prod_{t \in \mathcal{N}(i) \setminus s} \mu_{ti}(x_i)$$

$$v_{1a}(x_1) = \mu_{d1}(x_1), \quad v_{3c}(x_3) = \mu_{e3}(x_3)$$



# Relation Between Sum-Product for UGMs and Factor Graph

•  $m_{ji}(x_i)$  in the undirected graph is equal to  $\mu_{si}(x_i)$  in the factor graph!

#### **Proof:**

UGM:

$$m_{ji}(x_i) = \sum_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{k \in \mathcal{N}(j) \setminus i} m_{kj}(x_j) \right)$$

#### Factor Graph:

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

$$= \sum_{x_j} \psi(x_i, x_j) \nu_{js}(x_j)$$

$$= \sum_{x_j} \psi(x_i, x_j) \prod_{t \in \mathcal{N}(j)\setminus s} \mu_{tj}(x_j)$$

$$= \sum_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{t \in \mathcal{N}'(j)\setminus s} \mu_{tj}(x_j) \right)$$

N'(j) denotes the neighbourhood of  $X_j$ , omitting the singleton factor node associated with  $\psi^E(x_j)$ .



#### Maximum a Posterior Probabilities

- Marginalization problem: summing over all configurations of sets of random variables.
- Maximum a Posterior (MAP) problem: maximizing over all sets of random variables.
- Two aspects to MAP:
  - 1. Finding the maximal probability.
  - 2. Finding a configuration that achieves the maximal probability.



# Maximal Probability

• Given a probability distribution  $p(x \mid \bar{x}_E)$ , the maximum a posterior probability is given by:

$$\max_{x} p(x \mid \bar{x}_{E}) = \max_{x} \frac{p(x, \bar{x}_{E})}{p(\bar{x}_{E})}$$
 Can be removed since we are finding max over  $X$ .
$$= \max_{x} p(x, \bar{x}_{E})$$

$$= \max_{x} p(x) \delta(x_{E}, \bar{x}_{E})$$

$$= \max_{x} p(x)^{E}$$

#### where

- $\bar{X}_E$  is the set of observed variables, and
- $p(x)^E$  is the unnormalized representation of the conditional probability  $p(x, \bar{x}_E)$ .



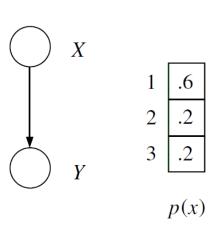
# Fallacy

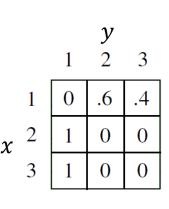
- Can we solve the MAP problem by computing the:
  - 1. marginal probability for each variable, and
  - 2. assignment of each variable that maximizes its individual marginal?

**NO!!!** 

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#### Illustration:





 $p(y \mid x)$ 

1	2	3
.4	.36	.24

p(y)

Marginal probabilities:

$$\max_{x} p(x) = p(x = 1) = 0.6$$

$$\max_{y} p(y) = p(y = 1) = 0.4$$

But

$$\max_{x,y} p(x,y) = p(x = 1, y = 2)$$
  
= 0.36

#### From Marginal to MAP Algorithms

• Distributive law of multiplication over addition:

$$a.b_1 + a.b_2 + ... + a.b_n = a.(b_1 + b_2 + ... + b_n)$$

• Plays a key role in elimination and sum-product algorithms:

$$p(x_1, x_2, ..., x_5) = \sum_{x_6} p(x_1) p(x_2 | x_1) p(x_3 | x_1) p(x_4 | x_2) p(x_5 | x_3) p(x_6 | x_2, x_5)$$

$$= \sum_{x_6} a. p(x_6 | x_2, x_5)$$

$$= a. p(x_6 = 0 | x_2, x_5) + \dots + a. p(x_6 = k | x_2, x_5)$$

$$= a. \left( p(x_6 = 0 | x_2, x_5) + \dots + p(x_6 = k | x_2, x_5) \right) \quad \text{(Distributive law)}$$

$$= p(x_1) p(x_2 | x_1) p(x_3 | x_1) p(x_4 | x_2) p(x_5 | x_3) \sum_{x_6} p(x_6 | x_2, x_5)$$



#### From Marginal to MAP Algorithms

Distributive law applies to the "max" operator too!

$$\max(a, b_1, a, b_2, ..., a, b_n) = a \cdot \max(b_1 + b_2 + ... + b_n)$$

 Turn the elimination algorithm into the "MAP-elimination" algorithm by replacing the "sum" with "max" operator:

$$\max_{x_6} p(x_1, x_2, ..., x_6) = \max_{x_6} p(x_1) p(x_2|x_1) p(x_3|x_1) p(x_4|x_2) p(x_5|x_3) p(x_6|x_2, x_5)$$

$$\text{"max" operator can be pushed in!}$$

$$= p(x_1) p(x_2|x_1) p(x_3|x_1) p(x_4|x_2) p(x_5|x_3) \max_{x_6} p(x_6|x_2, x_5)$$

$$\text{independent of } x_6$$

• Becomes the "max-product" algorithm.



# MAP-Elimination Algorithm

```
// main steps of the "MAP-Elimination Algorithm"
   MAP-ELIMINATE(\mathcal{G}, E)
        Initialize(\mathcal{G})
1.
        EVIDENCE(E)
        Update(\mathcal{G})
        Maximum
                                   // choose elimination ordering, and add local condition probabilities in active list
1. Initialize(\mathcal{G})
        choose an ordering I // same as the "variable elimination algorithm"
        for each node X_i in \mathcal{V}
              place p(x_i | x_{\pi_i}) on the active list
2. Evidence(E)
                                                              // add evidence potentials in active list
        for each i in E
                                                              // same as the "variable elimination algorithm"
              place \delta(x_i, \bar{x}_i) on the active list
3. Update(\mathcal{G})
                                   // maximization, and update active list
        for each i in I
              find all potentials from the active list that reference x_i and remove them from the active list
              let \phi_i^{\max}(x_{T_i}) denote the product of these potentials
              \det \overline{m_i^{\max}(x_{S_i})} = \max_{x_i} \phi_i^{\max}(x_{T_i})
              place m_i^{\max}(x_{S_i}) on the active list
```

4. Maximum

 $\max_{x} p^{E}(x) =$ the scalar value on the active list



Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

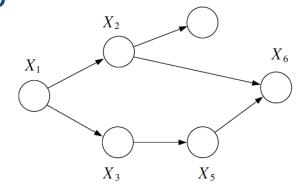
CS5340 :: G.H. Lee 36

### MAP-Elimination Algorithm

#### **Example:**

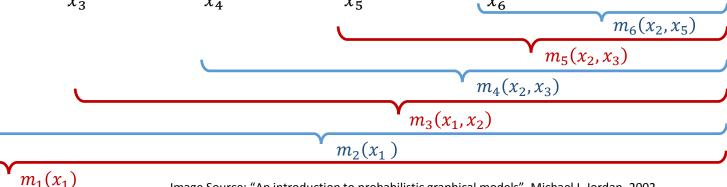
Elimination order:  $I = \{6, 5, 4, 3, 2, 1\}$ 

$$p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_4|x_2)p(x_5|x_3)p(x_6|x_2,x_5)$$



$$\max_{x} p(x_1, x_2, x_3, x_5 | \bar{x}_6) = \max_{x_1} \max_{x_2} \max_{x_3} \max_{x_4} \max_{x_5} \max_{x_6} \frac{p(x_1, x_2, x_3, x_5, \bar{x}_6)}{p(\bar{x}_6)}$$

- $= \max_{x_1} \max_{x_2} \max_{x_3} \max_{x_4} \max_{x_5} \max_{x_6} p(x_1, x_2, x_3, x_5, \bar{x}_6)$
- $= \max_{x_1} \max_{x_2} \max_{x_3} \max_{x_4} \max_{x_5} \max_{x_6} p(x_1) p(x_2|x_1) p(x_3|x_1) p(x_4|x_2) p(x_5|x_3) p(x_6|x_2, x_5) \delta(x_6, \bar{x}_6)$
- $= \max_{x_1} p(x_1) \max_{x_2} p(x_2|x_1) \max_{x_3} p(x_3|x_1) \max_{x_4} p(x_4|x_2) \max_{x_5} p(x_5|x_3) \max_{x_6} p(x_6|x_2,x_5) \delta(x_6,\bar{x}_6)$





 $Image\ Source:\ "An\ introduction\ to\ probabilistic\ graphical\ models",\ Michael\ I.\ Jordan,\ 2002.$ 

#### Underflow Problem

- Products of probabilities (numbers between 0 and 1) tend to underflow!
- Can be overcome by transforming to the monotone log scale:

$$\max_{x} p^{E}(x) = \max_{x} \log p^{E}(x)$$

Fortunately, the distributive law still holds:

$$\max(a + b_1, a + b_2, ..., a + b_n) = a + \max(b_1, b_2, ..., b_n)$$

 Turns the "max-product" algorithm into the "maxsum" algorithm.

- Find the MAP probability for a tree.
- We choose any node  $X_f$  as the root of the tree, and messages are propagated (inward pass) from the leaves to the root.
- Message from  $X_i$  to  $X_i$  (closer to root):

$$m_{ji}^{\max}(x_i) = \max_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{k \in \mathcal{N}(j) \backslash i} m_{kj}^{\max}(x_j) \right) X_i$$

$$\prod_{k \in \mathcal{N}(j) \backslash i} m_{kj}^{\max}(x_j)$$

$$\prod_{k \in \mathcal{N}(j) \backslash i} m_{kj}^{\max}(x_j)$$



Collect all messages at the root and compute the MAP probability as:

$$\max_{x} p^{E}(x) = \max_{x_{i}} \left( \psi^{E}(x_{f}) \prod_{e \in N(f)} m_{ef}^{\max}(x_{f}) \right)$$

$$\dots$$

$$X_{e \in N(f)} m_{ef}^{\max}(x_{f})$$

$$\dots$$

$$X_{e \in N(f)}$$

Do we need to pass the messages back to the leaves?

#### No!

MAP probabilities for all choices of the root node are the same.



#### Maximum a Posteriori Configurations

• This is the problem of finding a configuration  $x^*$  such that:

$$x^* \in \operatorname*{argmax} p^E(x)$$

• Making use of the messages to the root  $X_f$  from the sum-product algorithm, we obtain a value:

$$x_f^* \in \arg\max_{x_f} \left( \psi^E(x_f) \prod_{e \in \mathcal{N}(f)} m_{ef}^{\max}(x_f) \right)$$

that necessarily belongs to a maximum configuration.



#### Maximum a Posteriori Configurations

 Can we perform an outward pass of the messages from the root to leaves so that we can find the MAP configurations for all x?

#### NO!

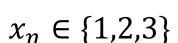
• No guarantee that the values  $x^*$  found this way belong to the same maximizing configuration.



#### Maximum a Posteriori Configurations

#### **Example:**

A lattice, or trellis, diagram shows two sets of configurations (black paths) in a chain model that give rise to the same MAP probability.



Trellis diagram shows each possible state of the random variable.

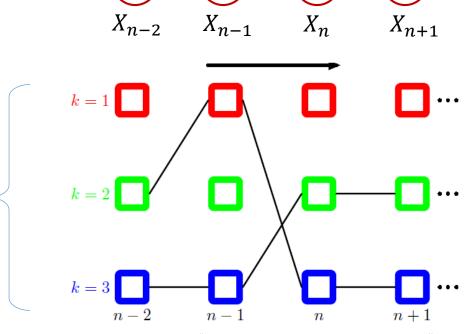




Image source: "Pattern recognition and machine learning", Christopher Bishop

• **Solution**: we also have to record the maximizing values in a table  $\delta_{ji}(x_i)$  when a message  $m_{ji}^{\max}(x_i)$  is sent from  $X_j$  to  $X_i$  (closer to root):

$$\delta_{ji}(x_i) \in \arg\max_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{k \in \mathcal{N}(j) \setminus i} m_{kj}^{\max}(x_j) \right)$$

• More precisely, for each  $X_i$ , the function  $\delta_{ji}(x_i)$  picks out a value of  $X_j$  (can be several) that achieves the maximum.



• Having defined  $\delta_{ji}(x_i)$  during the inward pass, we use  $\delta_{ji}(x_i)$  to define a consistent maximizing configuration during an outward pass:

- 1. Choose a maximizing value  $x_f^*$  at the root  $X_f$ .
- 2. Set  $x_e^* = \delta_{ef}(x_f^*)$  for each  $e \in N(f)$ .
- 3. Procedure continues outward to the leaves.



```
// main steps of the "MAP-Product Algorithm" for a tree \mathcal{T}(\mathcal{V}, \mathcal{E})
     Max-Product(\mathcal{T}, E)
           EVIDENCE(E)
           f = \text{ChooseRoot}(\mathcal{V})
          for e \in \mathcal{N}(f)
                 Collect(f, e)
          MAP = \max_{x_f} (\psi^E(x_f) \prod_{e \in \mathcal{N}(f)} m_{ef}^{\max}(x_f))
                                                                           // compute MAP probability at root
          x_f^* = \arg\max_{x_f} (\psi^E(x_f) \prod_{e \in \mathcal{N}(f)} m_{ef}^{\max}(x_f))
                                                                          // get MAP configuration at root
                 DISTRIBUTE(f, e)
1. Collect(i, j)
                                           // inward message passing
          for k \in \mathcal{N}(j) \setminus i
                Collect(j, k)
          SENDMESSAGE(i, i)
                                          // outward message passing
2. DISTRIBUTE(i, j)
          SetValue(i, j)
          for k \in \mathcal{N}(j) \setminus i
                DISTRIBUTE(j, k)
    SENDMESSAGE(j, i)
         m_{ji}^{\max}(x_i) = \max_{x_j} (\psi^E(x_j) \psi(x_i, x_j) \prod_{k \in \mathcal{N}(j) \setminus i} m_{kj}^{\max}(x_j)) // compute MAP probability message
         \delta_{ji}(x_i) \in \arg \max_{x_j} (\psi^E(x_j) \psi(x_i, x_j) \quad \prod \quad m_{kj}^{\max}(x_j)) \quad // \text{ get MAP configurations}
   SetValue(i, j) // get MAP configuration in outward pass
          x_i^* = \delta_{ii}(x_i^*)
```



## From Variable Elimination to Junction Tree

• Variable Elimination is query sensitive: we must rerun the entire algorithm for each query node.

• The Junction Tree algorithm generalizes Variable Elimination to avoid this.



# From Variable Elimination to Junction Tree

- Main idea behind Junction Trees:
  - Probability distributions corresponding to loopy undirected graphs can be re-parameterized as trees.
  - > We can run the Sum-Product algorithm on the tree re-parameterization.



### Cluster Graphs

- Undirected graph such that:
  - 1. Nodes are clusters  $C_i \subseteq \{X_1, ..., X_n\}$ , where  $X_i$  are the random variables.
  - 2. Edge between  $C_i$  and  $C_j$  associated with sepset  $S_{ij} = C_i \cap C_j$ .
- Family preservation: given a set of potentials  $\Psi \in \{\psi_1, ..., \psi_k\}$  from an UGM, we assign each  $\psi_k$  to a cluster  $C_{\alpha(k)}$  s.t.  $Scope[\psi_k] \subseteq C_{\alpha(k)}$ .
- Cluster potential is defined as:

$$\phi_i(C_i) = \prod_{k:\alpha(k)=i} \psi_k$$



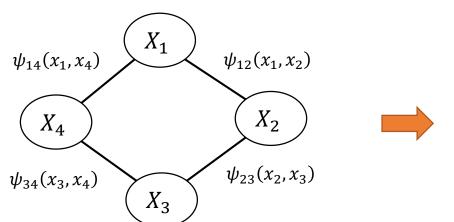
### Cluster Graphs

#### Example:

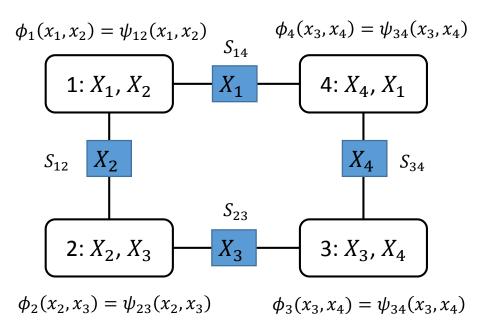
#### **Cluster Graph**

Sepset:  $S_{ij} \subseteq C_i \cap C_j$ 

**Undirected Graphical Model** 



Cluster potential:  $\phi_i(C_i) = \prod_{k:\alpha(k)=i} \psi_k$ 







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• For each pair of clusters  $C_i$ ,  $C_j$  and variable  $X \in C_i \cap C_j$ :

There exists an unique path between  $C_i$  and  $C_j$  for which all clusters and sepsets contain X.

• Equivalently: For any *X*, the set of clusters and sepsets containing *X* form a tree.

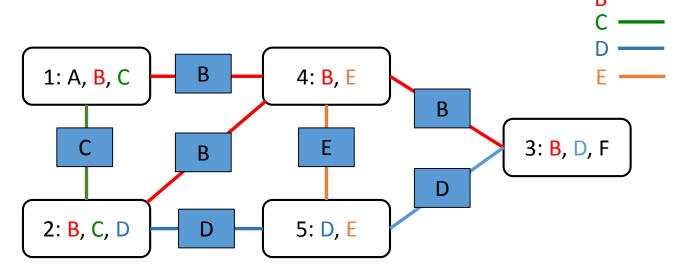


• A valid cluster graph must fulfil the running intersection property.

Example: Legal cluster graph

Trees formed by:

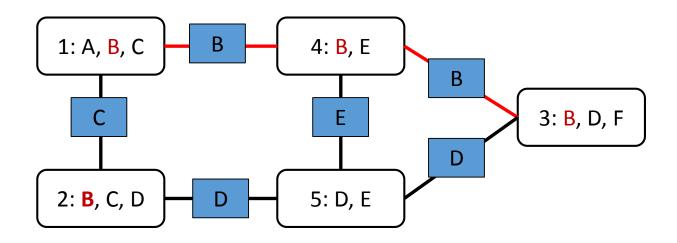
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Adapted from: "Probabilitistic Graphical Models", Daphne Koller



**Example**: Illegal cluster graph I



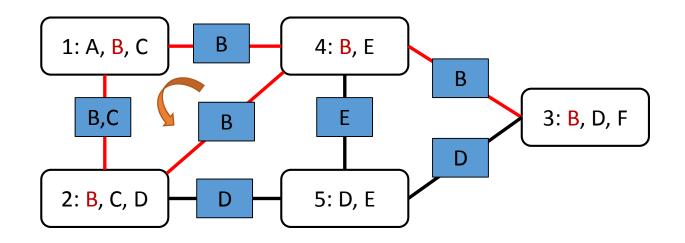
B is disconnected from the path!



Adapted from: "Probabilitistic Graphical Models", Daphne Koller

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**Example**: Illegal cluster graph II



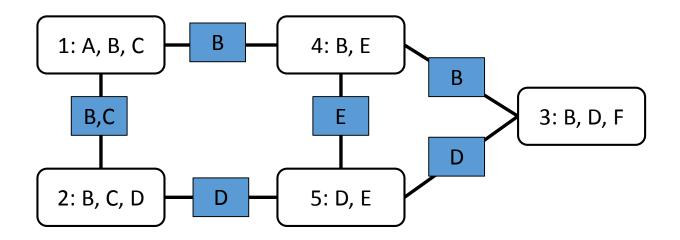
B forms a cycle!



Adapted from: "Probabilitistic Graphical Models", Daphne Koller

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Example: Alternative legal cluster graph





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### Clique Trees a.k.a. Junction Trees

- A cluster graph without cycles is known as the cluster tree.
- A cluster tree that fulfills the running intersection property is called the clique tree, a.k.a. junction tree.
- We refer to a "cluster" in a clique tree as "clique", and "cluster potential" as "clique potential".



### Clique Trees a.k.a. Junction Trees

We will first look at how to compute all marginals via the junction tree, before looking at how to convert a DGM/UGM into a junction tree.



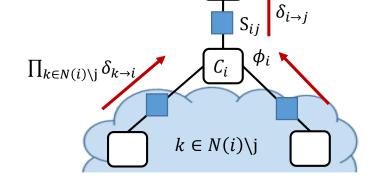
- We first randomly choose a root clique, followed by message passing:
  - Inward messages towards the root clique from the leaf cliques.
  - Outward messages from the root clique towards the leaf cliques.
- Message passing protocol:  $C_i$  is ready to pass message to a neighbour  $C_j$  when it has received messages from all neighbors except for  $C_i$ .



Use the sum-product algorithm to compute messages

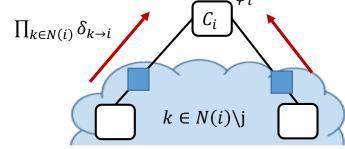
from  $C_i$  to  $C_j$ :

$$\delta_{i\to j} = \sum_{C_i \setminus S_{ij}} \phi_i \cdot \prod_{k \in N(i) \setminus j} \delta_{k\to i}$$



• The unnormalized\* marginal probability of clique  $C_i$  is given by:

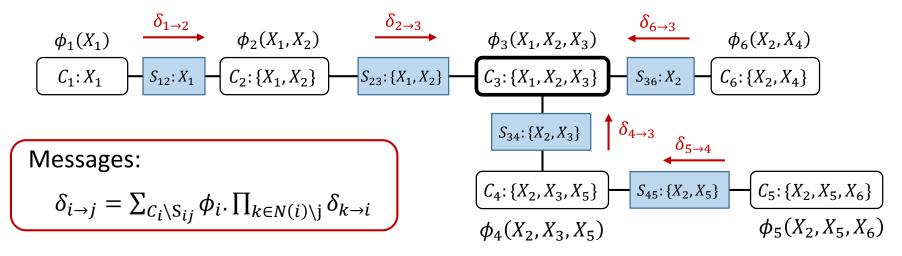
$$\tilde{p}(C_i) = \phi_i \cdot \prod_{k \in N(i)} \delta_{k \to i}$$



\*Unnormalized probability because the clique potentials come from the UGM potentials, where we ignored the partition function



#### **Example:** Let's choose $C_3$ as the root



#### Inward pass:

$$\delta_{1\to 2} = \sum_{C_1 \setminus S_{12}} \phi_1 = \phi_1$$

$$\delta_{2\to 3} = \sum_{C_2 \setminus S_{23}} \phi_2 \cdot \delta_{1\to 2} = \phi_2 \cdot \phi_1$$

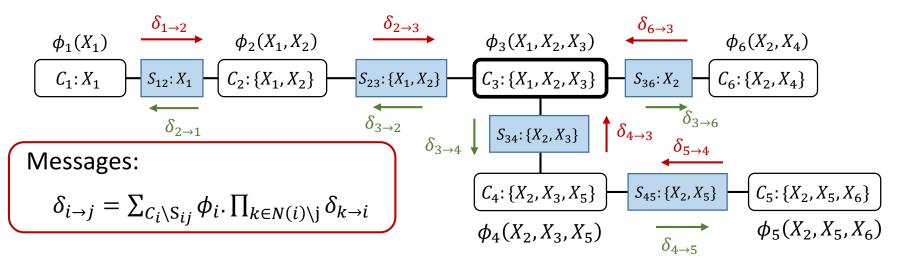
$$\delta_{5\to 4} = \sum_{C_5 \setminus S_{45}} \phi_5 = \sum_{X_6} \phi_5$$

$$\delta_{4\to 3} = \sum_{C_4 \setminus S_{34}} \phi_4 \cdot \delta_{5\to 3} = \sum_{X_5} \phi_4 \sum_{X_6} \phi_5$$

$$\delta_{6\to 3} = \sum_{C_6 \setminus S_{36}} \phi_6 = \sum_{X_4} \phi_6$$



#### **Example:** Let's choose $C_3$ as the root



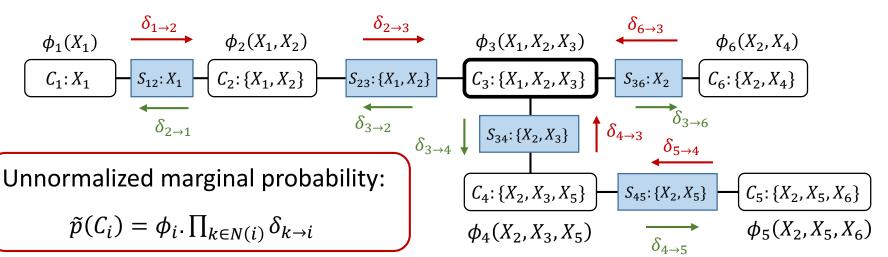
#### Inward pass:

$$\begin{split} \delta_{1\to 2} &= \sum_{C_1 \setminus S_{12}} \phi_1 = \phi_1 \\ \delta_{2\to 3} &= \sum_{C_2 \setminus S_{23}} \phi_2 \cdot \delta_{1\to 2} = \phi_2 \cdot \phi_1 \\ \delta_{5\to 4} &= \sum_{C_5 \setminus S_{45}} \phi_5 = \sum_{X_6} \phi_5 \\ \delta_{4\to 3} &= \sum_{C_4 \setminus S_{34}} \phi_4 \cdot \delta_{5\to 3} = \sum_{X_5} \phi_4 \sum_{X_6} \phi_5 \\ \delta_{6\to 3} &= \sum_{C_6 \setminus S_{36}} \phi_6 = \sum_{X_4} \phi_6 \end{split}$$

#### Outward pass:

$$\begin{split} \delta_{3\to 2} &= \sum_{C_3 \setminus S_{23}} \phi_3 \,.\, \delta_{6\to 3} \,.\, \delta_{4\to 3} \\ \delta_{2\to 1} &= \sum_{C_2 \setminus S_{12}} \phi_2 \,.\, \delta_{3\to 2} \\ \delta_{3\to 6} &= \sum_{C_3 \setminus S_{36}} \phi_3 \,.\, \delta_{2\to 3} \,.\, \delta_{4\to 3} \\ \delta_{3\to 4} &= \sum_{C_3 \setminus S_{34}} \phi_3 \,.\, \delta_{2\to 3} \,.\, \delta_{6\to 3} \\ \delta_{4\to 5} &= \sum_{C_4 \setminus S_{45}} \phi_4 \,.\, \delta_{3\to 4} \end{split}$$

#### **Example:** Let's choose $C_3$ as the root



$$\begin{split} \tilde{p}(C_1) &= \tilde{p}(X_1) = \phi_1. \prod_{k \in N(1)} \delta_{k \to 1} \\ &= \phi_1. \delta_{2 \to 1} \\ &= \phi_1. \sum_{C_2 \setminus S_{12}} \phi_2. \delta_{3 \to 2} \\ &= \phi_1. \sum_{X_2} \phi_2. \sum_{C_3 \setminus S_{23}} \phi_3. \delta_{6 \to 3}. \delta_{4 \to 3} \\ &= \phi_1. \sum_{X_2} \phi_2. \sum_{X_3} \phi_3. \sum_{X_4} \phi_6. \sum_{X_5} \phi_4. \sum_{X_6} \phi_5 \end{split}$$

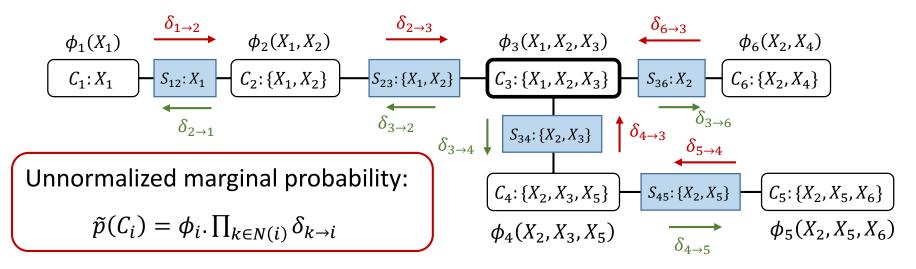
Result is equivalent to variable elimination!

#### Marginal probability:

$$p(X_1) = \frac{\tilde{p}(X_1)}{\sum_{X_1} \tilde{p}(X_1)}$$



#### **Example:** Let's choose $C_3$ as the root



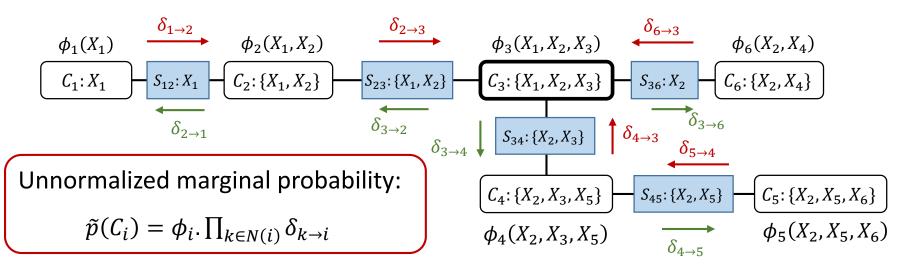
$$\begin{split} \widetilde{p}(C_2) &= \widetilde{p}(X_1, X_2) \\ &= \phi_2. \prod_{k \in N(2)} \delta_{k \to 2} \\ &= \phi_2. \delta_{1 \to 2} . \delta_{3 \to 2} \end{split}$$

#### Marginal probabilities:

$$p(X_1, X_2) = \frac{\tilde{p}(X_1, X_2)}{\sum_{X_1} \sum_{X_2} \tilde{p}(X_1, X_2)}$$
$$p(X_2) = \sum_{X_1} p(X_1, X_2)$$



#### **Example:** Let's choose $C_3$ as the root



$$\tilde{p}(C_{3}) = \tilde{p}(X_{1}, X_{2}, X_{3}) 
= \phi_{3} \cdot \delta_{2 \to 3} \cdot \delta_{6 \to 3} \cdot \delta_{4 \to 3} 
\tilde{p}(C_{5}) = \tilde{p}(X_{2}, X_{5}, X_{6}) 
= \phi_{5} \cdot \delta_{4 \to 5} 
\tilde{p}(C_{4}) = \tilde{p}(X_{2}, X_{3}, X_{5}) 
= \phi_{4} \cdot \delta_{3 \to 4} \cdot \delta_{5 \to 4} 
\tilde{p}(C_{6}) = \tilde{p}(X_{2}, X_{4}) 
= \phi_{6} \cdot \delta_{3 \to 6}$$



#### 1. Triangulation: Get the reconstituted graph

Choose an elimination ordering I

```
DIRECTEDGRAPHELIMINATE(G, I)

1. G^m = \text{Moralize}(G) // for DGM, skip this step if UGM

2. UndirectedGraphEliminate(G^m, I) // get reconstituted graph

1. Moralize(G)
```

for each node  $X_i$  in Iconnect all of the parents of  $X_i$ end drop the orientation of all edges
return G

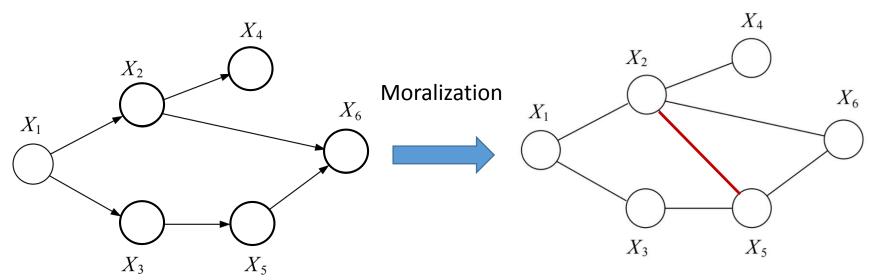
2. Underected Graph Eliminate (G, I) for each node  $X_i$  in I connect all of the remaining neighbors of  $X_i$  remove  $X_i$  from the graph end



Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

#### 1. Triangulation: Get the reconstituted graph

Choose an elimination ordering I = (6; 5; 4; 3; 2; 1)



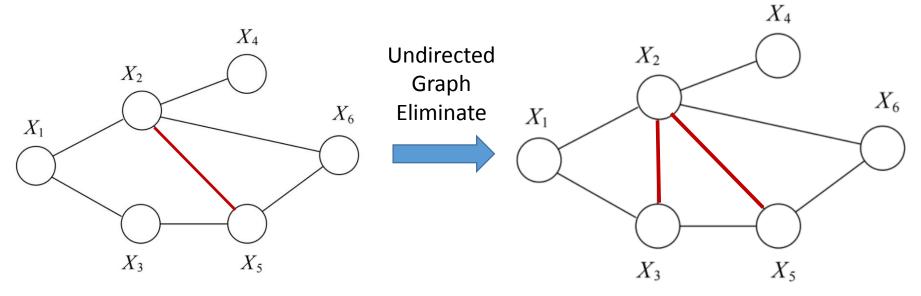
Parents are "married"



Source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

#### 1. Triangulation: Get the reconstituted graph

Choose an elimination ordering I = (6; 5; 4; 3; 2; 1)



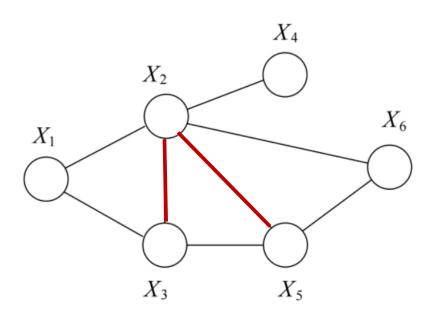
Parents are "married"

Reconstituted graph: additional edges (red) added during the elimination process

National University of Singapore of Computing

Image source: "An introduction to probabilistic graphical models", Michael I. Jordan, 2002.

2. Get all clusters and all possible sepsets: Use eliminate cliques as clusters, a possible sepset is  $S_{ij} = C_i \cap C_j$ .



$$C_5: \{X_2, X_5, X_6\}$$

$$C_4$$
: { $X_2$ ,  $X_3$ ,  $X_5$ }

$$C_6$$
: { $X_2$ ,  $X_4$ }

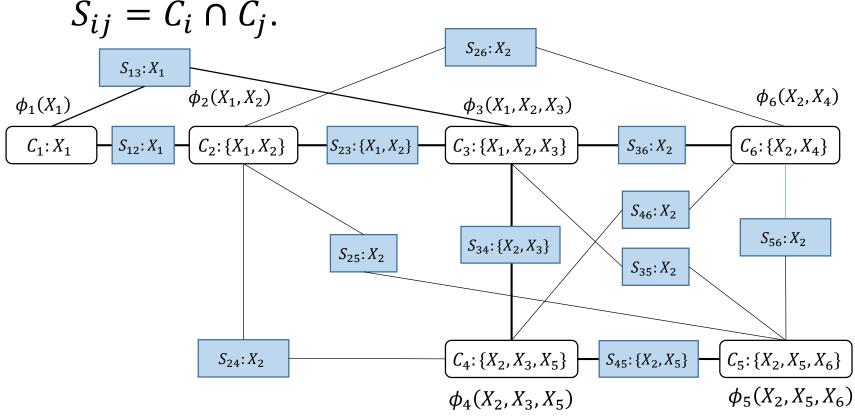
$$C_3$$
: { $X_1$ ,  $X_2$ ,  $X_3$ }

$$C_2$$
: { $X_1, X_2$ }

$$C_1: X_1$$



2. Get all clusters and all possible sepsets: Use eliminate cliques as clusters, a possible sepset is

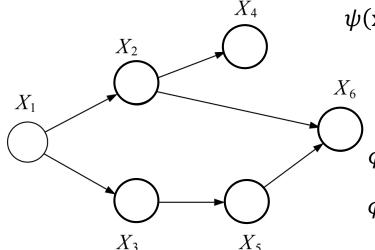




3. Assign cluster potentials: cluster potentials are formed by condition probabilities (DGM), or potentials (UGM).

 $p(\mathbf{x}_1)p(x_2|\mathbf{x}_1)p(x_3|\mathbf{x}_1)p(x_4|\mathbf{x}_2)p(x_5|\mathbf{x}_3)p(x_6|\mathbf{x}_2,\mathbf{x}_5)$  $\psi(\mathbf{x}_1)\psi(x_1,\mathbf{x}_2)\psi(x_1,\mathbf{x}_3)\psi(x_2,\mathbf{x}_4)\psi(x_3,\mathbf{x}_5)\psi(x_2,\mathbf{x}_5,\mathbf{x}_6)$ 





$$\phi_1(X_1) = p(x_1),$$
  $\phi_2(X_1, X_2) = p(x_2|x_1)$ 

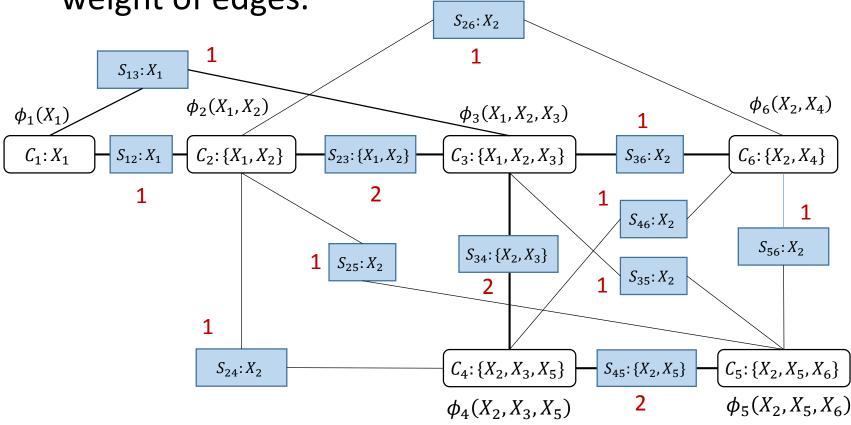
$$\phi_3(X_1, X_2, X_3) = p(x_3|x_1), \quad \phi_4(X_2, X_3, X_5) = p(x_5|x_3)$$

$$\phi_5(X_2, X_5, X_6) = p(x_6|x_2, x_5),$$

$$\phi_6(X_2, X_4) = p(x_4 | x_2)$$



3. Get clique tree / junction tree: find the maximum spanning tree with cardinality of sepsets as weight of edges.





3. Get clique tree / junction tree: find the maximum spanning tree with cardinality of sepsets as weight of edges.

**Theorem**: A cluster tree T is a clique tree / junction tree only if it is a maximal spanning tree.



#### **Proof**:

Consider a random variable  $X_k$  and a cluster tree T with cluster  $C_i$  and sepset  $S_i$ , the fact that T is a tree implies:

$$1(a): \text{indicator function that} \\ \text{returns 1 if $a$ is true, 0 otherwise} \\ \sum_{j=1}^{M-1} 1(X_k \in S_j) \leq \sum_{i=1}^{M} 1(X_k \in C_i) - 1, \\ \text{\# times $X_k$ appear in} \\ \text{the sepsets} \\ \text{\# times $X_k$ appear in} \\ \text{the cluster} \\ \text{$M:$ \# clusters} \\ \text{$M:$$$

The inequality sign becomes equality when  $X_k$  forms a subtree, i.e. running intersection property is fulfilled.



#### **Proof**:

Total weight of a cluster tree w(T) is equal to the sum of the cardinalities of its sepsets:

$$w(T) = \sum_{j=1}^{M-1} |S_j|$$

$$= \sum_{j=1}^{M-1} \sum_{k=1}^{N} 1(X_k \in S_j)$$

$$= \sum_{k=1}^{N} \sum_{j=1}^{M-1} 1(X_k \in S_j)$$

sum of cardinalities of all sepsets

sum of cardinalities of all clusters minus # random variables

$$= \sum_{k=1}^{N} \sum_{j=1}^{M-1} 1(X_k \in S_j) \leq \sum_{k=1}^{N} \left[ \sum_{i=1}^{M} 1(X_k \in C_i) - 1 \right]$$
 From the previous slide

 $= \sum_{i=1}^{M} \sum_{j=1}^{N} 1(X_k \in C_i) - N$ 

$$= \sum_{i=1}^{M} |C_i| - N$$

*M*: # cliques

*N*: # random variables



#### **Proof**:

$$w(T) = \sum_{i=1}^{M-1} |S_j| \le \sum_{k=1}^{N} \left[ \sum_{i=1}^{M} 1(X_k \in C_i) - 1 \right]$$

*M*: # cliques

*N*: # random variables

- We saw from previous slide that for the running intersection property, i.e. junction tree to hold, the inequality has to become equality.
- This implies a maximum sum of cardinalities of all sepsets,
   i.e. maximal spanning tree!

3. Get clique tree / junction tree: find the maximum spanning tree with cardinality of sepsets as weight of edges.

```
KRUSKAL(G):
1 A = Ø
2 foreach v ∈ G.V:
3    MAKE-SET(v)
4 foreach (u, v) in G.E ordered by weight(u, v), increasing:
5    if FIND-SET(u) ≠ FIND-SET(v):
6         A = A ∪ {(u, v)}
7         UNION(u, v)
8 return A
```

Can be more than 1 maximum spanning tree!

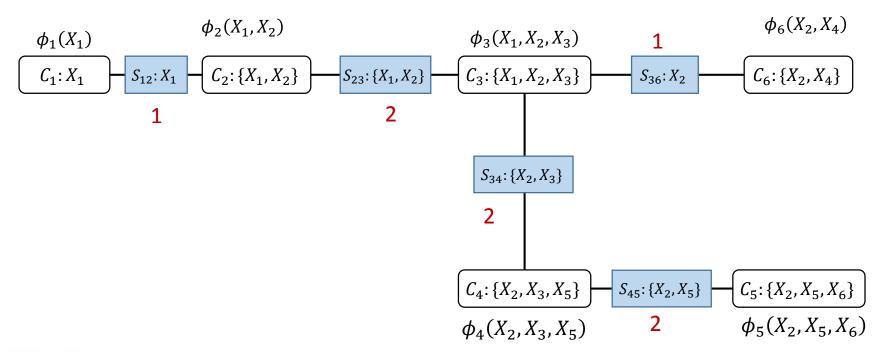


Source: https://en.wikipedia.org/wiki/Kruskal%27s\_algorithm

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3. Get clique tree / junction tree: find the maximum spanning tree with cardinality of sepsets as weight of edges.

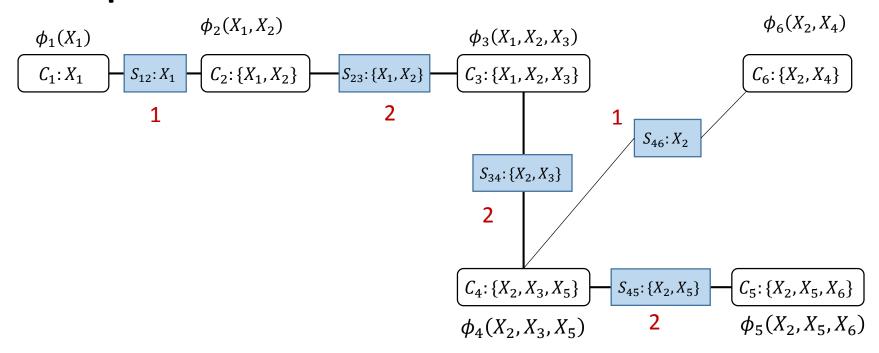
#### **Example:**





3. Get clique tree / junction tree: find the maximum spanning tree with cardinality of sepsets as weight of edges.

#### **Example:**





#### Summary

- We have looked at how to:
- Represent a joint distribution with a factor graph, and use it to compute the marginal/conditional probabilities.
- 2. Use the max-product algorithm to find the maximal probability and its configurations.
- 3. Convert a DGM/UGM into the junction tree and use it to compute the marginal/conditional probabilities.

