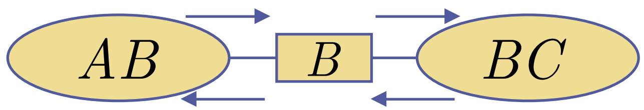
Machine Learning

Topic 18

- The Junction Tree Algorithm
- Collect & Distribute
- Algorithmic Complexity
- ArgMax Junction Tree Algorithm

Review: Junction Tree Algorithm

- Send message from each clique *to* its separators of what it thinks the submarginal on the separator is.
- Normalize each clique by incoming message *from* its separators so it agrees with them



$V = \{A, B\} \quad S = \{B\} \quad W = \{B, C\}$

If agree: $\sum_{V \setminus S} \psi_V = \phi_S = p(S) = \phi_S = \sum_{W \setminus S} \psi_W$ **...Done!**

Else:

Send message From V to W...

$$\phi_S^* = \sum_{V \setminus S} \psi_V$$
$$\psi_W^* = \frac{\phi_S^*}{\phi_S} \psi_W$$
$$\psi_V^* = \psi_V$$

Send message From W to V...

$$\phi_S^{**} = \sum_{W \setminus S} \psi_W^*$$
$$\psi_V^{**} = \frac{\phi_S^{**}}{\phi_S^*} \psi_V^*$$
$$\psi_W^{**} = \psi_W^*$$

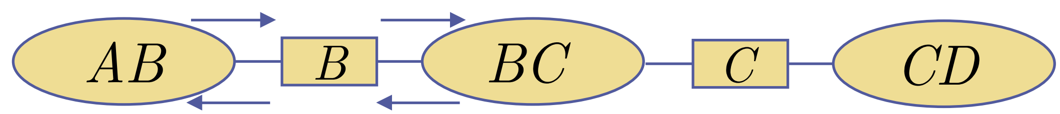
Now they Agree...Done!

$$\sum_{V \setminus S} \psi_V^{**} = \sum_{V \setminus S} \frac{\phi_S^{**}}{\phi_S^*} \psi_V^* = \frac{\phi_S^{**}}{\phi_S^*} \sum_{V \setminus S} \psi_V^* = \phi_S^{**} = \sum_{W \setminus S} \psi_W^{**}$$

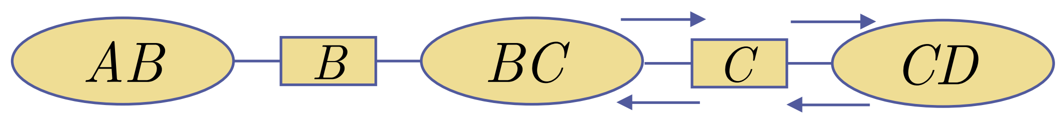
JTA with many cliques

- Problem: what if we have more than two cliques?

1) Update AB & BC



2) Update BC & CD



- Problem: AB has not heard about CD!
  After BC updates, it will be inconsistent for AB

- Need to iterate the pairwise updates many times
- This will eventually converge to consistent marginals
- But, inefficient… can we do better?

JTA: Collect & Distribute

- Use tree recursion rather than iterate messages mindlessly!

initialize(DAG){ Pick root
Set all variables as: $\psi_{C_i} = p\left(x_i \mid \pi_i\right), \phi_S = 1$ **}**

```
collectEvidence(node) {
   for each child of node {
      update1(node,collectEvidence(child)); }
   return(node); }

distributeEvidence(node) {
   for each child of node {
      update2(child,node);
      distributeEvidence(child); } }
```

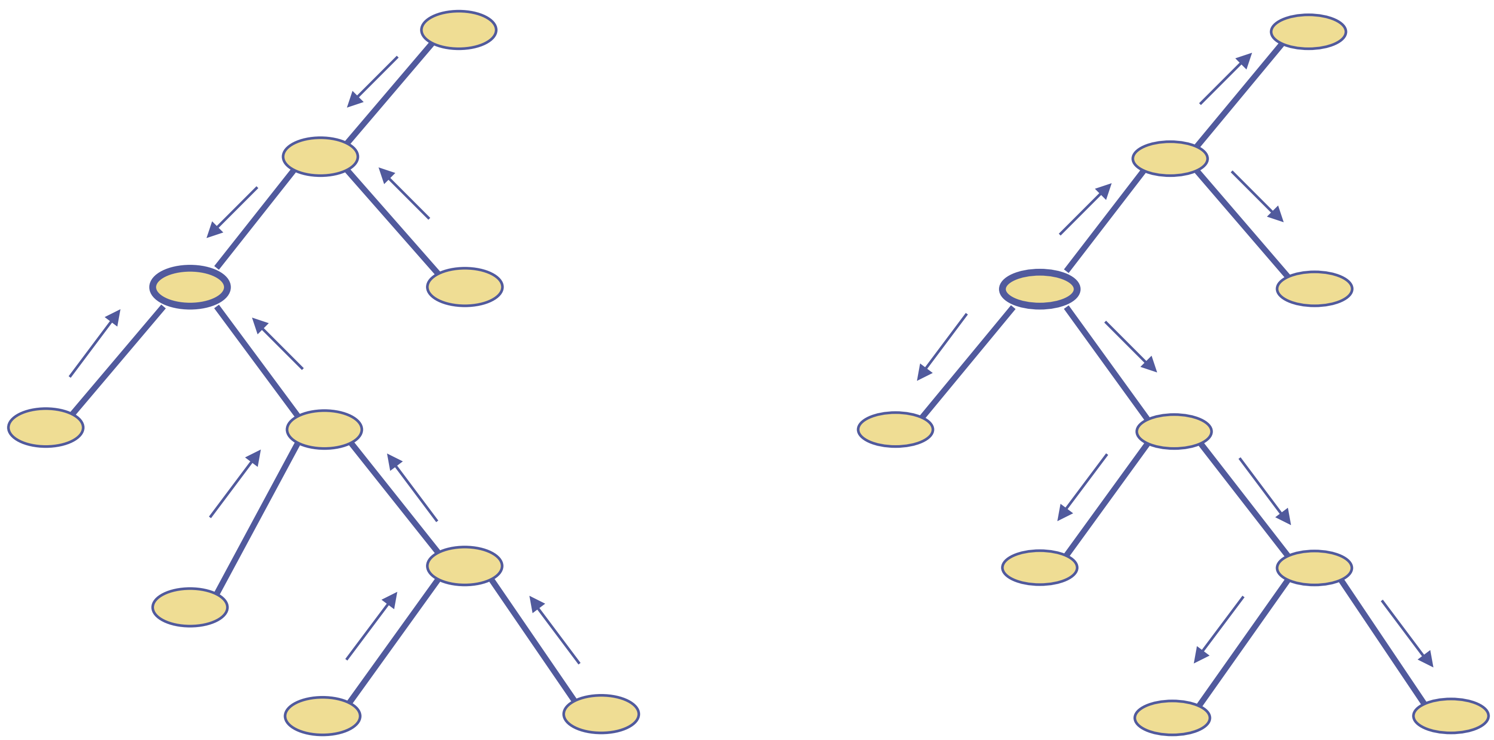
update1(node w,node v) { $\phi^{*}_{V\cap W} = \sum_{V\setminus(V\cap W)} \psi_V, \;\; \psi_W = \frac{\phi^{*}_{V\cap W}}{\phi_{V\cap W}} \psi_W$ **}**

update2(node w,node v) { $\phi^{**}_{V\cap W} = \sum_{V\setminus(V\cap W)} \psi_V, \;\; \psi_W = \frac{\phi^{**}_{V\cap W}}{\phi^{*}_{V\cap W}} \psi_W$ **}**

normalize() { $p\left(X_C\right) = \frac{1}{\sum_C \psi^{**}_C} \psi^{**}_C \;\; \forall C, \;\; p\left(X_S\right) = \frac{1}{\sum_S \phi^{**}_S} \phi^{**}_S \;\; \forall S$ **}**

Junction Tree Algorithm

- JTA: 1)*Initialize* 2)*Collect* 3)*Distribute* 4)*Normalize*



- Note: leaves do not change their ψ during *collect*
- Note: the first cliques *collect* changes are parents of leaves
- Note: root does not change its ψ during *distribute*

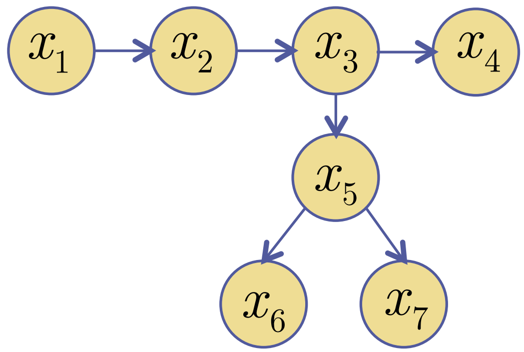
Algorithmic Complexity

- The 5 steps of JTA are all efficient:

1) Moralization
   Polynomial in # of nodes
2) Introduce Evidence (fixed or constant)
   Polynomial in # of nodes (convert pdf to slices)
3) Triangulate (Tarjan & Yannakakis 1984)
   Suboptimal=Polynomial, Optimal=NP
4) Construct Junction Tree (Kruskal)
   Polynomial in # of cliques
5) Junction Tree Algorithm (Init,Collect,Distribute,Normalize)
   Polynomial (linear) in # of cliques, *Exponential* in Clique Cardinality

Junction Tree Algorithm

- Convert Directed Graph to Junction Tree



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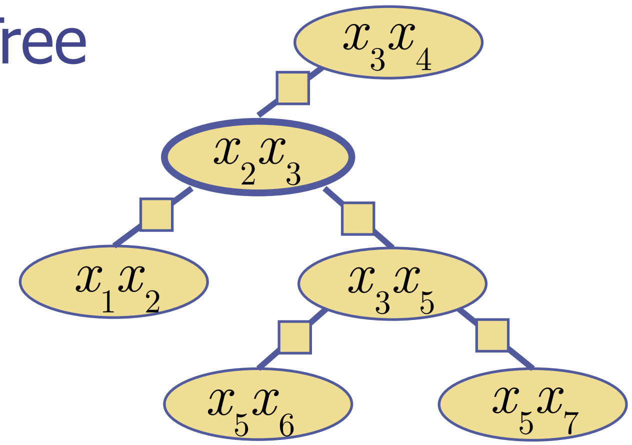


- *Initialize* separators to 1 (and Z=1) and set clique tables to the CPTs in the Directed Graph

$$p(X) = p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_2)p(x_4 \mid x_3)p(x_5 \mid x_3)p(x_6 \mid x_5)p(x_7 \mid x_5)$$

$$p(X) = \frac{1}{Z}\frac{\prod_C \psi(X_C)}{\prod_S \phi(X_S)} = \frac{1}{1}\frac{p(x_1,x_2)p(x_3 \mid x_2)p(x_4 \mid x_3)p(x_5 \mid x_3)p(x_6 \mid x_5)p(x_7 \mid x_5)}{1 \times 1 \times 1 \times 1 \times 1}$$

- Run *Collect, Distribute, Normalize*
- Get valid marginals from all ψ, ϕ tables

JTA with Extra Evidence

- If extra *evidence* is observed, must slice tables accordingly
- Example: $p(A,B,C,D) = \frac{1}{Z}\psi_{AB}\psi_{BC}\psi_{CD}$

$$Z = 1 \qquad AB - \boxed{B} - BC - \boxed{C} - CD$$

$$\psi_{AB} = \begin{array}{cc} \begin{bmatrix} 8 & 4 \\ 3 & 1 \end{bmatrix} & \begin{array}{l} A=0 \\ A=1 \end{array} \\ \begin{array}{cc} B=0 & B=1 \end{array} & \end{array} \qquad \psi_{BC} = \begin{array}{cc} \begin{bmatrix} 2 & 3 \\ 1 & 1 \end{bmatrix} & \begin{array}{l} B=0 \\ B=1 \end{array} \\ \begin{array}{cc} C=0 & C=1 \end{array} & \end{array} \qquad \psi_{CD} = \begin{array}{cc} \begin{bmatrix} 1 & 4 \\ 1 & 1 \end{bmatrix} & \begin{array}{l} C=0 \\ C=1 \end{array} \\ \begin{array}{cc} D=0 & D=1 \end{array} & \end{array}$$

- You are given *evidence*: A=0. Replace table with slices…

$$\psi_{AB} \to \begin{bmatrix} 8 & 4 \end{bmatrix} \qquad \psi_{BC} = \begin{bmatrix} 2 & 3 \\ 1 & 1 \end{bmatrix} \qquad \psi_{CD} = \begin{bmatrix} 1 & 4 \\ 1 & 1 \end{bmatrix}$$

- JTA now gives ψ, ϕ as marginals *conditioned* on evidence

$$p(B \mid A=0) = \frac{\psi_{AB}^{**}}{\sum_B \psi_{AB}^{**}} \qquad p(B,C \mid A=0) = \frac{\psi_{BC}^{**}}{\sum_{B,C} \psi_{BC}^{**}} \qquad p(C,D \mid A=0) = \frac{\psi_{CD}^{**}}{\sum_{C,D} \psi_{CD}^{**}}$$

- All denominators equal the new normalizer Z'

$$Z' = p(EVIDENCE) = \sum_B \psi_{AB}^{**} = \sum_{B,C} \psi_{BC}^{**} = \sum_{C,D} \psi_{CD}^{**}$$

ArgMax Junction Tree Algorithm

- We can also use JTA for finding the max not the sum over the joint to get argmax of marginals & conditionals
- Say have some evidence: $p\left(X_F, \bar{X}_E\right) = p\left(x_1, \ldots, x_n, \bar{x}_{n+1}, \ldots, \bar{x}_N\right)$
- Most likely (highest p) X_F? $X_F^* = \arg\max_{X_F} p\left(X_F, \bar{X}_E\right)$
- What is most likely state of patient with fever & headache?

$$\begin{aligned} p_F^* &= \max_{x_2,x_3,x_4,x_5} p\left(x_1 = 1, x_2, x_3, x_4, x_5, x_6 = 1\right) \\ &= \max_{x_2} p\left(x_2 \mid x_1 = 1\right) p\left(x_1 = 1\right) \max_{x_3} p\left(x_3 \mid x_1 = 1\right) \\ &\quad \max_{x_4} p\left(x_4 \mid x_2\right) \max_{x_5} p\left(x_5 \mid x_3\right) p\left(x_6 = 1 \mid x_2, x_5\right) \end{aligned}$$

- Solution: replace sum with max inside JTA update code

$$\phi_{V\cap W}^* = \max_{V\setminus(V\cap W)} \psi_V, \quad \psi_W = \frac{\phi_{V\cap W}^*}{\phi_{V\cap W}} \psi_W \qquad \phi_{V\cap W}^{**} = \max_{V\setminus(V\cap W)} \psi_V, \quad \psi_W = \frac{\phi_{V\cap W}^{**}}{\phi_{V\cap W}^*} \psi_W$$

- Final potentials are *max marginals*: $\psi^{**}\left(X_C\right) = \max_{U\setminus C} p\left(X\right)$
- Highest value in potential is most likely: $X_C^* = \arg\max_C \psi^{**}\left(X_C\right)$

ArgMax Junction Tree Algorithm

- Why do I need the ArgMax junction tree algorithm?
- Can't I just compute marginals using the Sum algorithm and then find the highest value in each marginal???
- No!! Here's a counter-example:

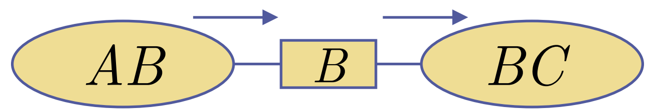
$$
p(x_1, x_2) = \begin{array}{cc} & \begin{array}{ccc} x_1 & x_1 & x_1 \\ A & B & C \end{array} \\ \begin{array}{c} x_2 = 0 \\ x_2 = 1 \end{array} & \begin{bmatrix} .14 & .05 & .27 \\ .24 & .20 & .10 \end{bmatrix} \end{array}
$$

- Most likely is $x_1^*=C$ and $x_2^*=0$
- But the sub-marginals $p(x_1)$ and $p(x_2)$ do not reveal this…

$$
p(x_1) = \begin{array}{c} \begin{array}{ccc} A & B & C \end{array} \\ \begin{bmatrix} 0.38 & 0.25 & 0.37 \end{bmatrix} \end{array}
\qquad
p(x_2) = \begin{array}{cc} \begin{array}{c} x_2 = 0 \\ x_2 = 1 \end{array} & \begin{bmatrix} .46 \\ .54 \end{bmatrix} \end{array}
$$

- The marginals would *falsely* imply that is $x_1^*=A$ and $x_2^*=1$

Example



- Note that products are element-wise
- Let us send a regular JTA message from AB to BC

$$\psi_{AB} = \begin{array}{cc} \begin{bmatrix} 8 & 4 \\ 3 & 1 \end{bmatrix} & \begin{array}{l} A=0 \\ A=1 \end{array} \\ \begin{array}{cc} B=0 & B=1 \end{array} & \end{array} \qquad \phi_B = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{array}{l} B=0 \\ B=1 \end{array} \qquad \psi_{BC} = \begin{array}{cc} \begin{bmatrix} 2 & 3 \\ 1 & 1 \end{bmatrix} & \begin{array}{l} B=0 \\ B=1 \end{array} \\ \begin{array}{cc} C=0 & C=1 \end{array} & \end{array}$$

$$\phi_B^* = \sum_A \psi_{AB} = \sum_A \begin{bmatrix} 8 & 4 \\ 3 & 1 \end{bmatrix} = \begin{array}{c} \begin{bmatrix} 11 & 5 \end{bmatrix} \\ \begin{array}{cc} B=0 & B=1 \end{array} \end{array} = \begin{bmatrix} 11 \\ 5 \end{bmatrix} \begin{array}{l} B=0 \\ B=1 \end{array}$$

$$\psi_{BC}^* = \frac{\phi_B^*}{\phi_B} \psi_{BC} = \frac{\begin{bmatrix} 11 \\ 5 \end{bmatrix}}{\begin{bmatrix} 1 \\ 1 \end{bmatrix}} \begin{bmatrix} 2 & 3 \\ 1 & 1 \end{bmatrix} = \begin{array}{cc} \begin{bmatrix} 22 & 33 \\ 5 & 5 \end{bmatrix} & \begin{array}{l} B=0 \\ B=1 \end{array} \\ \begin{array}{cc} C=0 & C=1 \end{array} & \end{array}$$

- If argmax JTA, just change the separator update to:

$$\phi_B^* = \max_A \psi_{AB} = \max_A \begin{bmatrix} 8 & 4 \\ 3 & 1 \end{bmatrix} = \begin{array}{c} \begin{bmatrix} 8 & 4 \end{bmatrix} \\ \begin{array}{cc} B=0 & B=1 \end{array} \end{array} = \begin{bmatrix} 8 \\ 4 \end{bmatrix} \begin{array}{l} B=0 \\ B=1 \end{array}$$