Advanced Machine Learning & Perception

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Graphical (Structured) Models

- From Structured Prediction to Graphical Models
- Inference
- From Logic Networks to Bayesian Networks
- A Review of Graphical Models
- Junction Tree Algorithm
- MAP Estimation (ArgMax Junction Tree Algorithm)
- Loopy Propagation

Structured Prediction

- The key of structured prediction is fast computation of:

$$\arg\max_{y \in Y} \mathbf{w}^T \phi\left(\mathbf{x}, y\right)$$

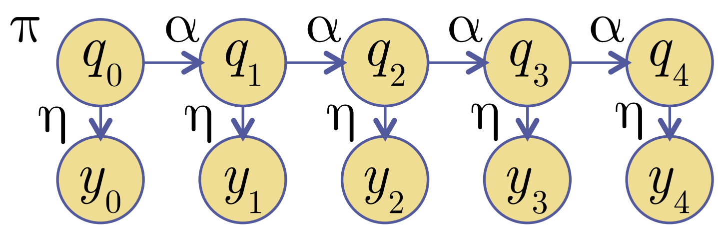
- Usually, the space Y is too huge to enumerate
- But, if it has independencies, we can quickly find the max
- This is equivalent to finding the max of a graphical model

$$p\left(y\right) = \tfrac{1}{Z} \exp\left(\mathbf{w}^T \phi\left(\mathbf{x}, y\right)\right)$$

- The argmax of p(y) is the same as the argmax of above
- If y splits into many conditionally independent terms
  → finding the max (Decoding) may be efficient
- Graphical models have three canonical problems to solve:
  1) Marginal inference, 2) Decoding and 3) Learning

Structured Prediction & HMMs

- Recall Hidden Markov Model (now y is observed, q hidden):



space of q's is $O(M^T)$

- Here, space of q's is *huge* just like in structure prediction
- Would like to do 3 basic things with graphical models:
  1) Evaluate: given $y_1,\ldots,y_T$ compute likelihood $p(y_1,\ldots,y_T)$
  2) Decode: given $y_1,\ldots,y_T$ compute best $q_1,\ldots,q_T$ or $p(q_t)$
  3) Learn: given $y_1,\ldots,y_T$ learn parameters θ
- Typically, HMMs use Baum-Welch, α-β or Viterbi algorithm
- More general graphical models use Junction Tree Algorithm
- The JTA is a way of performing efficient inference

Inference

- Inference: goal is to predict some variables given others
  - x1: flu
  - x2: fever
  - x3: sinus infection
  - x4: temperature
  - x5: sinus swelling
  - x6: headache

  Patient claims headache and high temperature. Does he have a flu?

  Given findings variables X_f and unknown variables X_u predict queried variables X_q

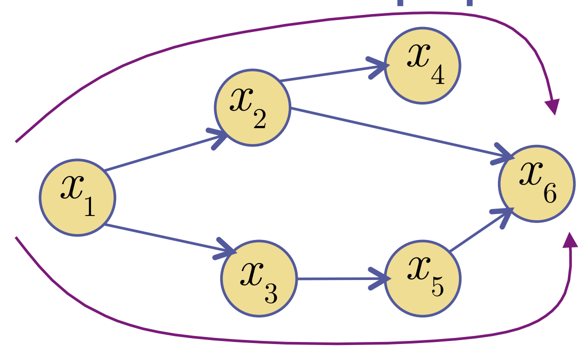
- Classical approach: truth tables (slow) or logic networks

- Modern approach: probability tables (slow) or Bayesian networks (fast belief propagation, junction tree algorithm)

Logic Nets to Bayesian Nets

- 1980's expert systems & logic networks became popular

x1	x2	x1 v x2	x1^x2	x1 -> x2
T	T	T	T	T
T	F	T	F	F
F	T	T	F	T
F	F	F	F	T



- Problem: inconsistency, 2 paths can give different answers
- Problem: rules are hard, instead use soft probability tables

x3 = x1 ^ x2

x3=0

	x2=0	x2=1
x1=0	1.0	1.0
x1=1	1.0	0.0

x3=1

	x2=0	x2=1
x1=0	0.0	0.0
x1=1	0.0	1.0

p(x3|x1,x2)

x3=0

	x2=0	x2=1
x1=0	0.8	0.7
x1=1	0.7	0.1

x3=1

	x2=0	x2=1
x1=0	0.2	0.3
x1=1	0.3	0.9

- These directed graphs are called Bayesian Networks

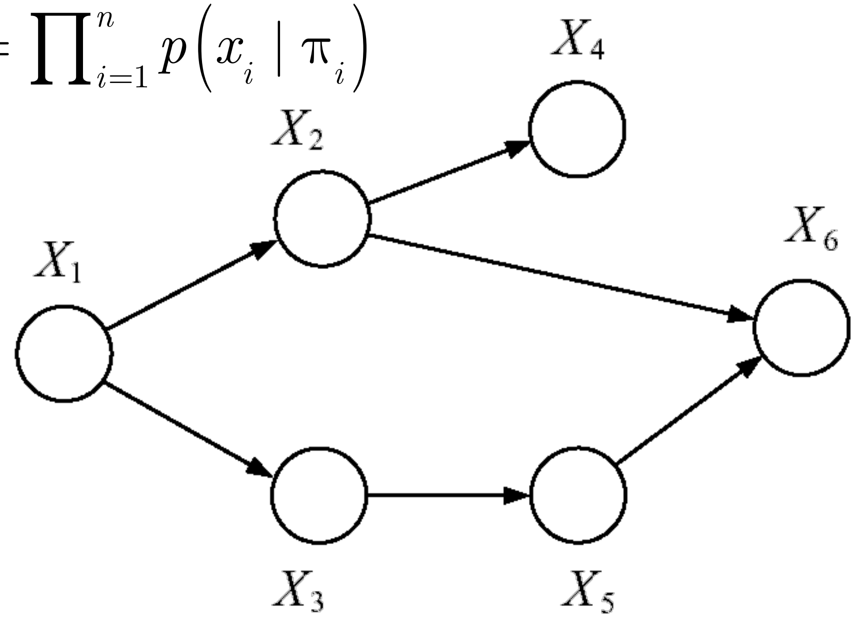
Aka Bayesian Networks

Directed Graphical Models

- Factorize a large (how big?) probability over several vars

$$p\left(x_1,\ldots,x_n\right) = \prod_{i=1}^{n} p\left(x_i \mid pa_i\right) = \prod_{i=1}^{n} p\left(x_i \mid \pi_i\right)$$

- Interpretation
  1: flu
  2: fever
  3: sinus infection
  4: temperature
  5: sinus swelling
  6: headache



$$p\left(x_1,\ldots,x_6\right) = p\left(x_1\right) p\left(x_2 \mid x_1\right) p\left(x_3 \mid x_1\right) p\left(x_4 \mid x_2\right) p\left(x_5 \mid x_3\right) p\left(x_6 \mid x_2, x_5\right)$$

2^6 $\quad 2^1 \quad 2^2 \quad 2^2 \quad 2^2 \quad 2^2 \quad 2^3$

Undirected Graphical Models

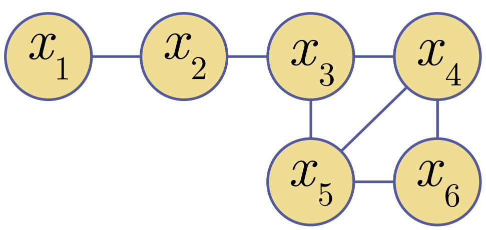
- Probability for undirected is defined via Potential Functions which are more flexible than conditionals or marginals

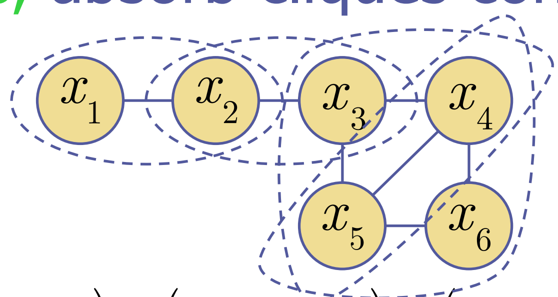
$$p(X) = p(x_1,\ldots,x_M) = \tfrac{1}{Z}\prod_C \psi(X_C) \qquad Z = \sum_X \prod_C \psi(X_C)$$

- Just a factorization of p(X), Z just normalizes the pdf
- Potential functions are positive functions of (not mutually exclusive) sub-groups of variables

0.1	**0.2**
0.05	**0.3**

- Potential functions are over complete sub-graphs or cliques C in the graph, clique is a set of fully-interconnected nodes
- Use maximal cliques, absorb cliques contained in larger ψ



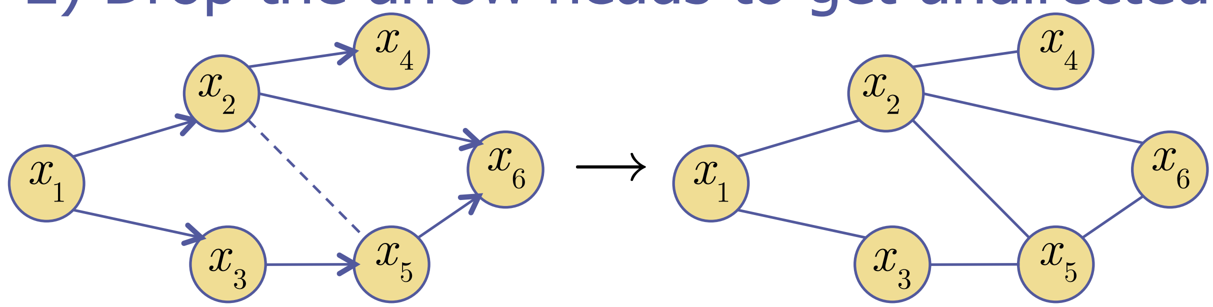


$$\psi(x_2,x_3)\,\psi(x_2)\,\psi(x_3) \rightarrow \psi(x_2,x_3)$$

$$p(X) = \tfrac{1}{Z}\psi(x_1,x_2)\,\psi(x_2,x_3)\,\psi(x_3,x_4,x_5)\,\psi(x_4,x_5,x_6)$$

Moralization

- Converts directed graph into undirected graph
- By moralization, marrying the parents:
  1) Connect nodes that have common children
  2) Drop the arrow heads to get undirected

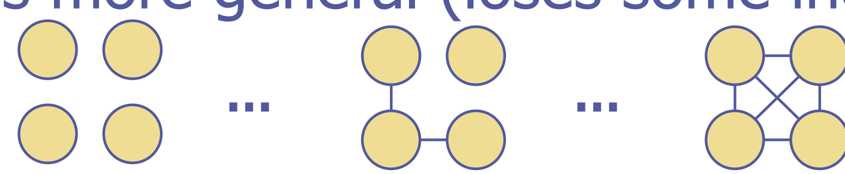


$$p(x_1)\,p(x_2 \mid x_1)\,p(x_3 \mid x_1)\,p(x_4 \mid x_2)\,p(x_5 \mid x_3)\,p(x_6 \mid x_2, x_5)$$
$$\rightarrow \tfrac{1}{Z}\,\psi(x_1, x_2)\,\psi(x_1, x_3)\,\psi(x_2, x_4)\,\psi(x_3, x_5)\,\psi(x_2, x_5, x_6)$$

$$p(x_1)\,p(x_2 \mid x_1) \rightarrow \psi(x_1, x_2)$$
$$p(x_4 \mid x_2) \rightarrow \psi(x_2, x_4)$$
$$Z \rightarrow 1$$

- Note: moralization resolves *coupling* due to marginalizing
- moral graph is more general (loses some independencies)

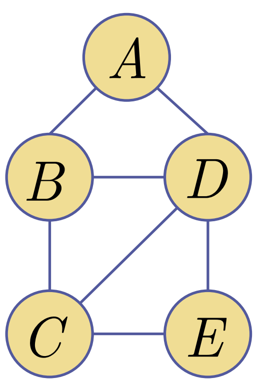
most specific



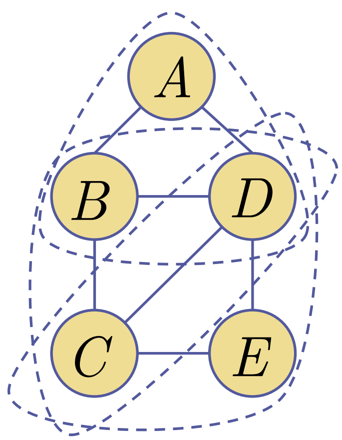
most general

Junction Trees

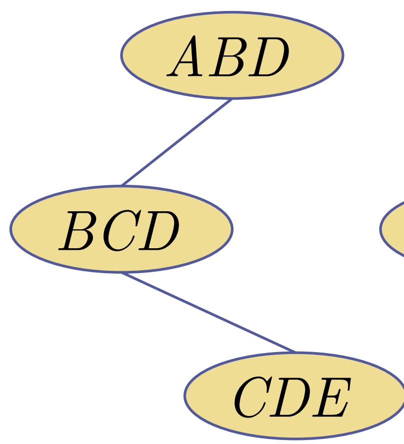
- Given moral graph want to build Junction Tree:
  - each node is a clique (ψ) of variables in moral graph
  - edges connect cliques of the potential functions
  - unique path between nodes & root node (tree)
  - between connected clique nodes, have separators (ϕ)
  - separator nodes contain intersection of variables



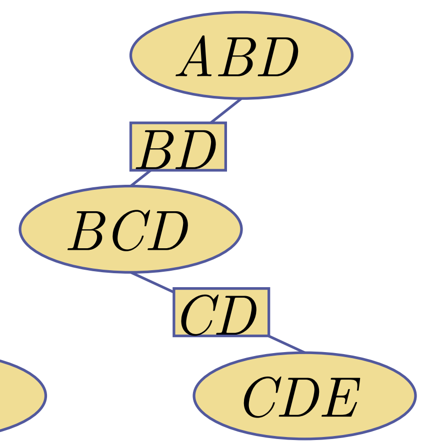
undirected



cliques



clique tree



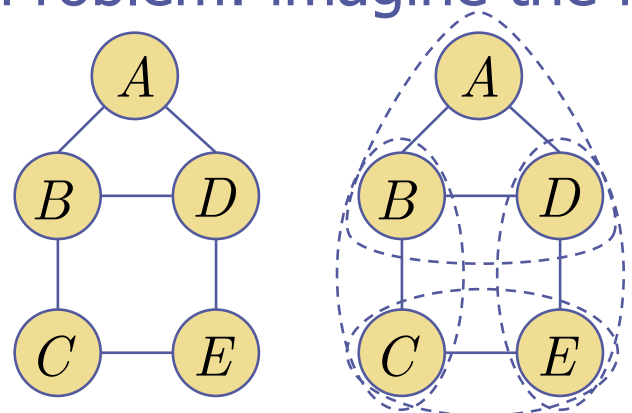
junction tree

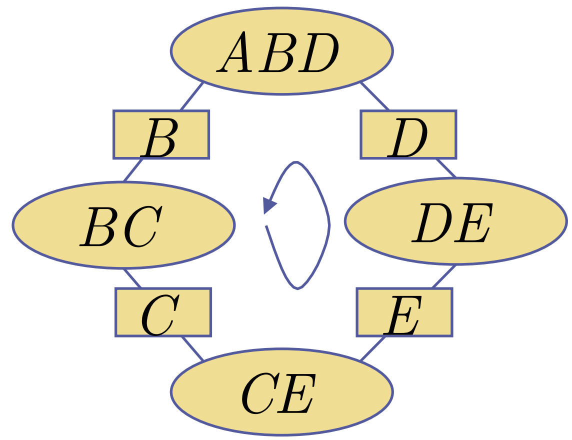
$$\psi\left(A,B,D\right)$$
$$\phi\left(B,D\right)$$
$$\psi\left(B,C,D\right)$$
$$\phi\left(C,D\right)$$
$$\psi\left(C,D,E\right)$$

$$p\left(X\right) = \tfrac{1}{Z}\psi\left(A,B,D\right)\psi\left(B,C,D\right)\psi\left(C,D,E\right)$$

Triangulation

- Problem: imagine the following undirected graph

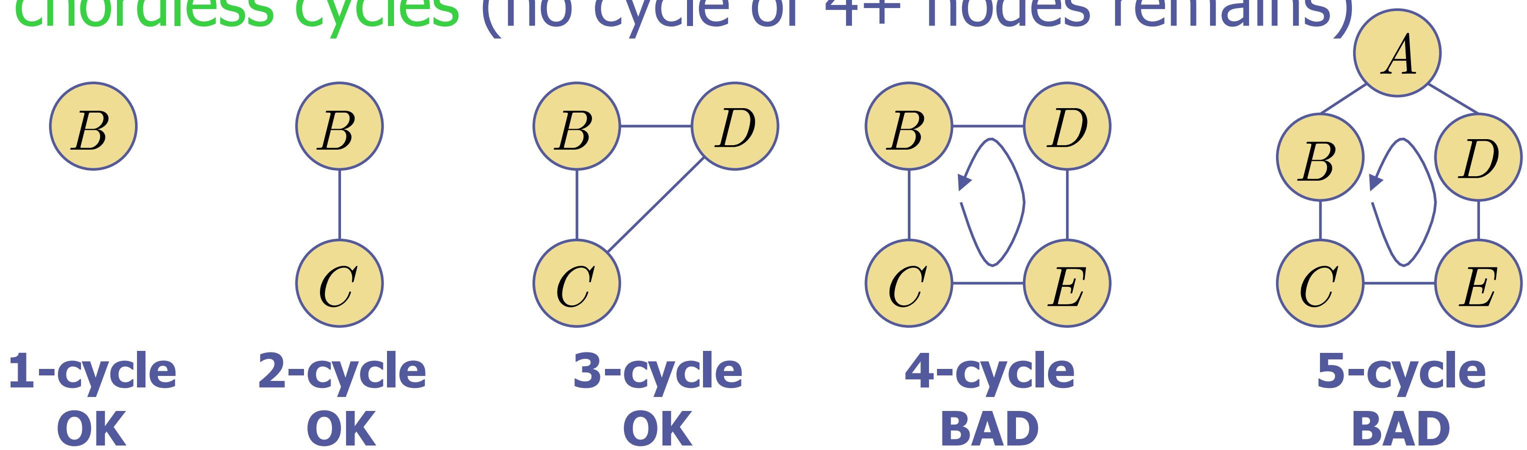




- Not a Tree!
- To ensure Junction Tree is a tree (no loops, etc.) before forming it must first Triangulate moral graph before finding the cliques…
- Triangulating gives more general graph (like moralization)
- Adds links to get rid of cycles or loops
- Triangulation: Connect nodes in moral graph such that no cycle of 4 or more nodes remains in the graph

Triangulation

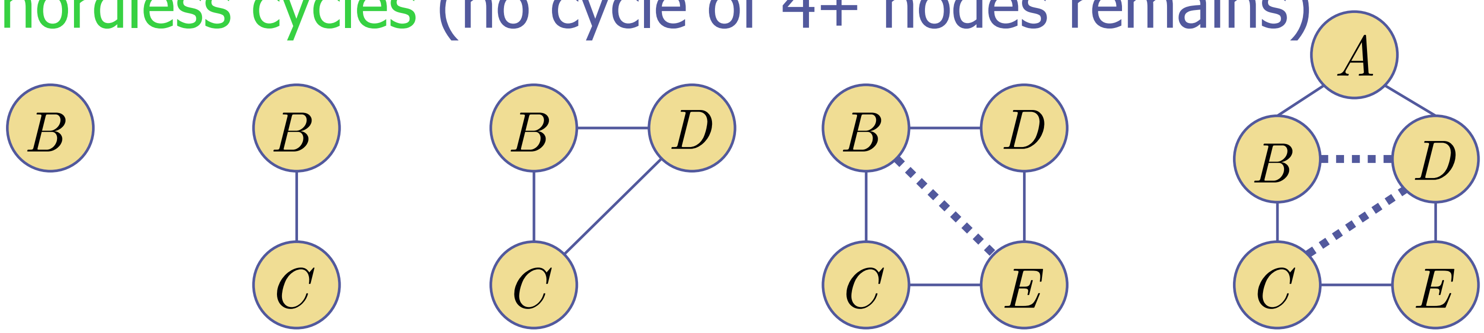
- Triangulation: Connect nodes in moral graph such that no chordless cycles (no cycle of 4+ nodes remains)



- So, *add links*, but many possible choices…
- HINT: keep largest clique size small (for efficient JTA)
- Chordless: no edges between successor nodes in cycle
- Sub-optimal triangulations of moral graph are Polynomial
- Triangulation that minimizes largest clique size is NP
- But, OK to use a suboptimal triangulation (slower JTA…)

Triangulation

•Triangulation: Connect nodes in moral graph such that no chordless cycles (no cycle of 4+ nodes remains)



1-cycle OK **2-cycle OK** **3-cycle OK** **3-cycle OK** **3-cycle OK**

•So, *add links*, but many possible choices…

•HINT: keep largest clique size small (for efficient JTA)

•Chordless: no edges between successor nodes in cycle

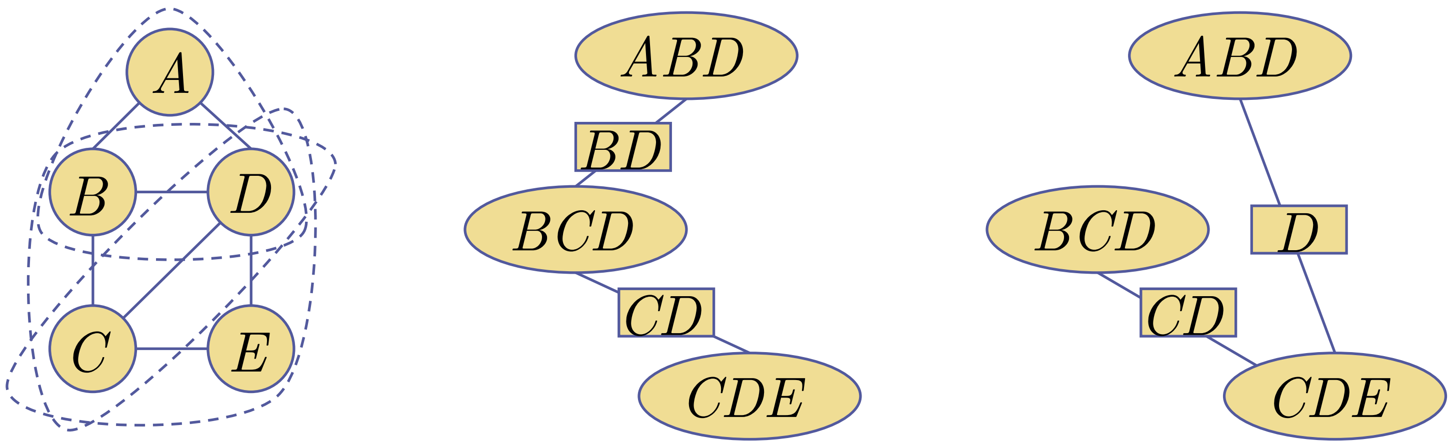
•Sub-optimal triangulations of moral graph are Polynomial

•Triangulation that minimizes largest clique size is NP

•But, OK to use a suboptimal triangulation (slower JTA…)

Running Intersection Property

- Junction Tree must satisfy Running Intersection Property
- RIP: On unique path connecting clique V to clique W, all other cliques share nodes in $V \cap W$



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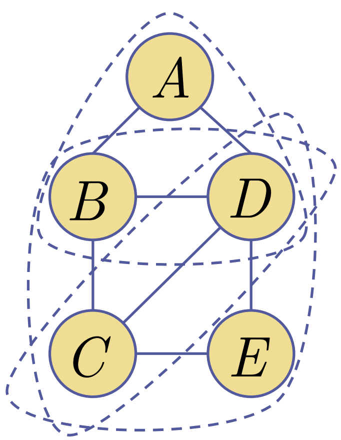
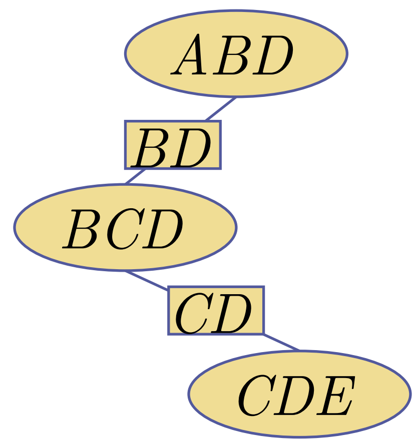
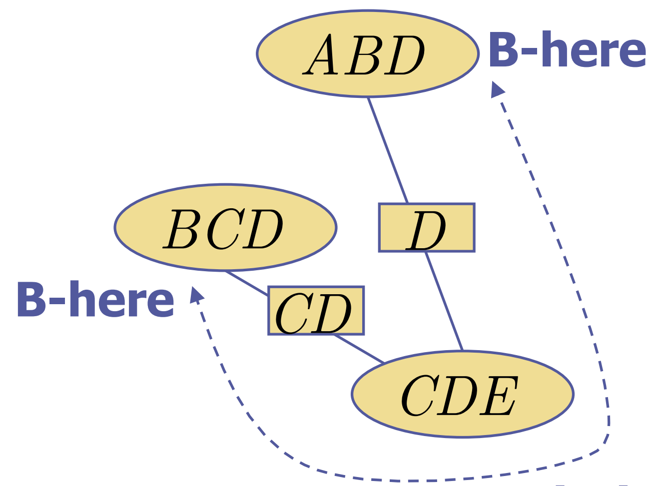






Missing More B's on path!

HINT: Junction Tree has largest total separator cardinality

$$\left|\Phi\right| = \left|\phi\left(B,C\right)\right| + \left|\phi\left(C,D\right)\right| = 2+2$$

$$\left|\Phi\right| = \left|\phi\left(C,D\right)\right| + \left|\phi\left(D\right)\right| = 2+1$$

Forming the Junction Tree

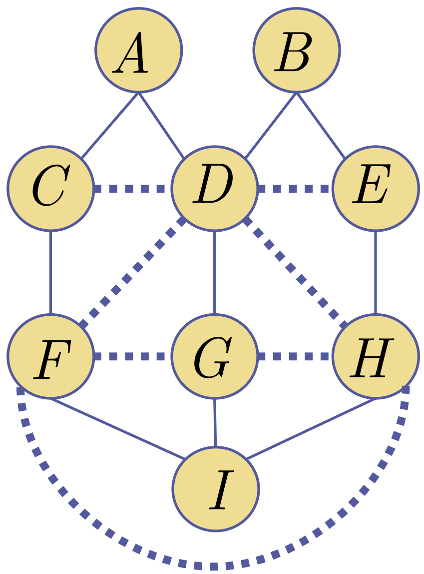
- Now need to connect the cliques into a Junction Tree
- But, must ensure Running Intersection Property
- Theorem: a valid (RIP) Junction Tree connection is one that maximizes the cardinality of the separators

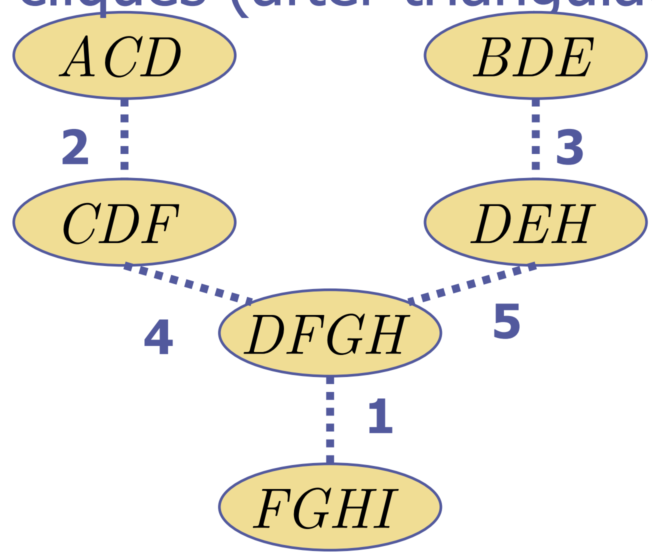
$$
\begin{aligned}
JT^* &= \max_{TREE\,STRUCTURES} \left|\Phi\right| \\
&= \max_{TREE\,STRUCTURES} \sum\nolimits_S \left|\phi\left(X_S\right)\right|
\end{aligned}
$$

- Use Kruskal's algorithm:
  1) Init Tree with all cliques unconnected (no edges)
  2) Compute size of separators between all pairs
  3) Connect the two cliques with the biggest separator cardinality which doesn't create a loop in current Tree (maintains Tree structure)
  4) Stop when all nodes are connected, else goto 3

Kruskal Example

- Start with unconnected cliques (after triangulation)





	ACD	BDE	CDF	DEH	DFGH	FGHI
ACD	-	1	2	1	1	0
BDE		-	1	2	1	0
CDF			-	1	2	1
DEH				-	2	1
DFGH					-	3
FGHI						-

Junction Tree Probabilities

- We now have a valid Junction Tree!
- What does that mean?
- Recall probability for undirected graphs:

$$p(X) = p(x_1, \ldots, x_M) = \frac{1}{Z} \prod_C \psi(X_C)$$

- Can write junction tree as potentials of its cliques:

$$p(X) = \frac{1}{Z} \prod_C \tilde{\psi}(X_C)$$

- Alternatively: clique potentials over separator potentials:

$$p(X) = \frac{1}{Z} \frac{\prod_C \psi(X_C)}{\prod_S \phi(X_S)}$$

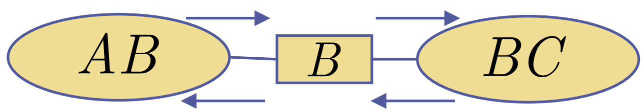
- This doesn't change/do anything! Just less compact...
- Like *de-absorbing* smaller cliques from maximal cliques:

$$\tilde{\psi}(A,B,D) = \frac{\psi(A,B,D)}{\phi(B,D)} \longleftarrow$$

...gives back original formula if $\phi(B,D) \triangleq 1$

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…

$$\boxed{\begin{aligned} \phi_S^* &= \sum_{V \setminus S} \psi_V \\ \psi_W^* &= \frac{\phi_S^*}{\phi_S} \psi_W \\ \psi_V^* &= \psi_V \end{aligned}}$$

Send message From W to V…

$$\boxed{\begin{aligned} \phi_S^{**} &= \sum_{W \setminus S} \psi_W^* \\ \psi_V^{**} &= \frac{\phi_S^{**}}{\phi_S^*} \psi_V^* \\ \psi_W^{**} &= \psi_W^* \end{aligned}}$$

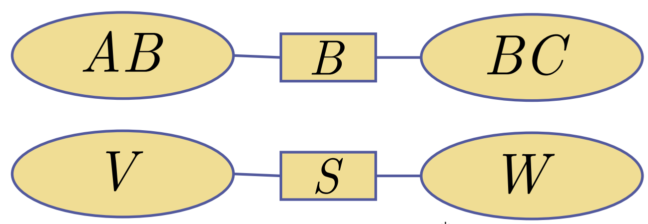
Now they Agree…Done!

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

Junction Tree Algorithm

- When "Done", all clique potentials are marginals and all separator potentials are submarginals!
- Note that p(X) is unchanged by message passing step:

$$\boxed{\begin{aligned} \phi_S^* &= \sum\nolimits_{V \setminus S} \psi_V \\ \psi_W^* &= \frac{\phi_S^*}{\phi_S} \psi_W \\ \psi_V^* &= \psi_V \end{aligned}}$$



$$p(X) = \frac{1}{Z} \frac{\psi_V^* \psi_W^*}{\phi_S^*} = \frac{1}{Z} \frac{\psi_V \frac{\phi_S^*}{\phi_S} \psi_W}{\phi_S^*} = \frac{1}{Z} \frac{\psi_V \psi_W}{\phi_S}$$

- Example: if potentials are poorly initialized… get corrected!

$$\begin{aligned} \psi_{AB} &= p(B \mid A) p(A) \\ &= p(A, B) \\ \psi_{BC} &= \boxed{p(C \mid B)} \\ \phi_B &= \boxed{1} \end{aligned}$$

$$\longrightarrow \quad \phi_B^* = \sum\nolimits_A \psi_{AB} = \sum\nolimits_A p(A, B) = \boxed{p(B)}$$

$$\longrightarrow \quad \psi_{BC}^* = \frac{\phi_S^*}{\phi_S} \psi_{BC} = \frac{p(B)}{1} p(C \mid B) = \boxed{p(B, C)}$$

Junction Tree Algorithm

- Example: if *evidence* is observed… i.e. random var A:=1

  Initialize as before, cliques get underlying conditionals…

$$\psi_{AB} = p(A,B) \qquad \psi_{BC} = p(C \mid B) \qquad \phi_B = 1$$

  Update with slice…

$$\phi_B^* = \sum\nolimits_A \psi_{AB}\delta(A=1) = \sum\nolimits_A p(A,B)\delta(A=1) = p(A=1,B)$$

$$\psi_{BC}^* = \frac{\phi_S^*}{\phi_S}\psi_{BC} = \frac{p(A=1,B)}{1}p(C \mid B) = p(A=1,B,C)$$

$$\psi_{AB}^* = \psi_{AB} = p(A=1,B)$$

  To get conditionals…

$$p(B,C \mid A=1) = \frac{\psi_{BC}^*}{\sum_{B,C}\psi_{BC}^*}$$

- Problem: if send message to neighbor & he changes, we must re-update! Could keep looping for a long time.

JTA: Collect & Distribute

- Trees: recursive, no need to reiterate messages mindlessly!
- Send a message only after hearing from all neighbors…

initialize(DAG){ Pick root
Set all variables as: $\psi_{C_i} = p\left(x_i \mid \pi_i\right) \; \forall i$
$\phi_S = 1 \quad \forall S$
$Z = 1$ **}**

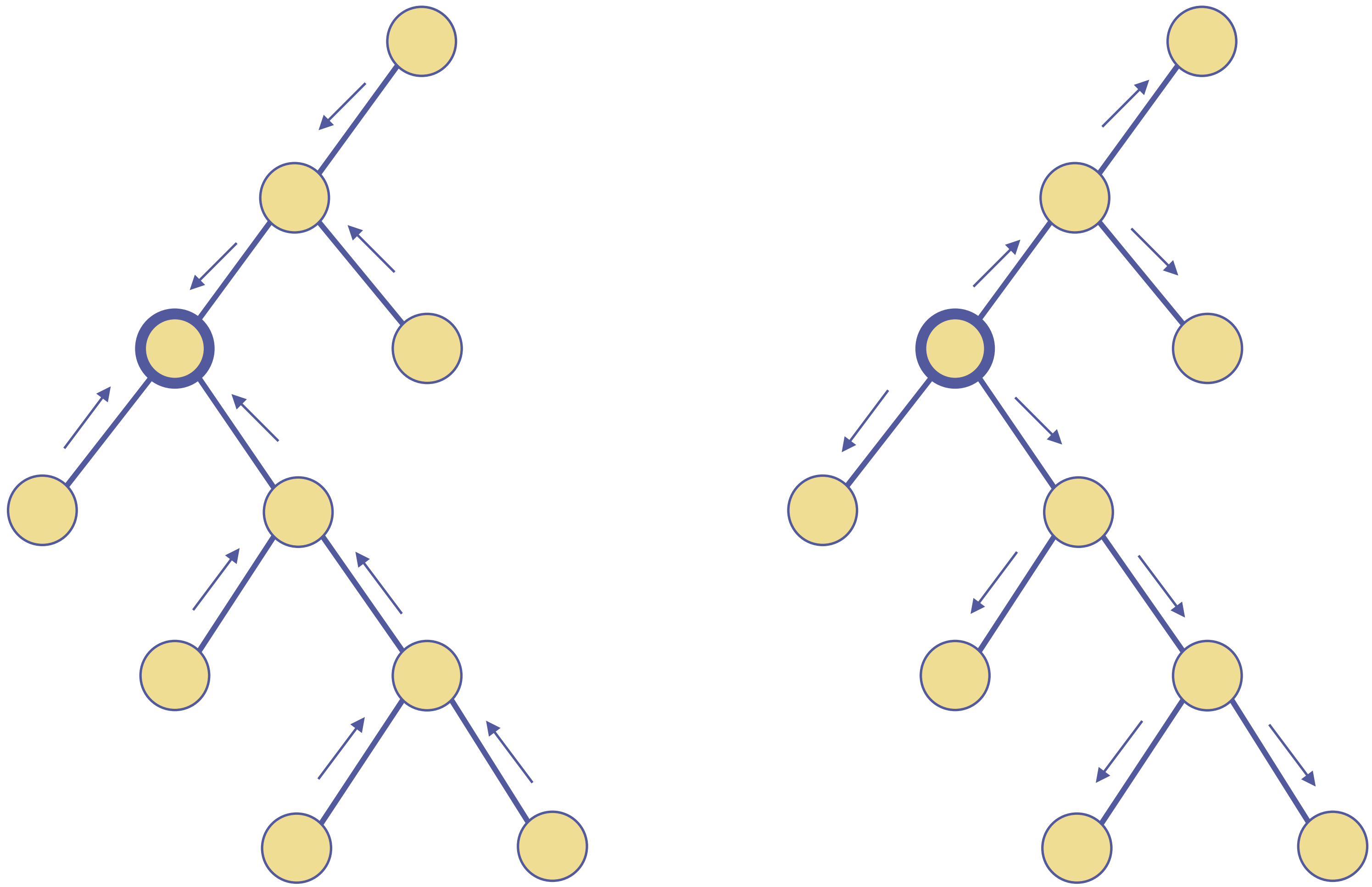
```
collectEvidence(node) {
   for each child of node  {
      update(node,collectEvidence(child)); }
   return(node); }

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

update(node,evidence) {
```

$$\psi_C^* = \frac{\phi_S^*}{\sum_{C \setminus S} \psi_C} \psi_C$$

}

Junction Tree Algorithm

• JTA: 1) *Initialize* 2) *Collect* 3) *Distribute*



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?

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

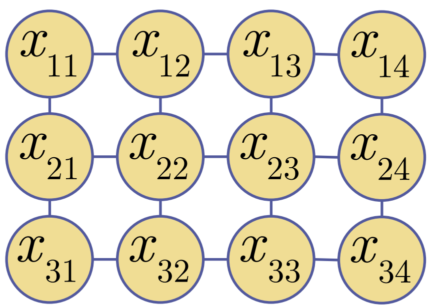
- Solution: update in JTA uses max instead of sum:

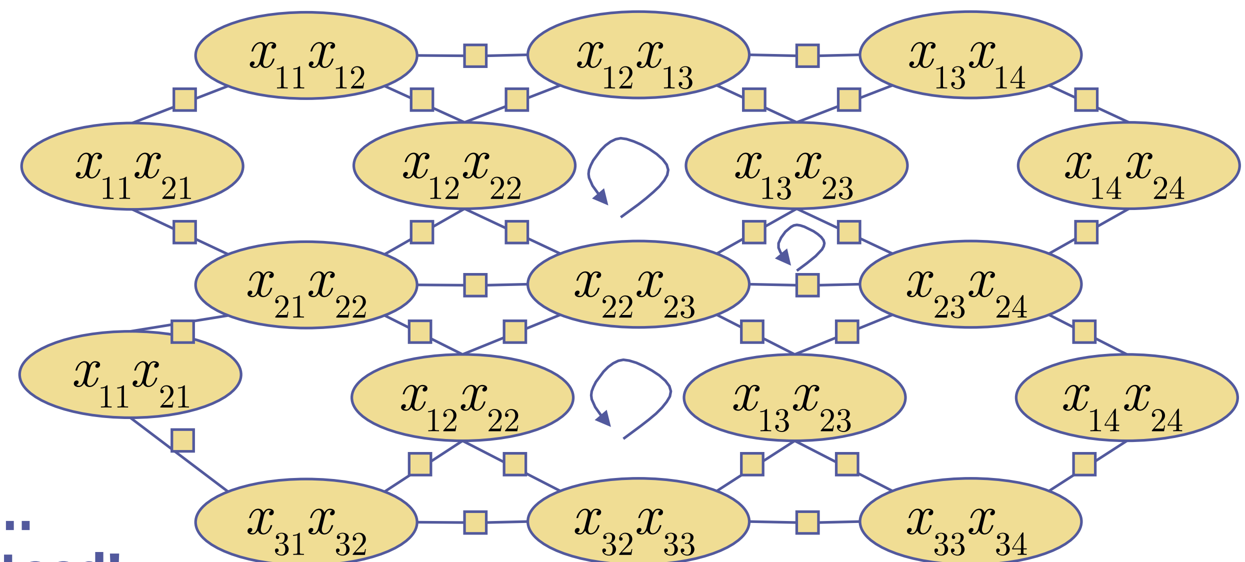
$$
\phi_S^* = \max_{V \setminus S} \psi_V \qquad \psi_W^* = \frac{\phi_S^*}{\phi_S} \psi_W \qquad \psi_V^* = \psi_V
$$

- Final potentials aren't marginals: $\psi\left(X_C\right) = \max_{U \setminus C} p\left(X\right)$
- Highest value in potential is most likely: $X_C^* = \arg\max_C \psi\left(X_C\right)$

Loopy Belief Propagation

- We *could* run junction tree algorithm on non-trees… but…
  - a) no guaranteed convergence
  - b) might get inexact marginals
  - c) might iterate indefinitely (not polynomial time)
- Called Loopy Propagation since messages loop indefinitely
- Example: Markov random field for images…





Just find cliques
Don’t triangulate
Keep iterating JTA…
Sometimes Guaranteed!