

## **Probabilistic Graphical Models**

## The Belief Propagation (Sum-Product) Algorithm



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Lecture 5, January 29, 2014

Reading: KF-chap 10

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# Pros and Cons of Procedure Elimination



• Algebraic elimination = graphical elimination





# Complexity

- The overall complexity is determined by the number of the largest elimination clique
  - What is the largest elimination clique? a pure graph theoretic question
  - **Tree-width** *k*: one less than the smallest achievable value of the cardinality of the largest elimination clique, ranging over all possible elimination ordering
  - "good" elimination orderings lead to **small cliques** and hence reduce complexity (what will happen if we eliminate "e" first in the above graph?)
  - Find the best elimination ordering of a graph --- NP-hard
  - → Inference is NP-hard
  - But there often exist "obvious" optimal or near-opt elimination ordering

# From Elimination to Message Passing



- Our algorithm so far answers only one query (e.g., on one node), do we need to do a complete elimination for every such query?
- Elimination = message passing on a clique tree



• Messages can be reused

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# From Elimination to Message Passing



- Our algorithm so far answers only one query (e.g., on one node), do we need to do a complete elimination for every such query?
- Elimination = message passing on a clique tree
  - Another query ...



• Messages  $m_f$  and  $m_h$  are reused, others need to be recomputed © Eric Xing @ CMU, 2005-2014

# **Tree GMs**







Undirected tree: a unique path between any pair of nodes Directed tree: all nodes except the root have exactly one parent

Poly tree: can have multiple parents

# Equivalence of directed and undirected trees



- Any undirected tree can be converted to a directed tree by choosing a root node and directing all edges away from it
- A directed tree and the corresponding undirected tree make the same conditional independence assertions
- Parameterizations are essentially the same.

• Undirected tree: 
$$p(x) = \frac{1}{Z} \left( \prod_{i \in V} \psi(x_i) \prod_{(i,j) \in E} \psi(x_i, x_j) \right)$$

- Directed tree:  $p(x) = p(x_r) \prod_{(i,j) \in E} p(x_j | x_i)$
- Equivalence:  $\psi(x_r) = p(x_r); \quad \psi(x_i, x_j) = p(x_j | x_i);$  $Z = 1, \quad \psi(x_i) = 1$
- Evidence:?

# From elimination to message passing



- Recall ELIMINATION algorithm:
  - Choose an ordering  $\mathcal{Z}$  in which query node f is the final node
  - Place all potentials on an active list
  - Eliminate node *i* by removing all potentials containing *i*, take sum/product over  $x_i$ .
  - Place the resultant factor back on the list

# **Elimination on a tree**







# Message passing on a tree



# From elimination to message passing



### • Recall ELIMINATION algorithm:

- Choose an ordering  $\mathcal{Z}$  in which query node f is the final node
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### • For a TREE graph:

- Choose query node *f* as the root of the tree
- View tree as a directed tree with edges pointing towards leaves from f
- Elimination ordering based on depth-first traversal
- Elimination of each node can be considered as message-passing (or Belief Propagation) directly along tree branches, rather than on some transformed graphs
- $\rightarrow$  thus, we can use the tree itself as a data-structure to do general inference!!

- A node can send a message to its neighbors when (and only when) it has received messages from all its *other* neighbors.
- Computing node marginals:
  - Naïve approach: consider each node as the root and execute the message passing algorithm



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# **Computing node marginals**

- Naïve approach:
  - Complexity: NC
    - N is the number of nodes
    - C is the complexity of a complete message passing
- Alternative dynamic programming approach
  - 2-Pass algorithm (next slide →)
  - Complexity: 2C!

• A two-pass algorithm:



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# **Belief Propagation (SP-algorithm): Sequential implementation**



# Belief Propagation (SP-algorithm): Parallel synchronous implementation





- For a node of degree d, whenever messages have arrived on any subset of d-1 node, compute the message for the remaining edge and send!
  - A pair of messages have been computed for each edge, one for each direction
  - All incoming messages are eventually computed for each node

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# **Correctness of BP on tree**

- Collollary: the synchronous implementation is "non-blocking"
- Thm: The Message Passage Guarantees obtaining all marginals in the tree

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

• What about non-tree?

# **Another view of SP: Factor Graph**

• Example 1



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### **Factor Graphs** • Example 2 $X_1$ X₁ $\mathbf{f}_{c}$ f<sub>a</sub> $X_3$ X<sub>3</sub> $X_2$ $X_2$ f<sub>b</sub> $\psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = f_a(\mathbf{x}_1, \mathbf{x}_2) f_b(\mathbf{x}_2, \mathbf{x}_3) f_c(\mathbf{x}_3, \mathbf{x}_1)$ Example 3 $X_1$ $X_1$ f<sub>a</sub> $X_2$ $X_3$ $X_3$ $X_2$ $\psi(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3) = f_a(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3)$

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# **Factor Tree**



• A Factor graph is a Factor Tree if the undirected graph obtained by ignoring the distinction between variable nodes and factor nodes is an undirected tree



# Message Passing on a Factor Tree

- Two kinds of messages
  - 1. v: from variables to factors
  - 2. µ: from factors to variables

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

# Message Passing on a Factor Tree, con'd



- Message passing protocol:
  - A node can send a message to a neighboring node only when it has received messages from all its *other* neighbors
- Marginal probability of nodes:





$$\begin{split} \mathsf{P}(\mathsf{x}_{\mathsf{i}}) & \propto \prod_{\mathsf{s} \ \in \ \mathsf{N}(\mathsf{i})} \mu_{\mathsf{s}\mathsf{i}}(\mathsf{x}_{\mathsf{i}}) \\ & \propto \nu_{\mathsf{i}\mathsf{s}}(\mathsf{x}_{\mathsf{i}}) \mu_{\mathsf{s}\mathsf{i}}(\mathsf{x}_{\mathsf{i}}) \end{split}$$

# **BP on a Factor Tree**



# Why factor graph?

• Tree-like graphs to Factor trees



# **Poly-trees to Factor trees**



# Why factor graph?





- Because FG turns tree-like graphs to factor trees,
- and trees are a data-structure that guarantees correctness of BP !

# Max-product algorithm: computing MAP probabilities



## Max-product algorithm: computing MAP configurations using a final bookkeeping backward pass



# Summary



- Sum-Product algorithm computes singleton marginal probabilities on:
  - Trees
  - Tree-like graphs
  - Poly-trees
- *Maximum a posteriori* configurations can be computed by replacing sum with max in the sum-product algorithm
  - Extra bookkeeping required

# Inference on general GM

- Now, what if the GM is not a tree-like graph?
- Can we still directly run message-passing protocol along its edges?
- For non-trees, we do not have the guarantee that message-passing will be consistent!
- Then what?
  - Construct a graph data-structure from P that has a tree structure, and run message-passing on it!
- $\rightarrow$  Junction tree algorithm

# **Elimination Clique**

- Recall that Induced dependency during marginalization is captured in elimination cliques
  - Summation <-> elimination
  - Intermediate term <-> elimination clique

P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f)

- $\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)\phi_{h}(e,f)$
- $\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)\phi_g(e)\phi_h(e,f)$
- $\Rightarrow P(a)P(b)P(c|b)P(d|a)P(e|c,d)\phi_f(a,e)$
- $\Rightarrow P(a)P(b)P(c|b)P(d|a)\phi_{e}(a,c,d)$
- $\Rightarrow P(a)P(b)P(c|b)\phi_d(a,c)$
- $\Rightarrow P(a)P(b)\phi_c(a,b)$
- $\Rightarrow P(a)\phi_b(a)$
- $\Rightarrow \phi(a)$ 
  - Can this lead to an generic inference algorithm?





# **Moral Graph**

• Note that for both directed GMs and undirected GMs, the joint probability is in a product form:

**BN**: 
$$P(\mathbf{X}) = \prod_{i=1:d} P(X_i | \mathbf{X}_{\pi_i})$$

**MRF:** 
$$P(\mathbf{X}) = \frac{1}{Z} \prod_{c \in C} \psi_c(\mathbf{X}_c)$$

- So let's convert local conditional probabilities into potentials; then the second expression will be generic, but how does this operation affect the directed graph?
  - We can think of a conditional probability, e.g., P(C|A,B) as a function of the three variables *A*, *B*, and *C* (we get a real number of each configuration):





- Problem: But a node and its parent are not generally in the same clique in a BN
- Solution: Marry the parents to obtain the "moral graph"

# Moral Graph (cont.)



- Define the potential on a clique as the product over all conditional probabilities contained within the clique
- Now the product of potentials gives the right answer:





 $P(X_{1}, X_{2}, X_{3}, X_{4}, X_{5}, X_{6})$   $= P(X_{1})P(X_{2})P(X_{3} | X_{1}, X_{2})P(X_{4} | X_{3})P(X_{5} | X_{3})P(X_{6} | X_{4}, X_{5})$   $= \psi(X_{1}, X_{2}, X_{3})\psi(X_{3}, X_{4}, X_{5})\psi(X_{4}, X_{5}, X_{6})$ where  $\psi(X_{1}, X_{2}, X_{3}) = P(X_{1})P(X_{2})P(X_{3} | X_{1}, X_{2})$   $\psi(X_{3}, X_{4}, X_{5}) = P(X_{4} | X_{3})P(X_{5} | X_{3})$   $\psi(X_{4}, X_{5}, X_{6}) = P(X_{6} | X_{4}, X_{5})$ Note the interpretion of concentration of the con

Note that here the interpretation of potential is ambivalent: it can be either *marginals* or *conditionals* 

# **Clique trees**



• A clique tree is an (undirected) tree of cliques



• Consider cases in which two neighboring cliques V and W have an overlap S (e.g.,  $(X_1, X_2, X_3)$  overlaps with  $(X_3, X_4, X_5)$ ),



 Now we have an alternative representation of the joint in terms of the potentials:

# **Clique trees**



• A clique tree is an (undirected) tree of cliques



• The alternative representation of the joint in terms of the potentials:

$$P(X_{1}, X_{2}, X_{3}, X_{4}, X_{5}, X_{6})$$

$$= P(X_{1})P(X_{2})P(X_{3} | X_{1}, X_{2})P(X_{4} | X_{3})P(X_{5} | X_{3})P(X_{6} | X_{4}, X_{5})$$

$$= P(X_{1}, X_{2}, X_{3}) \frac{P(X_{3}, X_{4}, X_{5})}{P(X_{3})} \frac{P(X_{4}, X_{5}, X_{6})}{P(X_{4}, X_{5})}$$

$$= \psi(X_{1}, X_{2}, X_{3}) \frac{\psi(X_{3}, X_{4}, X_{5})}{\psi(X_{3})} \frac{\psi(X_{4}, X_{5}, X_{6})}{\psi(X_{4}, X_{5})}$$
Now each isomorphism arginal set of values of values of values of the set of the se

Now each potential is isomorphic to the *cluster marginal* of the attendant set of variables

# Why this is useful?

### • Propagation of probabilities

• Now suppose that some evidence has been "absorbed" (i.e., certain values of some nodes have been observed). How do we propagate this effect to the rest of the graph?



### • What do we mean by propagate?

Can we adjust all the potentials  $\{\psi\}$ ,  $\{\phi\}$  so that they still represent the correct cluster marginals (or unnormalized equivalents) of their respective attendant variables?

• Utility?  $P(X_1 | X_6 = x_6) = \sum_{X_2, X_3} \psi(X_1, X_2, X_3)$  $P(X_3 | X_6 = x_6) = \phi(X_3)$  $P(x_6) = \sum_{X_4, X_5} \psi(X_4, X_5, x_6)$ © Eric Xing @ CMU, 2005-2014



### Local operations!

# **Local Consistency**

• We have two ways of obtaining p(S)

$$P(S) = \sum_{V \setminus S} \psi(V) \qquad \qquad P(S) = \sum_{W \setminus S} \psi(W)$$

and they must be the same

- The following update-rule ensures this:
  - Forward update:

**Backward update** 

$$\phi_{S}^{*} = \sum_{V \setminus S} \psi_{V}^{*} \qquad \psi_{W}^{*} = \frac{\phi_{S}^{*}}{\phi_{S}} \psi_{W}$$
$$\phi_{S}^{**} = \sum_{W \setminus S} \psi_{W}^{*} \qquad \psi_{V}^{**} = \frac{\phi_{S}^{**}}{\phi_{S}^{*}} \psi_{V}^{*}$$

• Two important identities can be proven

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

Local Consistency

 $\cdot = \frac{\psi_V^{**}\psi_W^{**}}{\phi^{**}} = \frac{\psi_V\psi_W}{\phi_S}$ 

 $\psi(V)$ 

V

 $\phi(S)$ 

S

 $\psi(W)$ 

W

**Invariant Joint** 



# **Message Passing Algorithm**



$$\phi_{S}^{*} = \sum_{V \setminus S} \psi_{V}^{*} \qquad \psi_{W}^{*} = \frac{\phi_{S}^{*}}{\phi_{S}} \psi_{W}$$
$$\phi_{S}^{**} = \sum_{W \setminus S} \psi_{W}^{*} \qquad \psi_{V}^{**} = \frac{\phi_{S}^{**}}{\phi_{S}^{*}} \psi_{V}^{*}$$

- This simple local message-passing algorithm on a clique tree defines the general probability propagation algorithm for directed graphs!
  - Many interesting algorithms are special cases:
    - Forward-backward algorithm for hidden Markov models,
    - Kalman filter updates
    - Pealing algorithms for probabilistic trees
  - The algorithm seems reasonable. Is it correct?

# A problem

• Consider the following graph and a corresponding clique tree



- Note that C appears in two non-neighboring cliques
- Question: with the previous message passage, can we ensure that the probability associated with C in these two (non-neighboring) cliques consistent?
- Answer: No. It is not true that in general local consistency implies global consistency
- What else do we need to get such a guarantee?

# Triangulation

- A triangulated graph is one in which *no cycles* with four or more nodes exist in which there is no *chord*
- We triangulate a graph by adding chords:
- Now we no longer have our global inconsistency problem.
  - A clique tree for a triangulated graph has the *running intersection property*: If a node appears in two cliques, it appears everywhere on the path between the cliques
  - Thus local consistency implies global consistency



D



С



# **Junction trees**



- A clique tree for a triangulated graph is referred to as a *junction tree*
- In junction trees, local consistency implies global consistency. Thus the local message-passing algorithms is (provably) correct
- It is also possible to show that *only* triangulated graphs have the property that their clique trees are junction trees. Thus if we want local algorithms, we *must* triangulate
- Are we now all set?
  - How to triangulate?
  - The complexity of building a JT depends on how we triangulate!!
  - Consider this network: it turns out that we will need to pay an O(2<sup>4</sup>) or O(2<sup>6</sup>) cost depending on how we triangulate!



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# How to triangulate

• A graph elimination algorithm



moralization

graph elimination

- Intermediate terms correspond to the cliques resulted from elimination
  - "good" elimination orderings lead to **small cliques** and hence reduce complexity (what will happen if we eliminate "e" first in the above graph?)
  - finding the optimum ordering is NP-hard, but for many graph optimum or nearoptimum can often be heuristically found

# A junction tree







# **Message-passing algorithms**





- Message update
  - The Hugin update
  - The Shafer-Shenoy update

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

$$m_{i \to j}(S_{ij}) = \sum_{C_i \setminus S_{ij}} \psi_{C_i} \prod_{k \neq j} m_{k \to i}(S_{ki})$$

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# A Sketch of the Junction Tree Algorithm



### • The algorithm

- 1. Moralize the graph (trivial)
- 2. Triangulate the graph (good heuristic exist, but actually NP hard)
- 3. Build a clique tree (e.g., using a maximum spanning tree algorithm
- 4. Propagation of probabilities --- a local message-passing protocol
- Results in marginal probabilities of all cliques --- solves all queries in a single run
- A **generic** exact inference algorithm for any GM
- **Complexity**: exponential in the size of the maximal clique --- a good elimination order often leads to small maximal clique, and hence a good (i.e., thin) JT

# Recall the Elimination and Message Passing Algorithm



• Elimination = message passing on a clique tree

$$m_e(a,c,d)$$
  
=  $\sum_e p(e \mid c,d) m_g(e) m_f(a,e)$ 



$$(y_1 \rightarrow y_2 \rightarrow y_3 \rightarrow \dots \rightarrow y_T)$$

$$(x_1 \rightarrow x_2 \rightarrow x_3 \rightarrow \dots \rightarrow x_T)$$

$$\alpha_t^k = p(x_t \mid y_t^k = 1) \sum_i \alpha_{t-1}^i a_{i,k}$$

$$P(\mathbf{x}) = \sum_{k} \alpha_T^k$$

# **Shafer Shenoy for HMMs**

• Recap: Shafer-Shenoy algorithm



• Message from clique *i* to clique *j* :

$$\mu_{i \to j} = \sum_{C_i \setminus S_{ij}} \psi_{C_i} \prod_{k \neq j} \mu_{k \to i}(S_{ki})$$

• Clique marginal

$$p(C_i) \propto \psi_{C_i} \prod_k \mu_{k \to i}(S_{ki})$$

# Message Passing for HMMs (cont.)

• A junction tree for the HMM



- Rightward pass  $\mu_{t \to t+1}(y_{t+1}) = \sum_{y_t} \psi(y_t, y_{t+1}) \mu_{t-1 \to t}(y_t) \mu_{t\uparrow}(y_{t+1})$   $= \sum_{y_t}^{y_t} p(y_{t+1} | y_t) \mu_{t-1 \to t}(y_t) p(x_{t+1} | y_{t+1})$   $= p(x_{t+1} | y_{t+1}) \sum_{y_t} a_{y_t, y_{t+1}} \mu_{t-1 \to t}(y_t)$ 
  - This is exactly the *forward algorithm*!
- Leftward pass ...

$$\mu_{t-1\leftarrow t}(y_t) = \sum_{y_{t+1}} \psi(y_t, y_{t+1}) \mu_{t\leftarrow t+1}(y_{t+1}) \mu_{t\uparrow}(y_{t+1})$$
$$= \sum_{\mathbf{y}_{t+1}} p(\mathbf{y}_{t+1} | \mathbf{y}_t) \mu_{t\leftarrow t+1}(\mathbf{y}_{t+1}) p(\mathbf{x}_{t+1} | \mathbf{y}_{t+1})$$

• This is exactly the backward algorithm!







# Summary

- Junction tree data-structure for exact inference on general graphs
- Two methods
  - Shafer-Shenoy
  - Belief-update or Lauritzen-Speigelhalter
- Constructing Junction tree from chordal graphs
  - Maximum spanning tree approach