## Probabilistic Graphical Models

## The Belief Propagation (Sum-Product) Algorithm



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## Pros and Cons of Procedure Elimination

- Algebraic elimination $\equiv$ 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
$\rightarrow$ 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 $\equiv$ message passing on a clique tree

- Messages can be reused


## 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 $\equiv$ message passing on a clique tree
- Another query ...

- Messages $m_{f}$ and $m_{h}$ are reused, others need to be recomputed


## 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

We will come back to this later

## 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: $\quad p(x)=\frac{1}{Z}\left(\prod_{i \in V} \psi\left(x_{i}\right) \prod_{(i, j) \in E} \psi\left(x_{i}, x_{j}\right)\right)$
- Directed tree:

$$
p(x)=p\left(x_{r}\right) \prod_{(i, j) \in E} p\left(x_{j} \mid x_{i}\right)
$$

- Equivalence:

$$
\begin{aligned}
& \psi\left(x_{r}\right)=p\left(x_{r}\right) ; \quad \psi\left(x_{i}, x_{j}\right)=p\left(x_{j} \mid x_{i}\right) ; \\
& Z=1, \quad \psi\left(x_{i}\right)=1
\end{aligned}
$$

- Evidence:?


## From elimination to message passing

- Recall ELIMINATION algorithm:
- Choose an ordering $z$ 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

- Elimination on trees is equivalent to message passing along



## From elimination to message passing

- Recall ELIMINATION algorithm:
- Choose an ordering $z$ 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
- 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!!


## The message passing protocol:

- 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


Computing $\mathrm{P}\left(\mathrm{X}_{1}\right)$

## The message passing protocol:

- 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


Computing $\mathrm{P}\left(\mathrm{X}_{2}\right)$

## The message passing protocol:

- 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


Computing $\mathrm{P}\left(\mathrm{X}_{3}\right)$

## Computing node marginals

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


## The message passing protocol:

- A two-pass algorithm:



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

$\operatorname{Sum}-\operatorname{Product}(\mathcal{T}, E)$
Evidence( $E$ )
$f=$ СноoseRoot $(\mathcal{V})$
for $e \in \mathcal{N}(f)$
$\operatorname{Collect}(f, e)$
for $e \in \mathcal{N}(f)$
Distribute $(f, e)$
for $i \in \mathcal{V}$
Computemarginal $(i)$
Evidence( $E$ )
for $i \in E$
$\psi^{E}\left(x_{i}\right)=\psi\left(x_{i}\right) \delta\left(x_{i}, \bar{x}_{i}\right)$
for $i \notin E$
$\psi^{E}\left(x_{i}\right)=\psi\left(x_{i}\right)$
$\operatorname{Collect}(i, j)$
for $k \in \mathcal{N}(j) \backslash i$
$\operatorname{Collect}(j, k)$
SendMessage $(j, i)$
Distribute $(i, j)$
$\operatorname{SendMESSAGE}(i, j)$
for $k \in \mathcal{N}(j) \backslash i$
Distribute $(j, k)$
SendMessage $(j, i)$

$$
m_{j i}\left(x_{i}\right)=\sum_{x_{j}}\left(\psi^{E}\left(x_{j}\right) \psi\left(x_{i}, x_{j}\right) \prod_{k \in \mathcal{N}(j) \backslash i} m_{k j}\left(x_{j}\right)\right)
$$

Computemarginal $(i)$
$p\left(x_{i}\right) \propto \psi^{E}\left(x_{i}\right) \prod_{j \in \mathcal{N}(i)} m_{j i}\left(x_{i}\right)$

## 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


## Correctness of BP on tree

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

$$
m_{j i}\left(x_{i}\right)=\sum_{x_{j}}\left(\psi\left(x_{j}\right) \psi\left(x_{i}, x_{j}\right) \prod_{k \in N(j) \backslash i} m_{k j}\left(x_{j}\right)\right)
$$

- What about non-tree?


## Another view of SP: Factor Graph

- Example 1



## Factor Graphs

- Example 2

- Example 3


$$
\psi\left(\mathrm{x}_{1}, \mathrm{x}_{2}, \mathrm{x}_{3}\right)=\mathrm{f}_{\mathrm{a}}\left(\mathrm{x}_{1}, \mathrm{x}_{2}, \mathrm{x}_{3}\right)
$$



## 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. $\quad v$ : from variables to factors
2. $\mu$ : from factors to variables


$$
\nu_{i s}\left(x_{i}\right)=\prod_{t \in \mathcal{N}(i) \backslash s} \mu_{t i}\left(x_{i}\right)
$$

$$
\mu_{s i}\left(x_{i}\right)=\sum_{x_{\mathcal{N}}(s) \backslash i}\left(f_{s}\left(x_{\mathcal{N}(s)}\right) \prod_{j \in \mathcal{N}(s) \backslash i} \nu_{j s}\left(x_{j}\right)\right)
$$

## 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:


$$
\begin{aligned}
\mathrm{P}\left(\mathrm{x}_{\mathrm{i}}\right) & \propto \prod_{\mathrm{s} \in \mathrm{~N}(\mathrm{i})} \mu_{\mathrm{si}}\left(\mathrm{x}_{\mathrm{i}}\right) \\
& \propto v_{\mathrm{is}}\left(\mathrm{x}_{\mathrm{i}}\right) \mu_{\mathrm{si}}\left(\mathrm{x}_{\mathrm{i}}\right)
\end{aligned}
$$

## BP on a Factor Tree



## Why factor graph?

- Tree-like graphs to Factor trees



## Poly-trees to Factor trees

## :\%\%  $\because \circ$



## 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: <br> 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

$$
\begin{aligned}
& P(a) P(b) P(c \mid b) P(d \mid a) P(e \mid c, d) P(f \mid a) P(g \mid e) P(h \mid e, f) \\
\Rightarrow & P(a) P(b) P(c \mid b) P(d \mid a) P(e \mid c, d) P(f \mid a) P(g \mid e) \phi_{h}(e, f) \\
\Rightarrow & P(a) P(b) P(c \mid b) P(d \mid a) P(e \mid c, d) P(f \mid a) \phi_{g}(e) \phi_{h}(e, f) \\
\Rightarrow & P(a) P(b) P(c \mid b) P(d \mid a) P(e \mid c, d) \phi_{f}(a, e) \\
\Rightarrow & P(a) P(b) P(c \mid b) P(d \mid a) \phi_{e}(a, c, d) \\
\Rightarrow & P(a) P(b) P(c \mid b) \phi_{d}(a, c) \\
\Rightarrow & P(a) P(b) \phi_{c}(a, b) \\
\Rightarrow & P(a) \phi_{b}(a) \\
\Rightarrow & \phi(a)
\end{aligned}
$$

- 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:

$$
\mathrm{BN}: P(\mathbf{X})=\prod_{i=1: d} P\left(X_{i} \mid \mathbf{X}_{\pi_{i}}\right) \quad \text { MRF: } P(\mathbf{X})=\frac{1}{Z} \prod_{c \in C} \psi_{c}\left(\mathbf{X}_{c}\right)
$$

- 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,. $P(C \mid A, B)$ 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:


$$
\begin{aligned}
& P\left(X_{1}, X_{2}, X_{3}, X_{4}, X_{5}, X_{6}\right) \\
= & P\left(X_{1}\right) P\left(X_{2}\right) P\left(X_{3} \mid X_{1}, X_{2}\right) P\left(X_{4} \mid X_{3}\right) P\left(X_{5} \mid X_{3}\right) P\left(X_{6} \mid X_{4}, X_{5}\right) \\
= & \psi\left(X_{1}, X_{2}, X_{3}\right) \psi\left(X_{3}, X_{4}, X_{5}\right) \psi\left(X_{4}, X_{5}, X_{6}\right)
\end{aligned}
$$

where

$$
\begin{gathered}
\psi\left(X_{1}, X_{2}, X_{3}\right)=P\left(X_{1}\right) P\left(X_{2}\right) P\left(X_{3} \mid X_{1}, X_{2}\right) \\
\psi\left(X_{3}, X_{4}, X_{5}\right)=P\left(X_{4} \mid X_{3}\right) P\left(X_{5} \mid X_{3}\right) \\
\psi\left(X_{4}, X_{5}, X_{6}\right)=P\left(X_{6} \mid X_{4}, X_{5}\right)
\end{gathered}
$$

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., $\left(X_{1}, X_{2}, X_{3}\right)$ overlaps with $\left(X_{3}, X_{4}, X_{5}\right)$ ),

- 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:

$$
\begin{aligned}
& P\left(X_{1}, X_{2}, X_{3}, X_{4}, X_{5}, X_{6}\right) \\
= & P\left(X_{1}\right) P\left(X_{2}\right) P\left(X_{3} \mid X_{1}, X_{2}\right) P\left(X_{4} \mid X_{3}\right) P\left(X_{5} \mid X_{3}\right) P\left(X_{6} \mid X_{4}, X_{5}\right) \\
= & P\left(X_{1}, X_{2}, X_{3}\right) \frac{P\left(X_{3}, X_{4}, X_{5}\right)}{P\left(X_{3}\right)} \frac{P\left(X_{4}, X_{5}, X_{6}\right)}{P\left(X_{4}, X_{5}\right)} \\
= & \psi\left(X_{1}, X_{2}, X_{3}\right) \frac{\psi\left(X_{3}, X_{4}, X_{5}\right)}{\phi\left(X_{3}\right)} \frac{\psi\left(X_{4}, X_{5}, X_{6}\right)}{\phi\left(X_{4}, X_{5}\right)} \\
& P\left(\begin{array}{l}
\text { Now eacl } \\
\text { isomorph } \\
\text { marginal } \\
\text { set of var }
\end{array}\right. \\
\hline \prod_{C} \psi_{C}\left(\mathbf{X}_{C}\right) &
\end{aligned}
$$

- Generally:

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?

$$
\begin{array}{ll}
P\left(X_{1} \mid X_{6}=x_{6}\right)=\sum_{X_{2}, X_{3}} \psi\left(X_{1}, X_{2}, X_{3}\right) & \text { Local operations! } \\
P\left(X_{3} \mid X_{6}=x_{6}\right)=\phi\left(X_{3}\right) & \\
P\left(X_{6}\right)=\sum_{X_{4}, X_{5}} \psi\left(X_{4}, X_{5}, x_{6}\right) & \text { ©Eric Xing @ CмU, 2005-2014 }
\end{array} \quad
$$



## Local Consistency

- We have two ways of obtaining $p(S)$

$$
P(S)=\sum_{V \backslash S} \psi(V) \quad P(S)=\sum_{W \backslash S} \psi(W)
$$


and they must be the same

- The following update-rule ensures this:
- Forward update: $\phi_{S}^{*}=\sum_{V \backslash S} \psi^{*}{ }_{V} \quad \psi_{W}^{*}=\frac{\phi_{S}^{*}}{\phi_{S}} \psi_{W}$
- Backward update $\phi_{S}^{* *}=\sum_{W \backslash S} \psi_{W}^{*} \quad \psi_{V}^{* *}=\frac{\phi_{S}^{* *}}{\phi_{S}^{*}} \psi_{V}^{*}$
- Two important identities can be proven

$$
\begin{array}{cc}
\sum_{V \backslash S} \psi_{V}^{* * *}=\sum_{W \backslash S} \psi_{W}^{*}=\phi_{S}^{* *} & \frac{\psi_{V}^{*} \psi_{W}^{*}}{\phi_{S}^{*}}=\frac{\psi_{V}^{* *} \psi_{W}^{* *}}{\phi_{S}^{* *}}=\frac{\psi_{V} \psi_{W}}{\phi_{S}} \\
\text { Local Consistency } & \text { Invariant Joint }
\end{array}
$$

## Message Passing Algorithm



- 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 (nonneighboring) 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



## 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 $\mathrm{O}\left(2^{4}\right)$ or $\mathrm{O}\left(2^{6}\right)$ cost depending on how we triangulate!



## How to triangulate

- A graph elimination algorithm

- 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

$$
\phi_{S}^{*}=\sum_{V \backslash S} \psi_{V} \quad \psi_{W}^{*}=\frac{\phi_{S}^{*}}{\phi_{S}} \psi_{W}
$$

- The Shafer-Shenoy update

$$
m_{i \rightarrow j}\left(S_{i j}\right)=\sum_{C_{i} \backslash S_{i j}} \psi_{C_{i}} \prod_{k \neq j} m_{k \rightarrow i}\left(S_{k i}\right)
$$

## 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 $\equiv$ message passing on a clique tree


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

$$
\alpha_{t}^{k}=p\left(x_{t} \mid y_{t}^{k}=1\right) \sum_{i} \alpha_{t-1}^{i} a_{i, k}
$$

## Shafer Shenoy for HMMs

- Recap: Shafer-Shenoy algorithm

- Message from clique $i$ to clique $j$ :
- Clique marginal

$$
\mu_{i \rightarrow j}=\sum_{C_{i} S_{i j}} \psi_{C_{i}} \prod_{k \neq j} \mu_{k \rightarrow i}\left(S_{k i}\right)
$$

$$
p\left(C_{i}\right) \propto \psi_{C_{i}} \prod_{k} \mu_{k \rightarrow i}\left(S_{k i}\right)
$$

## Message Passing for HMMs (cont.)

- A junction tree for the HMM

- Rightward pass


$$
\begin{aligned}
\mu_{t \rightarrow t+1}\left(y_{t+1}\right) & =\sum_{y_{t}} \psi\left(y_{t}, y_{t+1}\right) \mu_{t-1 \rightarrow t}\left(y_{t}\right) \mu_{t \uparrow}\left(y_{t+1}\right) \\
& =\sum_{y_{t}} p\left(y_{t+1} \mid y_{t}\right) \mu_{t-1 \rightarrow t}\left(y_{t}\right) p\left(x_{t+1} \mid y_{t+1}\right) \\
& =p\left(x_{t+1} \mid y_{t+1}\right) \sum_{y_{t}} a_{y_{t}, y_{t+1}} \mu_{t-1 \rightarrow t}\left(y_{t}\right)
\end{aligned}
$$

- This is exactly the forward algorithm!

- Leftward pass ...

$$
\begin{aligned}
\mu_{t-1 \leftarrow t}\left(y_{t}\right) & =\sum_{y_{t+1}} \psi\left(y_{t}, y_{t+1}\right) \mu_{t \leftarrow t+1}\left(y_{t+1}\right) \mu_{t \uparrow}\left(y_{t+1}\right) \\
& =\sum_{y_{t+1}} p\left(y_{t+1} \mid y_{t}\right) \mu_{t+t+1}\left(y_{t+1}\right) p\left(x_{t+1} \mid y_{t+1}\right)
\end{aligned}
$$

- This is ${ }_{5}^{Y_{t+1}}$ 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

