## L11 – Undirected Graphical Models

#### [Barber](http://web4.cs.ucl.ac.uk/staff/D.Barber/textbook/200620.pdf) 4.1, 4.2, 4.4, 5.1 (Notice that we are changing texts.)

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## What you should know after this lecture

- How a factor graph represents a distribution
- Relationship between factor graphs and Bayes nets
- How to use the sum-product algorithm to compute marginals in a factor graph

# Probabilistic reasoning about partially-specified world states

Factored states Discrete-valued factors Probability over possible worlds!



## Undirected models

- Directed models (Bayes nets) are good for many problems, particularly when there is a causal interpretation of the arrows. (Though causality is not necessary)
- Relationship between pixels in an image or adjacent plots of property is not independent but there's no sensible way to assign a direction.
- Can make graphical models with nodes and undirected arcs: Markov random fields
- We will skip that step and go straight to a formalism called factor graphs that can represent both directed and undirected models.

# Factor graphs



Undirected bipartite graph: factors only connect to variables

- Round nodes are random variables V
- Square nodes are factors φ: tables specifying, for each tuple of value of the connected variables, a non-negative number
- Represent a probability distribution (e.g. left graph above)

$$
P((a, b, c, d, e, f)) = \frac{1}{Z} \phi_1(a) \phi_2(b) \phi_3(a, b, d) \phi_4(a, c) \phi_5(d, g) \phi_6(c, e) \phi_7(c, f)
$$

where Z is a normalizer

$$
Z=\sum_{6.0411/16.420\, \text{Fall }2023}\varphi_1(a)\varphi_2(b)\varphi_3(a,b,d)\varphi_4(a,c)\varphi_5(d,g)\varphi_6(c,e)\varphi_7(c,f)
$$

# Bayes nets to factor graphs

- Variable nodes are the same
- Add one factor for each CPT
- Connect it to the "output" node and all parents
- Note that, for this construction  $Z = 1$  (no need to normalize!) Prove this to yourself by recalling the probability distribution represented by a Bayes net.

# Independence relations in factor graphs

- The Markov blanket of a node V consists of all nodes that are connected to any factor connected to V.
- The Markov blanket of A in our example is  $\{B, D, C\}$
- A node V is not independent of any node in its MB
- A node V is conditionally independent of the rest of the graph, conditioned on  $mb(V)$
- There are some sets of independence relations that are describable by a Bayes net but not describable by a factor graph (and vice versa)

Inference in factor graphs

Some inference problems:

• Joint distribution: In a factor graph, use table multiplication to compute a big table

$$
\frac{1}{Z}\prod_k \varphi_k
$$

where Z is the sum of all table entries

- Marginal distribution:  $P(Y)$  where  $Y \subset V$
- Conditional probability:  $P(Y | E = e)$ , where  $Y \subset V$ ,  $E \subset V$ , and  $Y \cap E = \emptyset$ ; and e is the observed values of the variables in E. Note that it is not necessary that  $Y \cup E = \mathcal{V}$ .
- Most probable assignment (MAP):

$$
argmax yP(Y=y \mid E=e) \enspace .
$$

Note that the MAP of a set of variables is not necessarily  $t_{6.0411/16.426r}$  set of MAPs of the individual variables.

# Computing all the individual marginals

- This method only applies if your factor graph does not have any cycles!
- Awesome algorithm with many names: belief propagation, sum-product, message passing
- Runs in time  $O(N \cdot |T^*|)$  where N is the number of nodes and |T<sup>\*</sup>| is number of entries in the largest table (exponential in the number of variables it is connected to).
- Can parallelize the computation.

# Belief propagation idea

- Pick an arbitrary variable  $V_i \in \mathcal{V}$  to be the root node
- Let  $N(V)$  be the factors connected to  $V$ ,  $N(\phi)$  vars connected to  $\phi$

$$
\begin{aligned} P(V_i) &= \sum_{\mathbf{V} \setminus V_i} P(\tilde{\mathbf{v}}) \\ &= \sum_{\mathbf{V} \setminus V_i} \prod_j \varphi_j(\tilde{\mathbf{v}}) \\ &= \sum_{\mathbf{V} \setminus V_i} \prod_{\varphi \in N(V_i)} F_{\varphi}(\tilde{\mathbf{v}}) \\ &= \prod_{\varphi \in N(V_i)} \sum_{V \in N(\varphi) \setminus V_i} F_{\varphi}(\tilde{\mathbf{v}}) \\ &= \prod_{\varphi \in N(V_i)} \mu_{\varphi \to V}(\mathbf{v}) \end{aligned}
$$

where  $F_{\phi}$  is the product of all the factors in the subtree attached to factor φ

• Recursive algorithm passes messages from leaves up to root, and then back down again 6.0411/16.420 Fall 2023 10

### Factor-to-variable messages

 $\mu_{\phi \to V}(v)$  expresses the  $\phi$  subtree's preference over the vector of possible values v for variable V

Let  $N(\phi)$  be the set of variables connected to factor  $\phi$ 

$$
\mu_{\varphi \to V}(\nu) = \sum_{W \in N(\varphi) \setminus V} \varphi(\nu, \bar{w}) \prod_{W \in N(\varphi) \setminus V} \mu_{W \to \varphi}(w)
$$

Base case if  $\phi$  is a leaf:

$$
\mu_{\varphi \to V}(\nu) = \varphi(\nu)
$$

Think of  $\mu_{\phi \to V}$  as representing P(V) if all subtrees except  $\phi$ were cut off. Slight abuse of notation:  $\prod$  is multiplying tables,  $\Sigma$  is marginalizing out variables.

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## Variable-to-factor messages

 $\mu_{V\rightarrow\phi}(v)$  expresses the V subtree's preference over the vector of possible values v for variable V

$$
\mu_{V\to \varphi}(\nu)=\prod_{\psi\in N(V)\setminus \varphi}\mu_{\psi\to V}(\nu)
$$

Base case if  $X_i$  is a leaf:

$$
\mu_{V\to\varphi}(\nu)=1
$$

Think of  $\mu_{V\rightarrow\phi}$  as representing P(V) if factor  $\phi$  were cut off.

## Sum-Product

- 1. Select  $V_i$  as root
- 2. Recursively compute  $P(V_i) \propto \prod_{\phi \in N(V_i)} \mu_{\phi \to V_i}$
- 3. Pass messages back down the tree, at each node computing marginal  $P(V_j) \propto \prod_{\Phi \in N(V_j)} \mu_{\Phi \to V_j}$



Recall that  $\propto$  means "proportional to," and we generally need to normalize to  $gct$  a distribution.  $13$ 

## Handling evidence

To compute  $P(V | E = e)$ , add a new potential for every variable  $V_i \in E$  that assigns 1 to  $V_i = e_i$  and 0 to all other values for  $V_i$ . Then run sum-product.

## More than marginal!

Easy to compute  $P(V_i, V_j)$  if they are connected in the graph via one factor φ:

$$
P(V_i,V_j) \propto \varphi \prod_{\varphi_i \in N(V_i) \setminus \varphi} \mu_{\varphi_i \rightarrow V_i} \prod_{\varphi_j \in N(V_j) \setminus \varphi} \mu_{\varphi_j \rightarrow V_j} \prod_{V_k \in N(\varphi) \setminus \{V_i,V_j\}} \mu_{V_k \rightarrow \varphi}
$$

Multiply everything coming into  $V_i$ ,  $V_j$ , and  $\phi$  from elsewhere, and normalize

If they aren't neighbors, then for each value  $V_i = v_i$ , compute

$$
P(V_i = v_i, V_j = v_j) = P(V_i = v_i | V_j = v_j)P(V_j = v_j)
$$

using tools we have already established.

# Handling loopy factor graphs

Exact inference is exponential in the number of variables in the "tree width" (largest group of variables that has to be considered jointly)

- 1. Cutset conditioning: pick a subset of nodes C such that, if they were removed, the remaining graph would be a tree. Iterate over assignments to C, do inference, and then reassemble the answers.
- 2. Variable elimination: iteratively,
	- Pick a variable V (efficiency depends on how you do this)
	- Define new  $\phi' = \sum_{v} \prod_{\phi \in N(V)} \phi$
	- Remove V and all  $\phi \in N(V)$  from graph
	- Add  $\phi'$  (defined on all neighboring variables)
	- Until you have a tree (or one big table!)
- 3. Junction tree alg : complicated!

# Approximation methods

1. Keep iterating belief propagation. It might converge... 2. Sampling : later!

### Next time

- Approximate inference via sampling
- Finding the most likely assignment
- Temporal models

#### Sum-Product Practice





• Suppose

$$
\varphi_{f_1}(C,A) = \begin{bmatrix} A & C & \varphi_{f_1}(A,C) \\ T & T & 0.05 \\ T & F & 0.45 \\ F & T & 0.45 \\ F & F & 0.05 \end{bmatrix}
$$

• Suppose

$$
\varphi_{f_2}(B,A)=\begin{bmatrix}B&C&\varphi_{f_1}(A,C)\\T&T&0.0\\T&F&0.5\\F&T&0.0\\F&T&0.5\end{bmatrix}
$$

• Which means

$$
P(C) = (1/Z)(\mu_{f_1 \to C} \times \mu_{f_2 \to C})
$$
  
= 1/Z  $\begin{bmatrix} C & \mu \\ T & .5 \end{bmatrix} \times \begin{bmatrix} C & \mu \\ T & 0 \end{bmatrix}$   
=  $\begin{bmatrix} C & P(C) \\ T & 0 \end{bmatrix}$  where Z = 0.5  
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#### $\mu_{f_1 \to C} = \begin{bmatrix} C \\ T \end{bmatrix}$  $\begin{bmatrix} C & \mu \\ T & .5 \\ F & .5 \end{bmatrix}$

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Then

Then

$$
\mu_{f_2\to C}=\begin{bmatrix}C&\mu\\T&0\\F&1\end{bmatrix}
$$

#### Sum-Product Practice



$$
P(C) = 1/Z \prod_{i=1}^{2} \mu_{f_1 \to C}
$$

$$
\mu_{f_1 \to C} = \sum_{A} \varphi_{f_1} \mu_{A \to f_1}
$$

$$
\mu_{A \to f_1} = 1
$$

$$
\mu_{f_2 \to C} = \sum_{A} \varphi_{f_2} \mu_{B \to f_2}
$$

$$
\mu_{B \to f_2} = 1
$$



$$
\begin{aligned} &\mu_{f_3\to A}=f_3\\ &\mu_{A\to f_1}=\mu_{f_3\to A}\\ &\mu_{f_1\to C}=\sum_{f}f_1\cdot\mu_{A\to f_1}\\ &\mu_{E\to f_4}=1\\ &\mu_{f_4\to B}=\sum_{f}f_4\cdot\mu_{E\to f_4}\\ &\mu_{G\to f_5}=1\\ &\mu_{f_5\to B}=\sum_{G}f_5\cdot\mu_{G\to f_5}\\ &\mu_{B\to f_2}=\mu_{f_4\to B}\cdot\mu_{f_5\to B}\\ &\mu_{F\to f_2}=1\\ &\mu_{f_2\to C}=\sum_{g,f}f_2\cdot\mu_{B\to f_2}\cdot\mu_{F\to f_2}\\ &P(C)\propto\mu_{f_1\to C}\cdot\mu_{f_2\to C}\end{aligned}
$$

Note that, to do the backward pass, you **do not** pass P(C) back out. So  $\mu_{C \to f_1} = \mu_{f_2 \to C}$ . Similarly  $\mu_{C \to f_2} = \mu_{f_1 \to C}$ . And then  $\mu_{f_2\to F} = \sum_{C,B} f_2 \cdot \mu_{C\to f_2} \cdot \mu_{B\to f_2}.$