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Summer Semester 2015/2016

8. Belief Propagation



Recall: Inference *

Inference means the procedure to estimate the probability distribution, encoded by a graphical model, for a given data (or observation).

Assume we are given a factor graph $G = (\mathcal{V}, \mathcal{E}, \mathcal{F})$ and the observation \mathbf{x} .

Maximum A Posteriori (MAP) inference: find the state $\mathbf{y}^* \in \mathcal{Y}$ of maximum probability,

$$\mathbf{y}^* \in \underset{\mathbf{y} \in \mathcal{Y}}{\operatorname{argmax}} p(\mathbf{y} \mid \mathbf{x}) = \underset{\mathbf{y} \in \mathcal{Y}}{\operatorname{argmin}} E(\mathbf{y}; \mathbf{x}) .$$

Probabilistic inference: find the value of the partition function $Z(\mathbf{x})$ and the marginal distributions $\mu_F(\mathbf{y}_F)$ for each factor $F \in \mathcal{F}$,

$$Z(\mathbf{x}) = \sum_{\mathbf{y} \in \mathcal{Y}} \exp(-E(\mathbf{y}; \mathbf{x})) ,$$

$$\mu_F(\mathbf{y}_F) = p(\mathbf{y}_F \mid \mathbf{x}) .$$

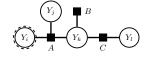


Sum-product algorithm

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Agenda for today's lecture *

Today we are going to learn about belief propagation to perform exact inference on graphical models having tree structure.



- Probabilistic inference: Sum-product algorithm
- MAP inference: Max-sum algorithm

We also extend belief propagation for general factor graphs, which results in an approximate inference.

Probabilistic inference on chains

Assume that we are given the following factor graph and a corresponding energy function $E(\mathbf{y})$, where $\mathcal{Y} = \mathcal{Y}_i \times \mathcal{Y}_j \times \mathcal{Y}_k \times \mathcal{Y}_l$.



We want to compute $p(\mathbf{y})$ for any $\mathbf{y} \in \mathcal{Y}$ by making use of the factorization

$$p(\mathbf{y}) = \frac{1}{Z} \exp(-E(\mathbf{y})) = \frac{1}{Z} \exp(-E_A(y_i, y_j)) \exp(-E_B(y_j, y_k)) \exp(-E_C(y_k, y_l)).$$

Problem: we also need to calculate the partition function

$$Z = \sum_{\mathbf{y} \in \mathcal{Y}} \exp(-E(\mathbf{y})) = \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \sum_{y_k \in \mathcal{Y}_k} \sum_{y_l \in \mathcal{Y}_l} \exp(-E(y_i, y_j, y_k, y_l)) ,$$

which looks expensive (the sum has $|\mathcal{Y}_i| \cdot |\mathcal{Y}_j| \cdot |\mathcal{Y}_k| \cdot |\mathcal{Y}_l|$ terms)

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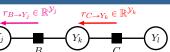
Partition function



We can expand the partition function as

$$\begin{split} Z &= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \sum_{y_k \in \mathcal{Y}_k} \sum_{y_l \in \mathcal{Y}_l} \exp(-E(y_i, y_j, y_k, y_l)) \\ &= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \sum_{y_k \in \mathcal{Y}_k} \sum_{y_l \in \mathcal{Y}_l} \exp\left(-\left(E_A(y_i, y_j) + E_B(y_j, y_k) + E_C(y_k, y_l)\right)\right) \\ &= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \sum_{y_k \in \mathcal{Y}_k} \sum_{y_l \in \mathcal{Y}_l} \exp(-E_A(y_i, y_j)) \exp(-E_B(y_j, y_k)) \exp(-E_C(y_k, y_l)) \\ &= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_i \in \mathcal{Y}_j} \exp(-E_A(y_i, y_j)) \sum_{y_k \in \mathcal{Y}_k} \exp(-E_B(y_j, y_k)) \sum_{y_l \in \mathcal{Y}_l} \exp(-E_C(y_k, y_l)) \;. \end{split}$$

Elimination



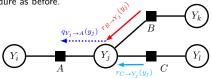
ote that we can successively *eliminate* variables, that is

$$Z = \sum_{y_l \in \mathcal{Y}_l} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_A(y_i, y_j)) \sum_{y_k \in \mathcal{Y}_k} \exp(-E_B(y_j, y_k)) \underbrace{\sum_{y_l \in \mathcal{Y}_l} \exp(-E_C(y_k, y_l))}_{}$$

$$= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_A(y_i, y_j)) \underbrace{\sum_{y_k \in \mathcal{Y}_k} \exp(-E_B(y_j, y_k)) r_{C \to Y_k}(y_k)}_{r_{B \to Y_j}(y_j)}$$

$$= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_A(y_i, y_j)) r_{B \to Y_j}(y_j) = \sum_{y_i \in \mathcal{Y}_i} r_{A \to Y_i}(y_i) \ .$$

Now we are assuming a tree-structured factor graph and applying the same elimination procedure as before.



$$Z = \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_A(y_i, y_j)) \sum_{\substack{y_k \in \mathcal{Y}_k \\ r_{\mathcal{B} \to \mathcal{Y}_i}(y_j)}} \exp(-E_B(y_j, y_k)) \sum_{\substack{y_l \in \mathcal{Y}_l \\ r_{\mathcal{C} \to \mathcal{Y}_j}(y_j)}} \exp(-E_C(y_j, y_l))$$

$$_{B\rightarrow Y_{j}}(y_{j})$$

$$= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_A(y_i, y_j)) \underbrace{r_{B \to Y_j}(y_j) r_{C \to Y_j}(y_j)}_{q_{Y_j \to A}(y_j)}$$

$$= \sum_{y_i \in \mathcal{Y}_i} \sum_{y_i \in \mathcal{Y}_i} \exp(-E_A(y_i, y_j)) q_{Y_j \to A}(y_j)$$

elimination procedure as before.

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Messages



Message: pair of vectors at each factor graph edge $(i, F) \in \mathcal{E}$.

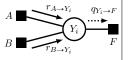


1. Variable-to-factor message $q_{Y_i \to F} \in \mathbb{R}^{\mathcal{Y}_i}$ is given by

$$q_{Y_i \to F}(y_i) = \prod_{F' \in M(i) \backslash \{F\}} r_{F' \to Y_i}(y_i) \;,$$

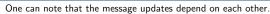
where $M(i) = \{F \in \mathcal{F} : (i, F) \in \mathcal{E}\}$ denotes the set of factors adjacent to Y_i .

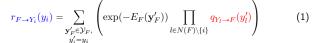
Factor-to-variable message: $r_{F \to Y_i} \in \mathbb{R}^{\mathcal{Y}_i}$.



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Message scheduling *





$$q_{Y_i \to F}(y_i) = \prod_{F' \in M(i) \setminus \{F\}} r_{F' \to Y_i}(y_i) \tag{2}$$

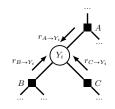
The messages that do not depend on previous computation are the following.

- The factor-to-variable messages in which no other variable is adjacent to the factor; then the product in (1) will be empty.
- The variable-to-factor messages in which no other factor is adjacent to the variable; then the product in (2) is empty and the message will be one.

Inference result: partition function Z

Partition function is evaluated at the (root) node i

$$Z = \sum_{y_i \in \mathcal{Y}_i} \prod_{F \in M(i)} r_{F \to Y_i}(y_i) .$$



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Factor-to-variable message

 $Z = \sum_{y_i \in \mathcal{Y}_i} \sum_{y_j \in \mathcal{Y}_j} \exp(-E_A(y_i, y_j)) q_{Y_j \to A}(y_j)$

Inference on trees (cont.)

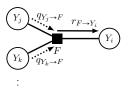
Now we are assuming a tree-structured factor graph and applying the same

2. Factor-to-variable message $r_{F \to Y_i} \in \mathbb{R}^{\mathcal{Y}_i}$ is given by

 $= \sum_{y_i \in \mathcal{Y}_i} r_{A \to Y_i}(y_i) .$

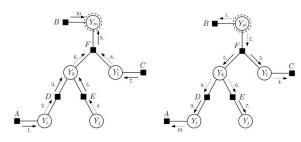
$$r_{F \to Y_i}(y_i) = \sum_{\substack{\mathbf{y}_F' \in \mathcal{Y}_F, \\ y_i' = y_i}} \left(\exp(-E_F(\mathbf{y}_F')) \prod_{l \in N(F) \setminus \{i\}} q_{Y_l \to F}(y_l') \right),$$

where $N(F) = \{i \in V : (i, F) \in \mathcal{E}\}$ denotes the set of variables adjacent to F.



Message scheduling on trees

For tree-structured factor graphs there always exist at least one such message that can be computed initially, hence all the dependencies can be resolved.



- Select one variable node as root of the tree (e.g., Y_m)
- Compute leaf-to-root messages (e.g., by applying depth-first-search)
- Compute root-to-leaf messages (reverse order as before)

Inference result: the marginals $\mu_F(\mathbf{y}_F)$

The marginal distribution for each factor can be computed as

Optimality and complexity *

Assume a tree-structured factor graph. If the messages are computed based on depth-first search order for the sum-product algorithm, then it converges after 2|V| iterations and provides the **exact** marginals.

If $|\mathcal{Y}_i| \leq K$ for all $i \in \mathcal{V}$, then the complexity of the algorithm $\mathcal{O}(|\mathcal{V}| \cdot K^{F_{\text{max}}})$, where $F_{\text{max}} = \max_{F \in \mathcal{F}} |N(F)|$.

$$r_{F \to Y_i}(y_i) = \sum_{\substack{\mathbf{y}_F' \in \mathcal{Y}_F, \\ y_i' \to y_i}} \left(\exp(-E_F(\mathbf{y}_F')) \prod_{l \in N(F) \setminus \{i\}} q_{Y_l \to F}(y_l') \right).$$

Note that the complexity of the naïve way is $\mathcal{O}(K \cdot m^{|V|})$.

Reminder. Assuming $f,g:\mathbb{R}\to\mathbb{R}$, the notation $f(x)=\mathcal{O}(g(x))$ means that there exists C>0 and $x_0\in\mathbb{R}$ such that $|f(x)|\leqslant C|g(x)|$ for all $x>x_0$.

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MAP inference

$$\mathbf{y}^* \in \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} p(\mathbf{y}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} \frac{1}{Z} \tilde{p}(\mathbf{y}) = \operatorname*{argmax}_{\mathbf{y} \in \mathcal{Y}} \tilde{p}(\mathbf{y}) \; .$$

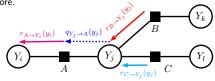
Similar to the sum-product algorithm one can obtain the so-called max-sum algorithm to solve the above maximization.

By applying the \ln function, we have

$$\begin{split} \ln \max_{\mathbf{y} \in \mathcal{Y}} \tilde{p}(\mathbf{y}) &= \max_{\mathbf{y} \in \mathcal{Y}} \ln \tilde{p}(\mathbf{y}) \\ &= \max_{\mathbf{y} \in \mathcal{Y}} \ln \prod_{F \in \mathcal{F}} \exp(-E_F(\mathbf{y}_F)) \\ &= \max_{\mathbf{y} \in \mathcal{Y}} \sum_{F \in \mathcal{F}} -E_F(\mathbf{y}_F) \; . \end{split}$$

MAP inference on trees (cont.)

Now we are assuming a tree-structured factor graph and applying an elimination procedure as before.



$$\max_{\mathbf{y} \in \mathcal{Y}} \sum_{F \in \mathcal{F}} -E_F(\mathbf{y}_F) = \max_{y_i} \underbrace{\max_{y_j} -E_A(y_i, y_j) + q_{Y_j \to A}(y_j)}_{r_{A \to Y_i}(y_i)} = \max_{y_i} r_{A \to Y_i}(y_i)$$

The solution is then obtained as:

$$y_i^* \in \operatorname{argmax} r_{A \to Y_i}(y_i),$$

$$y_j^* \in \underset{y_j}{\operatorname{argmax}} -E_A(y_i^*, y_j) + q_{Y_j \to A}(y_j),$$

$$y_k^* \in \operatorname{argmax} -E_B(y_j^*, y_k),$$

$$y_l^* \in \operatorname{argmax} -E_C(y_j^*, y_l)$$
.

Choosing an optimal state st

Sum-product algorithm Max-sum algorithm Loopy belief propagation

The following **back-tracking** algorithm is applied for choosing an optimal y^* .

1. Initialize the procedure at the root node (Y_i) by choosing any

$$y_i^* \in \underset{y_i \in \mathcal{Y}_i}{\operatorname{argmax}} \max_{\mathbf{y}' \in \mathcal{Y}, y_i' = y_i} \tilde{p}(\mathbf{y}')$$
,

and set $\mathcal{I} = \{i\}$.

- 2. Based on (reverse) depth-first search order, for each $j \in V \setminus I$
 - (a) choose a configuration y_i^* at the node Y_j such that

$$\begin{aligned} y_j^* \in \underset{y_j \in \mathcal{Y}_j}{\operatorname{argmax}} & \underset{\mathbf{y}' \in \mathcal{Y}, \\ y_j' = y_j, \\ y_i' = y_i^* & \forall i \in \mathcal{I} \end{aligned},$$

(b) update $\mathcal{I} = \mathcal{I} \cup \{j\}$.

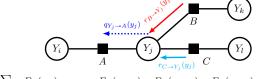


Max-sum algorithm

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MAP inference on trees

Now we are assuming a tree-structured factor graph and applying an elimination procedure as before.



$$\begin{split} \max_{\mathbf{y} \in \mathcal{Y}} \sum_{F \in \mathcal{F}} -E_F(\mathbf{y}_F) &= \max_{\mathbf{y}} -E_A(y_i, y_j) - E_B(y_j, y_k) - E_C(y_j, y_l) \\ &= \max_{y_i, y_j} -E_A(y_i, y_j) + \max_{\underbrace{y_k} -E_B(y_j, y_k) + \max_{y_l} -E_C(y_j, y_l)}_{r_{C \to Y_j}(y_j)} \\ &= \max_{y_i, y_j} -E_A(y_i, y_j) + \underbrace{r_{B \to Y_j}(y_j) + r_{C \to Y_j}(y_j)}_{q_{Y_j \to A}(y_j)} \end{split}$$

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Messages

The messages become as follows

$$\begin{split} q_{Y_i \to F}(y_i) &= \sum_{F' \in M(i) \backslash \{F\}} r_{F' \to Y_i}(y_i) \\ r_{F \to Y_i}(y_i) &= \max_{\substack{y_F' \in \mathcal{Y}_F, \\ y_i' = y_i}} \left(-E_F(y_F') + \sum_{l \in N(F) \backslash \{i\}} q_{Y_l \to F}(y_l') \right). \end{split}$$

The max-sum algorithm provides exact MAP inference for tree-structured factor

Sum-product and Max-sum comparison *

In general, for graphs with cycles there is no guarantee for convergence.

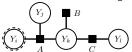
■ Sum-product algorithm

$$\begin{aligned} q_{Y_i \to F}(y_i) &= \prod_{F' \in M(i) \setminus \{F\}} r_{F' \to Y_i}(y_i) \\ r_{F \to Y_i}(y_i) &= \sum_{\substack{y'_F \in \mathcal{Y}_F, \\ y'_i = y_i}} \left(\exp(-E_F(y'_F)) \prod_{l \in N(F) \setminus \{i\}} q_{Y_l \to F}(y'_l) \right) \end{aligned}$$

Max-sum algorithm

$$\begin{aligned} q_{Y_i \to F}(y_i) &= \sum_{F' \in M(i) \setminus \{F\}} r_{F' \to Y_i}(y_i) \\ r_{F \to Y_i}(y_i) &= \max_{\substack{y_F' \in \mathcal{Y}_F, \\ y_i' = y_i}} \left(-E_F(y_F') + \sum_{l \in N(F) \setminus \{i\}} q_{Y_l \to F}(y_l') \right) \end{aligned}$$

Let us consider the following factor graph with

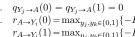


$E_A(0,y_j,y_k)$ $E_A(1,y_j,y_k)$					
	11(-)	y_k 0 1	11()	y_k 0 1	
	$y_j = 0$	1 0 0 1	$y_j = 0$	0 -1 0 0	

$E_C(y_k, y_l)$				
	y_l			
	0 1			
0	0 0.5			
g_k 1	0.5 0			

Let us chose the node Y_i as root. We calculate the messages for the \max -sum algorithm from leaf-to-root direction in a topological order as follows.

- $q_{Y_l\to C}(0)=q_{Y_l\to C}(1)=0$
- $r_{C \to Y_k}(0) = \max_{y_l \in \{0,1\}} \{-E_C(0,y_l) + q_{Y_l \to C}(0)\} = \max_{y_l \in \{0,1\}} -E_C(0,y_l) = 0$ $r_{C \to Y_k}(1) = \max_{y_l \in \{0,1\}} \{-E_C(1, y_l) + q_{Y_l \to C}(1)\} = \max_{y_l \in \{0,1\}} -E_C(1, y_l) = 0$
- $r_{B\to Y_k}(0) = -1$ $r_{B \to Y_k}(1) = -0.5$
- $\begin{aligned} q_{Y_k \to A}(0) &= r_{B \to Y_k}(0) + r_{C \to Y_k}(0) = -1 + 0 = -1 \\ q_{Y_k \to A}(1) &= r_{B \to Y_k}(1) + r_{C \to Y_k}(1) = -0.5 + 0 = -0.5 \end{aligned}$



 $r_{A \to Y_i}(0) = \max_{y_j, y_k \in \{0, 1\}} \{ -E_A(0, y_j, y_k) + q_{Y_j \to A}(y_j) + q_{Y_k \to A}(y_k) \} = -0.5$ $r_{A \to Y_i}(1) = \max_{y_i, y_k \in \{0,1\}} \{-E_A(1, y_j, y_k) + q_{Y_j \to A}(y_j) + q_{Y_k \to A}(y_k)\} = 0.5$

Example (cont.) *

In order to calculate the maximal state y^* we apply back-tracking

- 1. $y_i^* \in \operatorname{argmax}_{y_i \in \{0,1\}} r_{A \to Y_i}(y_i) = \{1\}$
- 2. $y_j^* \in \operatorname{argmax}_{y_j \max_{y_j, y_k \in \{0,1\}}} \{-E_A(1, y_j, y_k) + q_{Y_k \to A}(y_k)\} = \{0\}$
- $y_k^* \in \operatorname{argmax}_{y_k \in \{0,1\}} \{ -E_A(1,0,y_k) + r_{B \to Y_k}(y_k) + r_{C \to Y_k}(y_k) \} = \{1\}$
- 4. $y_l^* \in \operatorname{argmax}_{y_l \in \{0,1\}} \{-E_C(1, y_l) + r_{C \to Y_k}(1)\} = \{1\}$

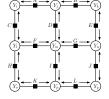
Therefore, the optimal state $y^* = (y_i^*, y_i^*, y_k^*, y_l^*) = (1, 0, 1, 1)$.

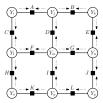
Loopy belief propagation

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Message passing in cyclic graphs

When the graph has cycles, then there is no well-defined *leaf-to-root* order. However, one can apply message passing on cyclic graphs, which results in loopy belief propagation





- Initialize all messages as constant 1
- $Pass\ factor-to-variables\ and\ variables-to-factor\ messages\ alternately\ until$
- Upon convergence, treat beliefs μ_F as approximate marginals

Messages

The factor-to-variable messages $r_{F o Y_i}$ remain well-defined and are computed

$$r_{F \to Y_i}(y_i) = \sum_{\substack{\mathbf{y}_F' \in \mathcal{Y}_F, \\ y_i' = y_i}} \left(\exp(-E_F(\mathbf{y}_F')) \prod_{j \in N(F) \setminus \{i\}} q_{Y_j \to F}(y_j') \right)$$

The variable-to-factor messages are normalized at every iteration as follows:

$$q_{Y_i \to F}(y_i) = \frac{\prod_{F' \in M(i) \backslash \{F\}} r_{F' \to Y_i}(y_i)}{\sum_{y_i' \in \mathcal{Y}_i} \prod_{F' \in M(i) \backslash \{F\}} r_{F' \to Y_i}(y_i')}$$

In case of tree structured graphs, in the sum-product algorithm these normalization constants are equal to 1, since the marginal distributions, calculated in each iteration, are exact.



Beliefs

The approximate marginals, i.e.beliefs, are computed as before but now a factor-specific normalization constant z_F is also used.

The factor marginals are given by

$$\mu_F(y_F) = \frac{1}{z_F} \exp(-E_F(y_F)) \prod_{i \in N(F)} q_{Y_i \to F}(y_i) ,$$

where the factor specific normalization constant is given by

$$z_F = \sum_{y_F \in \mathcal{Y}_F} \exp(-E_F(y_F)) \prod_{i \in N(F)} q_{Y_i \to F}(y_i) \ .$$

Beliefs (cont.) *

Loopy belief propagat

In addition to the factor marginals the algorithm also computes the variable marginals in a similar fashion.

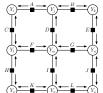
$$\mu_i(y_i) = \frac{1}{z_i} \prod_{F' \in M(i)} r_{F' \to Y_i}(y_i) ,$$

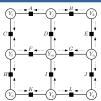
where the normalizing constant is given by

$$z_i = \sum_{y_i \in \mathcal{Y}_i} \prod_{F' \in M(i)} r_{F' \to Y_i}(y_i) \;.$$

Since the local normalization constant z_F differs at each factor for loopy belief propagation, the exact value of the normalizing constant Z cannot be directly calculated. Instead, an approximation to the log partition function can be computed.

Remarks on loopy belief propagation





Loopy belief propagation is very popular, but has some problems:

- It might not converge (e.g., it can oscillate).
- Even if it does, the computed probabilities are only approximate.
- If there is a single cycle only in the graph, then it converges.

Summary

We have discussed exact inference methods on tree-structured graphical models

Probabilistic inference: Sum-product algorithm

MAP inference: Max-sum algorithm

■ For general factor graphs: Loopy belief propagation

In the next lecture we will learn about

■ Human-pose estimation

White





Mean-field approximation: probabilistic inference via optimization (a.k.a. variational inference)

Literature

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