

# Probabilistic & Unsupervised Learning

## Belief Propagation

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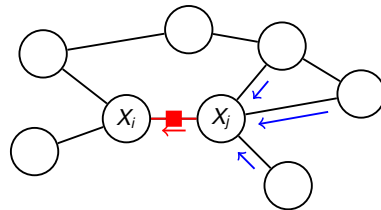
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### Loopy Belief Propagation

Joint distribution of undirected **graph**:

$$p(\mathcal{X}) = \frac{1}{Z} \prod_{\text{nodes } i} f_i(X_i) \prod_{\text{edges } (ij)} f_{ij}(X_i, X_j)$$



Messages computed recursively (**with few guarantees of convergence**):

$$M_{j \rightarrow i}(X_i) := \sum_{X_j} f_{ij}(X_i, X_j) f_j(X_j) \prod_{l \in \text{ne}(j) \setminus i} M_{l \rightarrow j}(X_j)$$

Marginal distributions are **approximate** in general:

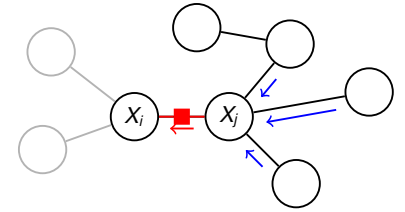
$$p(X_i) \approx b_i(X_i) \propto f_i(X_i) \prod_{k \in \text{ne}(i)} M_{k \rightarrow i}(X_i)$$

$$p(X_i, X_j) \approx b_{ij}(X_i, X_j) \propto f_{ij}(X_i, X_j) f_i(X_i) f_j(X_j) \prod_{k \in \text{ne}(i) \setminus j} M_{k \rightarrow i}(X_i) \prod_{l \in \text{ne}(j) \setminus i} M_{l \rightarrow j}(X_j)$$

### Recall: Belief Propagation on undirected trees

Joint distribution of undirected tree:

$$p(\mathcal{X}) = \frac{1}{Z} \prod_{\text{nodes } i} f_i(X_i) \prod_{\text{edges } (ij)} f_{ij}(X_i, X_j)$$



Messages computed recursively:

$$M_{j \rightarrow i}(X_i) := \sum_{X_j} f_{ij}(X_i, X_j) f_j(X_j) \prod_{l \in \text{ne}(j) \setminus i} M_{l \rightarrow j}(X_j)$$

Marginal distributions:

$$p(X_i) \propto f_i(X_i) \prod_{k \in \text{ne}(i)} M_{k \rightarrow i}(X_i)$$

$$p(X_i, X_j) \propto f_{ij}(X_i, X_j) f_i(X_i) f_j(X_j) \prod_{k \in \text{ne}(i) \setminus j} M_{k \rightarrow i}(X_i) \prod_{l \in \text{ne}(j) \setminus i} M_{l \rightarrow j}(X_j)$$

### Dealing with loops

► **Accuracy**: BP posterior marginals are **approximate** on all non-trees because evidence is **over counted**, but converged approximations are frequently found to be good (particularly in their means).

► **Convergence**: no general guarantee, but BP does converge in some cases:

- **Trees**.
- Graphs with a **single loop**.
- Distributions with sufficiently **weak** interactions.
- Graphs with **long** (and weak) loops
- **Gaussian** networks: means correct, variances may also converge.

► **Damping**: Common approach to encourage convergence (cf EP)

$$M_{i \rightarrow j}^{\text{new}}(X_j) := (1 - \alpha) M_{i \rightarrow j}^{\text{old}}(X_j) + \alpha \sum_{X_i} f_{ij}(X_i, X_j) f_i(X_i) \prod_{k \in \text{ne}(i) \setminus j} M_{k \rightarrow i}(X_i)$$

► **Grouping variables**: Variables can be grouped into cliques to improve accuracy.

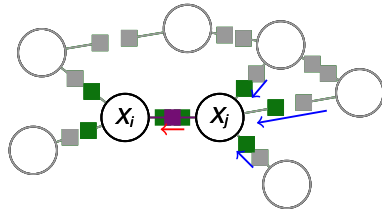
- Region graph approximations.
- Cluster variational method.
- Junction graph.

## Different Interpretations of Loopy Belief Propagation

Loopy BP can be interpreted as a fixed point algorithm from a few different perspectives:

- ▶ Expectation propagation.
- ▶ Tree-based reparametrization.
- ▶ Bethe free energy.

## Loopy BP as message-based EP



Then the EP updates to the messages are:

- ▶ **Deletion:**

$$q_{-ij}(X_i, X_j) = f_i(X_i) f_j(X_j) \prod_{k \in \text{ne}(i) \setminus j} M_{k \rightarrow i}(X_i) \prod_{l \in \text{ne}(j) \setminus i} M_{l \rightarrow j}(X_j) \prod_{s \neq i, j} f_s(X_s) \prod_{t \in \text{ne}(s)} M_{t \rightarrow s}(X_s)$$

- ▶ **Projection:**

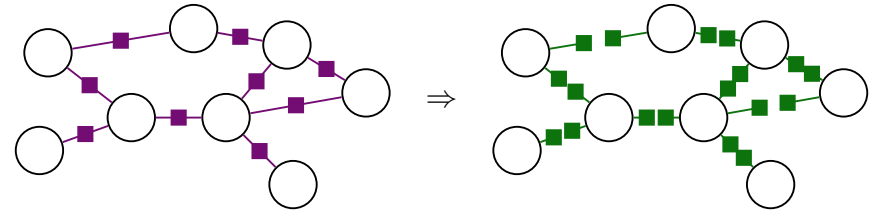
$$\{M_{i \rightarrow j}^{\text{new}}, M_{j \rightarrow i}^{\text{new}}\} = \text{argmin}_{\mathbf{KL}} [f_{ij}(X_i, X_j) q_{-ij}(X_i, X_j) \| M_{i \rightarrow j}(X_i) M_{j \rightarrow i}(X_j) q_{-ij}(X_i, X_j)]$$

Now,  $q_{-ij}(\cdot)$  factors  $\Rightarrow$  rhs factors  $\Rightarrow$  min is achieved by marginals of  $f_{ij}(\cdot) q_{-ij}(\cdot)$

$$M_{j \rightarrow i}^{\text{new}}(X_i) q_{-ij}(X_i) = \sum_{X_j} \left( f_{ij}(X_i, X_j) f_j(X_j) \prod_{l \in \text{ne}(j) \setminus i} M_{l \rightarrow j}(X_j) \right) f_i(X_i) \prod_{k \in \text{ne}(i) \setminus j} M_{k \rightarrow i}(X_i)$$

$$\Rightarrow M_{j \rightarrow i}^{\text{new}}(X_i) = \sum_{X_j} \left( f_{ij}(X_i, X_j) f_j(X_j) \prod_{l \in \text{ne}(j) \setminus i} M_{l \rightarrow j}(X_j) \right) \underbrace{q_{-ij}(X_i)}_{\text{marginal}}$$

## Loopy BP as message-based Expectation Propagation



Approximate pairwise factors  $f_{ij}$  by product of messages:

$$f_{ij}(X_i, X_j) \approx \tilde{f}_{ij}(X_i, X_j) = M_{i \rightarrow j}(X_j) M_{j \rightarrow i}(X_i)$$

Thus, the full joint is approximated by a factorised distribution:

$$p(\mathcal{X}) \approx \frac{1}{Z} \prod_{\text{nodes } i} f_i(X_i) \prod_{\text{edges } (ij)} \tilde{f}_{ij}(X_i, X_j) = \frac{1}{Z} \prod_{\text{nodes } i} \left( f_i(X_i) \prod_{j \in \text{ne}(i)} M_{j \rightarrow i}(X_i) \right) = \prod_{\text{nodes } i} b_i(X_i)$$

but with **multiple factors** for most  $X_i$ .

## Message-based EP

- ▶ Thus message-based EP in a loopy graph need not be seen as two separate approximations one to the sites and one to the cavity (as we had in the EP lecture).
- ▶ Instead, we can see it as a more severe constraint on the approximate sites: not just to an ExpFam factor, but to a product of ExpFam messages.
- ▶ On a tree-structured graph the message-factored version of EP finds the same marginals as standard EP.
  - ▶ Messages are calculated in exactly the same way as before (cf NLSSM).
  - ▶ Pairwise marginals can be found after convergence by computing  $\tilde{P}(\mathbf{y}_{i-1}, \mathbf{y}_i)$  as required (cf Forward-backward for HMMs).
  - ▶ Would not be true of fully-factored variational approximation.
- ▶ Factorisation view remains valid even when original sites lie in the appropriate ExpFam already – so loopy BP in (eg) discrete graphs can be seen as a form of EP.
- ▶ However, this view does not help us understand the convergence properties of BP.

## Loopy BP as tree-based reparametrisation

Tree-structured distributions can be parametrised in many ways:

$$\rho(\mathcal{X}) = \frac{1}{Z} \prod_{\text{nodes } i} f_i(X_i) \prod_{\text{edges } (ij)} f_{ij}(X_i, X_j) \quad \text{undirected tree} \quad (1)$$

$$= \rho(X_r) \prod_{i \neq r} \rho(X_i | X_{\text{pa}(i)}) \quad \text{directed (rooted) tree} \quad (2)$$

$$= \prod_{\text{nodes } i} \rho(X_i) \prod_{\text{edges } (ij)} \frac{\rho(X_i, X_j)}{\rho(X_i)\rho(X_j)} \quad \text{pairwise marginals} \quad (3)$$

where (3) requires that  $\sum_{X_j} \rho(X_i, X_j) = \rho(X_i)$ .

The undirected tree representation is not unique—multiplying a factor  $f_{ij}(X_i, X_j)$  by  $g(X_i)$  and dividing  $f_i(X_i)$  by the same  $g(X_i)$  does not change the distribution.

BP can be seen as an iterative replacement of  $f_i(X_i)$  by the local marginal of  $p_{ij}(X_i, X_j)$ , along with the corresponding reparametrisation of  $f_{ij}(X_i, X_j)$ . Cf. Hugin propagation.

Converged BP on a **tree** finds  $\rho(X_i)$  and  $\rho(X_i, X_j)$ , allowing us to transform (1) to (3).

## Reparametrisation on non-trees

- ▶ If BP converges on a non-tree, it will have successfully reparametrised the distribution to have **locally consistent** beliefs:

$$\rho(\mathcal{X}) \propto \prod_i b(X_i) \prod_{(ij)} \frac{b(X_i, X_j)}{b(X_i)b(X_j)} \quad \text{with} \quad \sum_{X_j} b(X_i, X_j) = b(X_i) \text{ etc.}$$

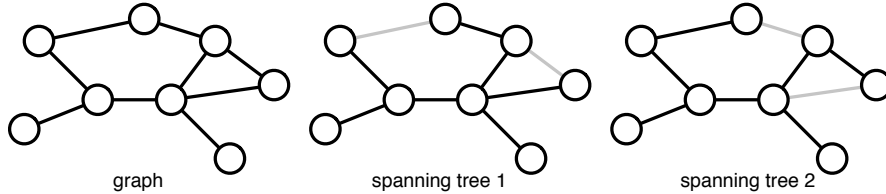
- ▶ However, the marginals will not usually be correct or **globally consistent**. That is

$$\sum_{X_{-i}} \left( \prod_i b(X_i) \prod_{(ij)} \frac{b(X_i, X_j)}{b(X_i)b(X_j)} \right) \neq b(X_i)$$

and the product will not generally be normalised.

- ▶ What can be said about these **pseudomarginals**?
- ▶ Consider the following (theoretical) message scheduling scheme:
  - ▶ Identify all the **spanning trees** of the graph.
  - ▶ Pass messages along edges of each spanning tree in turn.
  - ▶ Iterate over spanning trees to convergence

## Loopy BP as tree-based reparametrisation



$$\begin{aligned} \rho(\mathcal{X}) &= \frac{1}{Z} \prod_{\text{nodes } i} f_i^0(X_i) \prod_{\text{edges } (ij)} f_{ij}^0(X_i, X_j) \\ &= \frac{1}{Z} \prod_{\text{nodes } i \in T_1} f_i^0(X_i) \prod_{\text{edges } (ij) \in T_1} f_{ij}^0(X_i, X_j) \prod_{\text{edges } (ij) \notin T_1} f_{ij}^0(X_i, X_j) \\ &= \frac{1}{Z} \prod_{\text{nodes } i \in T_1} f_i^1(X_i) \prod_{\text{edges } (ij) \in T_1} f_{ij}^1(X_i, X_j) \prod_{\text{edges } (ij) \notin T_1} f_{ij}^1(X_i, X_j) \end{aligned}$$

where  $f_i^1(X_i) = \rho^{T_1}(X_i)$ ,  $f_{ij}^1(X_i, X_j) = \frac{\rho^{T_1}(X_i, X_j)}{\rho^{T_1}(X_i)\rho^{T_1}(X_j)}$ ,  $f_{ij}^1 = f_{ij}^0$ .

$$= \frac{1}{Z} \prod_{\text{nodes } i \in T_2} f_i^1(X_i) \prod_{\text{edges } (ij) \in T_2} f_{ij}^1(X_i, X_j) \prod_{\text{edges } (ij) \notin T_2} f_{ij}^1(X_i, X_j)$$

...

## Loopy BP as tree-based reparametrisation

At convergence, loopy BP has reparametrised the joint distribution as:

$$\rho(\mathcal{X}) = \frac{1}{Z} \prod_{\text{nodes } i} f_i^\infty(X_i) \prod_{\text{edges } (ij)} f_{ij}^\infty(X_i, X_j)$$

where for **any** tree  $T$  embedded in the graph,

$$\begin{aligned} f_i^\infty(X_i) &= \rho^T(X_i) \\ f_{ij}^\infty(X_i, X_j) &= \frac{\rho^T(X_i, X_j)}{\rho^T(X_i)\rho^T(X_j)} \end{aligned}$$

Thus, **the local marginals of all subtrees are locally consistent with each other**, and the pseudomarginals represent valid beliefs for any of the subtrees.

$$\rho(\mathcal{X}) = \frac{1}{Z} \prod_{\text{nodes } i} b_i(X_i) \prod_{\text{edges } (ij)} \frac{b_{ij}(X_i, X_j)}{b_i(X_i)b_j(X_j)}$$

## Loopy BP and Bethe free energy

In the reparametrisation view, BP solves for marginal beliefs  $b_{ij}(X_i, X_j)$  and  $b_i(X_i) = \sum_{x_j} b_{ij}(X_i, X_j)$  such that

$$p(\mathcal{X}) \propto \prod_i f_i(X_i) \prod_{(ij)} f_{ij}(X_i, X_j) \propto \prod_i b_i(X_i) \prod_{(ij)} \frac{b_{ij}(X_i, X_j)}{b_i(X_i)b_j(X_j)}$$

Another view of loopy BP is as a set of fixed point equations for finding stationary points of an objective function called the **Bethe free energy**, which is defined in terms of the locally consistent beliefs (or **pseudomarginals**)  $b_i \geq 0$  and  $b_{ij} \geq 0$ :

$$\begin{aligned} \sum_{x_i} b_i(x_i) &= 1 & \forall i \\ \sum_{x_j} b_{ij}(x_i, x_j) &= b_i(x_i) & \forall i, j \in \text{ne}(i), x_i \end{aligned}$$

## Bethe fixed point equations

The Bethe free-energy Lagrangian is:

$$\begin{aligned} \mathcal{L} &= \sum_i \sum_{x_i} b_i(x_i) \log f_i(x_i) + \sum_{(ij)} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \log f_{ij}(x_i, x_j) & [\mathcal{E}_{\text{bethe}}] \\ &- \sum_i \sum_{x_i} b_i(x_i) \log b_i(x_i) - \sum_{(ij)} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \log \frac{b_{ij}(x_i, x_j)}{b_i(x_i)b_j(x_j)} & [\mathcal{H}_{\text{bethe}}] \\ &+ \sum_i \xi_i \left( \sum_{x_i} b_i(x_i) - 1 \right) & [\text{norm } \forall i] \\ &+ \sum_{(ij)} \left[ \sum_{x_i} \xi_{ij}(x_i) \left( \sum_{x_j} b_{ij}(x_i, x_j) - b_i(x_i) \right) + \sum_{x_j} \xi_{ji}(x_j) \left( \sum_{x_i} b_{ij}(x_i, x_j) - b_j(x_j) \right) \right] & [\text{marg } \forall i, j, x_i] \end{aligned}$$

Setting derivatives wrt beliefs to 0 gives

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial b_i(x_i)} &= \log f_i(x_i) - \log b_i(x_i) + \underbrace{\sum_{j \in \text{ne}(i)} \sum_{x_j} \frac{b_{ij}(x_i, x_j)}{b_i(x_i)}}_{=1 \text{ by constraint}} + \xi_i - \sum_{j \in \text{ne}(i)} \xi_{ij}(x_i) + \text{const} = 0 \\ \Rightarrow b_i(x_i) &\propto f_i(x_i) \prod_{j \in \text{ne}(i)} e^{-\xi_{ij}(x_i)} \end{aligned}$$

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial b_{ij}(x_i, x_j)} &= \log f_{ij}(x_i, x_j) - \log b_{ij}(x_i, x_j) + \log b_i(x_i)b_j(x_j) + \xi_{ij}(x_i) + \xi_{ji}(x_j) + \text{const} = 0 \\ \Rightarrow b_{ij}(x_i, x_j) &\propto f_{ij}(x_i, x_j) b_i(x_i) b_j(x_j) e^{\xi_{ij}(x_i)} e^{\xi_{ji}(x_j)} \end{aligned}$$

## Loopy BP and Bethe free energy

Recall that the variational free energy is:  $\mathcal{F}(q) = \langle \log P(\mathcal{X}) \rangle_q + \mathbf{H}[q]$

We define the (negative) Bethe free energy:  $\mathcal{F}_{\text{bethe}}(\mathbf{b}) = \mathcal{E}_{\text{bethe}}(\mathbf{b}) + \mathcal{H}_{\text{bethe}}(\mathbf{b})$

- ▶ The Bethe average energy is the expected log-joint evaluated as though the pseudomarginals were correct:

$$\mathcal{E}_{\text{bethe}}(\mathbf{b}) = \sum_i \sum_{x_i} b_i(x_i) \log f_i(x_i) + \sum_{(ij)} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \log f_{ij}(x_i, x_j)$$

- ▶ The Bethe entropy is **approximate**: it is the sum of the pseudomarginal entropies corrected for pairwise (pseudo)interactions, but neglecting higher-order dependence:

$$\begin{aligned} \mathcal{H}_{\text{bethe}}(\mathbf{b}) &= \sum_i \mathbf{H}[b_i] - \sum_{(ij)} \mathbf{KL}[b_{ij} \| b_i b_j] \\ &= - \sum_i \sum_{x_i} b_i(x_i) \log b_i(x_i) - \sum_{(ij)} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \log \frac{b_{ij}(x_i, x_j)}{b_i(x_i)b_j(x_j)} \end{aligned}$$

- ▶ On a tree, both the beliefs and the Bethe entropy expression are correct, so  $\mathcal{F}_{\text{bethe}} = \mathcal{F}$ .
- ▶ Message updates in loopy BP can now be derived by finding the stationary points of a Lagrangian with local consistency and normalisation constraints. The BP messages are related to the Lagrange multipliers.

## Bethe fixed point messages

The Bethe Lagrangian fixed point equations are:

$$\begin{aligned} b_i(x_i) &\propto f_i(x_i) \prod_{j \in \text{ne}(i)} e^{-\xi_{ij}(x_i)} \\ b_{ij}(x_i, x_j) &\propto f_{ij}(x_i, x_j) b_i(x_i) b_j(x_j) e^{\xi_{ij}(x_i)} e^{\xi_{ji}(x_j)} \end{aligned}$$

Comparison with BP suggests that messages should have the form  $M_{j \rightarrow i}(x_i) = e^{-\xi_{ij}(x_i)}$ .

Indeed, solving for  $\xi_{ij}(x_i)$  by enforcing the constraint  $\sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i)$  we have:

$$\begin{aligned} \sum_{x_j} b_{ij}(x_i, x_j) &\propto \sum_{x_j} f_{ij}(x_i, x_j) b_i(x_i) b_j(x_j) e^{\xi_{ij}(x_i)} e^{\xi_{ji}(x_j)} \\ \Rightarrow b_i(x_i) &\propto b_i(x_i) e^{\xi_{ij}(x_i)} \sum_{x_j} f_{ij}(x_i, x_j) b_j(x_j) e^{\xi_{ji}(x_j)} \\ \Rightarrow e^{-\xi_{ij}(x_i)} &\propto \sum_{x_j} f_{ij}(x_i, x_j) b_j(x_j) e^{\xi_{ji}(x_j)} \\ &= \sum_{x_j} f_{ij}(x_i, x_j) f_j(x_j) \prod_{l \in \text{ne}(j) \setminus i} e^{-\xi_{jl}(x_j)} \end{aligned}$$

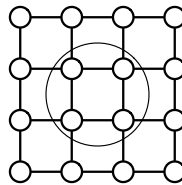
thus recovering the BP message passing rules.

## Loopy BP and Bethe free energy

- ▶ Fixed points of loopy BP are exactly the stationary points of the Bethe free energy.
- ▶ **Stable** fixed points of loopy BP are local maxima of Bethe free energy (note the negative definition of free energy for consistency with the variational free energy).
- ▶ For binary attractive networks, Bethe free energy at fixed points of loopy BP provides an upper bound on the log partition function  $\log Z$ —this is useful for learning undirected graphical models as it leads to a lower bound on the log likelihood.

## Extensions and variations

- ▶ Generalized BP: group variables together to treat their interactions exactly.
- ▶ Convergent alternatives: Fixed points of loopy BP are stationary points of the Bethe free energy. We can also derive algorithms that **increase** the Bethe free energy at every step, and are thus guaranteed to converge.
- ▶ Convex alternatives: We can derive convex cousins of the negative of the Bethe free energy. These give rise to algorithms that will converge to a unique global maximum.
- ▶ We have considered sum-product loopy BP to compute marginals. The treatment of loopy Viterbi or max-product algorithms is different.



## Loopy BP vs mean-field approximation

- ▶ Beliefs  $b_i$  and  $b_{ij}$  in loopy BP are only locally consistent pseudomarginals, not necessarily consistent marginals of the implied joint distribution.
- ▶ Bethe free energy accounts for interactions between different sites, while variational free energy assumes independence.
- ▶ The loop series or Plefka expansion of the log partition function  $Z$ : the variational free energy forms the first order terms, while Bethe free energy contains higher order terms (involving generalized loops).
- ▶ Loopy BP tends to be significantly more accurate whenever it converges.

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