Probabilistic & Unsupervised Learning
Approximate Inference

Belief Propagation

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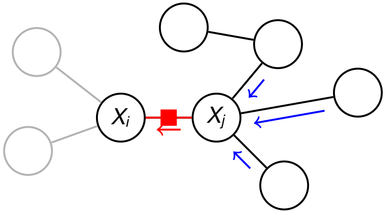
Recall: Belief Propagation on undirected trees



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:

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

Marginal distributions:

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

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

Loopy Belief Propagation

Joint distribution of undirected graph:

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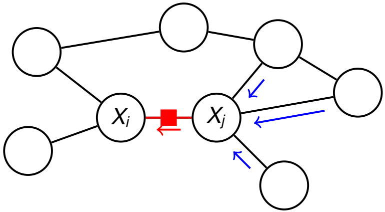

Messages computed recursively (with few guarantees of convergence):

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

Marginal distributions are approximate in general:

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

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

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).

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

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

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- **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:

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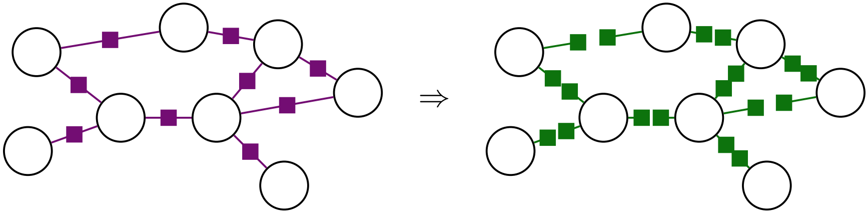
Loopy BP as message-based Expectation Propagation



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

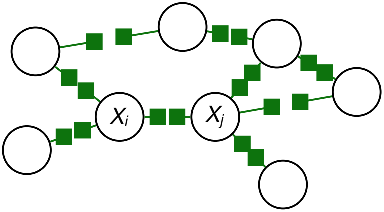
$$f_{ij}(X_i, X_j) \approx \tilde{f}_{ij}(X_i, X_j) = M_{i \to j}(X_j) M_{j \to i}(X_i)$$

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

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

but with multiple factors for most X_i.

Loopy BP as message-based EP



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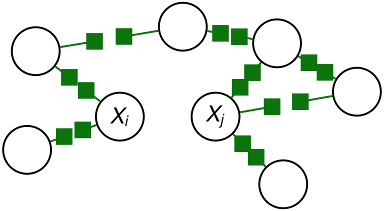

Then the EP updates to the messages are:

- Deletion:

$$q_{\neg ij}(\mathcal{X}) = f_i(X_i) f_j(X_j) \prod_{k \in \mathrm{ne}(i) \setminus j} M_{k \to i}(X_i) \prod_{l \in \mathrm{ne}(j) \setminus i} M_{l \to j}(X_j) \prod_{s \neq i,j} f_s(X_s) \prod_{t \in \mathrm{ne}(s)} M_{t \to s}(X_s)$$

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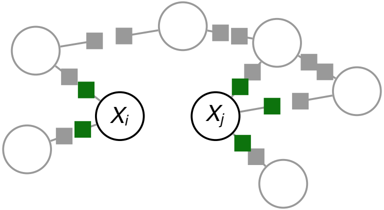

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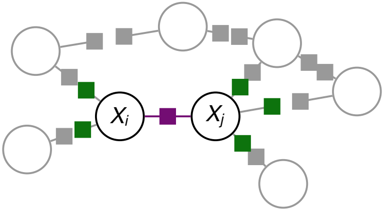

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- Projection:

$$\{M_{i \to j}^{\mathrm{new}}, M_{j \to i}^{\mathrm{new}}\} = \operatorname{argmin} \mathbf{KL}[f_{ij}(X_i, X_j) q_{\neg ij}(X_i, X_j) \| M_{j \to i}(X_i) M_{i \to j}(X_j) q_{\neg ij}(X_i, X_j)]$$

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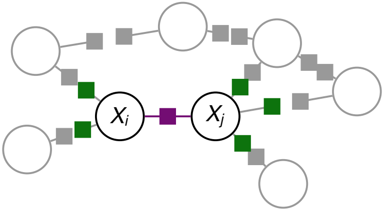

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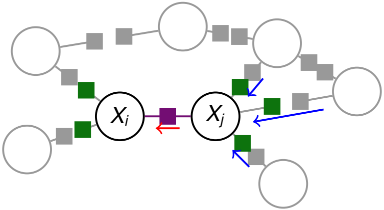

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$$M_{j \to i}^{\text{new}}(X_i) q_{\neg ij}(X_i) = \sum_{X_j} \left(f_{ij}(X_i, X_j) f_j(X_j) \prod_{l \in \text{ne}(j) \setminus i} M_{l \to j}(X_j) \right) \underbrace{f_i(X_i) \prod_{k \in \text{ne}(i) \setminus j} M_{k \to i}(X_i)}_{q_{\neg ij}(X_i)}$$

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

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  - 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.

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

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Loopy BP as tree-based reparametrisation

Tree-structured distributions can be parametrised in many ways:

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

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

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

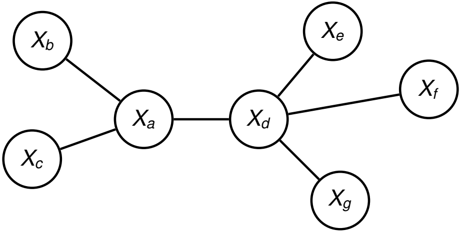
where (3) requires that $\sum_{X_j} p(X_i, X_j) = p(X_i)$.

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 $p(X_i)$ and $p(X_i, X_j)$, allowing us to transform (1) to (3).

Reparametrisation on trees



$$p(\mathcal{X}) \propto \prod_{(ij)} f_{ij}(X_i, X_j)$$

$$\Downarrow$$

$$p(\mathcal{X}) = \prod_i p(X_i) \prod_{(ij)} \frac{p(X_i, X_j)}{p(X_i)p(X_k)}$$

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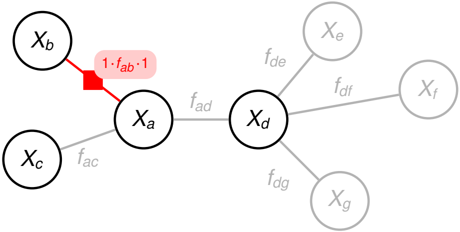

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$$p^n(X_i, X_j) = \frac{1}{Z_{ij}^n} f_i^{n-1}(X_i) f_{ij}^{n-1}(X_i, X_j) f_j^{n-1}(X_j) \quad \text{[store } Z_{ij}^n\text{s to obtain joint normaliser]}$$

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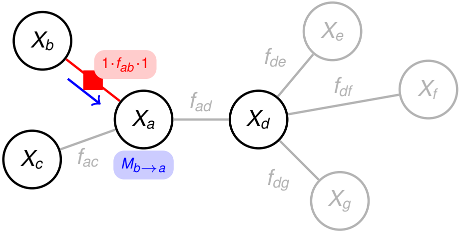

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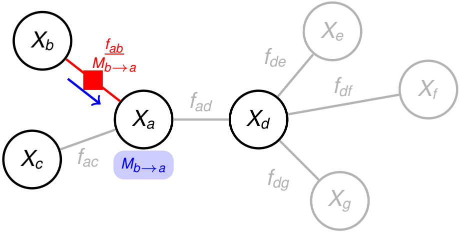

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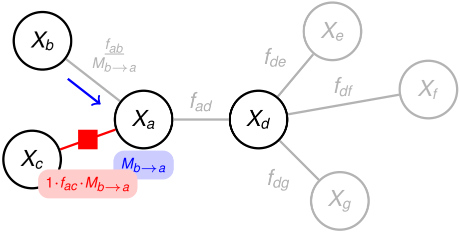

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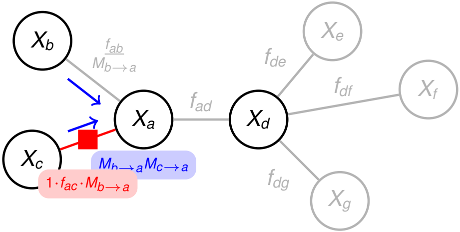

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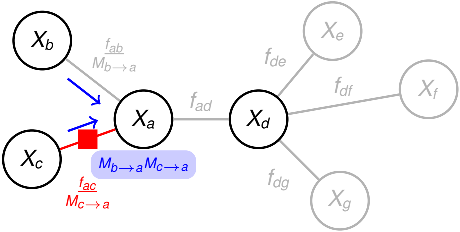
Reparametrisation on trees



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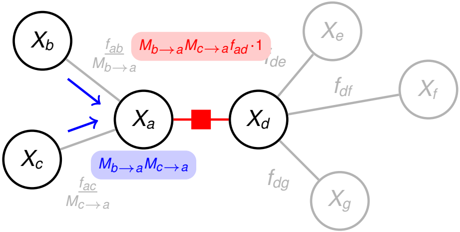

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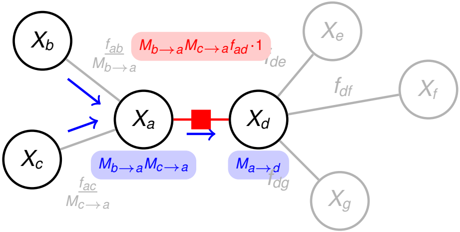

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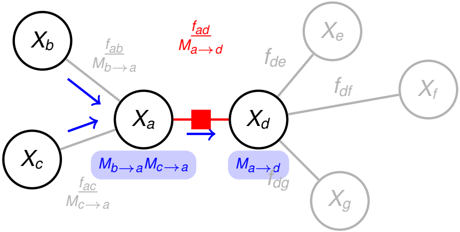

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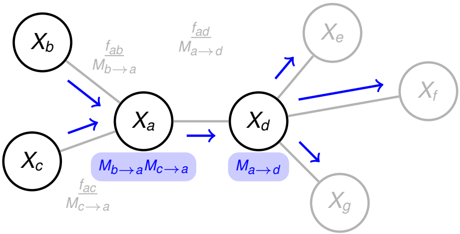

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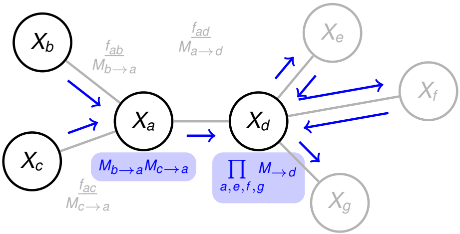

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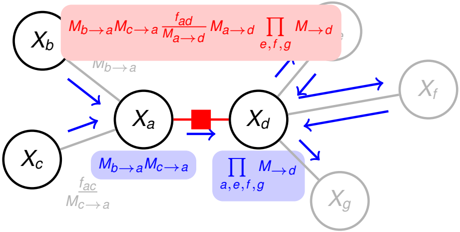

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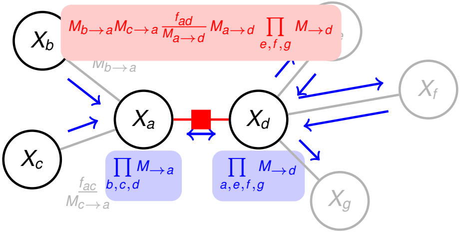

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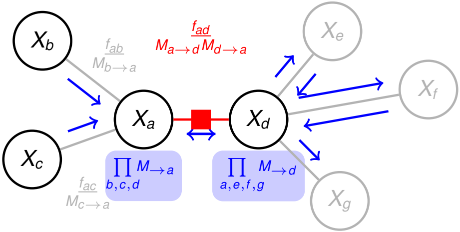

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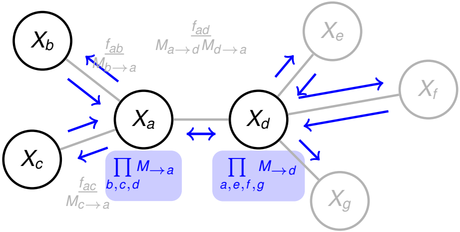

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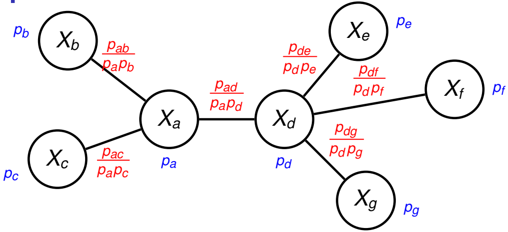

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After all messages have propagated:

$$f_i^\infty(X_i) = \prod_{j \in \mathrm{ne}(i)} M_{j\to i}(X_i) = p(X_i)$$

$$f_{ij}^\infty(X_i, X_j) = \frac{f_{ij}(X_i, X_j)}{M_{j\to i}(X_i) M_{i\to j}(X_j)} = \frac{\prod_{k\in \mathrm{ne}(i)\setminus j} M_{k\to i}(X_i) f_{ij}(X_i, X_j) \prod_{l \in \mathrm{ne}(j)\setminus i} M_{l\to j}(X_j)}{\prod_{k\in \mathrm{ne}(i)\setminus j} M_{k\to i}(X_i) M_{j\to i}(X_i) M_{i\to j}(X_j) \prod_{l\in \mathrm{ne}(j)\setminus i} M_{l\to j}(X_j)} = \frac{p(X_i, X_j)}{p(X_i)p(X_j)}$$

Reparametrisation on non-trees

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

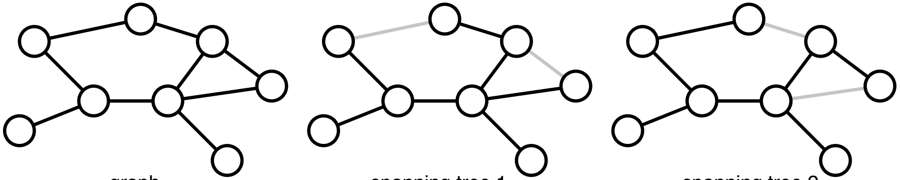
$$p(\mathcal{X}) \propto \prod_i b(X_i) \prod_{(ij)} \frac{b(X_i, X_j)}{b(X_i)b(X_j)} \quad \text{with} \quad \sum_{X_j} b(X_i, X_j) = b(X_i) \text{ etc.}$$

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

$$\sum_{\mathcal{X}_{\neg i}} \left(\prod_i b(X_i) \prod_{(ij)} \frac{b(X_i, X_j)}{b(X_i)b(X_j)} \right) \neq b(X_i)$$

  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



$$p(\mathcal{X}) = \frac{1}{Z} \prod_{\text{nodes } i} f_i^0(X_i) \prod_{\text{edges } (ij)} f_{ij}^0(X_i, X_j)$$

$$= \frac{1}{Z} \prod_{\text{nodes } i \in T_1} f_i^0(X_i) \prod_{\text{edges } (ij) \in T_1} f_{ij}^0(X_i, X_j) \prod_{\text{edges } (ij) \not\in T_1} f_{ij}^0(X_i, X_j)$$

$$= \frac{1}{Z} \prod_{\text{nodes } i \in T_1} f_i^1(X_i) \prod_{\text{edges } (ij) \in T_1} f_{ij}^1(X_i, X_j) \prod_{\text{edges } (ij) \not\in T_1} f_{ij}^1(X_i, X_j)$$

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

$$= \frac{1}{Z} \prod_{\text{nodes } i \in T_2} f_i^1(X_i) \prod_{\text{edges } (ij) \in T_2} f_{ij}^1(X_i, X_j) \prod_{\text{edges } (ij) \not\in T_2} f_{ij}^1(X_i, X_j)$$

$\ldots$

Loopy BP as tree-based reparametrisation

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

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

where for any tree T embedded in the graph,

$$f_i^{\infty}(X_i) = p^T(X_i)$$

$$f_{ij}^{\infty}(X_i, X_j) = \frac{p^T(X_i, X_j)}{p^T(X_i)p^T(X_j)}$$

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

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

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 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

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

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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 $b_{ij} \geq 0$:

$$\sum_{x_i} b_i(x_i) = 1 \qquad \forall i$$

$$\sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i) \qquad \forall i,\ j \in \text{ne}(i), x_i$$

Loopy BP and Bethe free energy

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

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

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

$$\begin{aligned}
\mathcal{H}_{\text{bethe}}(b) &= \sum_i \mathbf{H}[b_i] - \sum_{(ij)} \mathbf{KL}[b_{ij} \| b_i b_j] \\
&= -\sum_i \sum_{x_i} b_i(x_i) \log b_i(x_i) - \sum_{(ij)} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \log \frac{b_{ij}(x_i, x_j)}{b_i(x_i) b_j(x_j)}
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$$\mathcal{E}_{\text{bethe}}(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 the sum of the pseudomarginal entropies corrected for pairwise (pseudo)interactions, but neglecting higher-order dependence:

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

- On a tree, both the beliefs and the Bethe entropy expression are correct, so $\mathcal{F}_{\text{bethe}} = \mathcal{F}$.

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: $\mathcal{F}_{\text{bethe}}(b) = \mathcal{E}_{\text{bethe}}(b) + \mathcal{H}_{\text{bethe}}(b)$ where both terms are approximations to the corresponding variational likelihood terms.

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

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

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

$$\mathcal{H}_{\text{bethe}}(b) = \sum_i \mathbf{H}[b_i] - \sum_{(ij)} \mathbf{KL}[b_{ij} \| b_i b_j]$$

$$= -\sum_i \sum_{x_i} b_i(x_i) \log b_i(x_i) - \sum_{(ij)} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \log \frac{b_{ij}(x_i, x_j)}{b_i(x_i) b_j(x_j)}$$

- 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 equations

The Bethe free-energy Lagrangian is:

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

$$- \sum_i \sum_{x_i} b_i(x_i) \log b_i(x_i) - \sum_{(ij)} \sum_{x_i,x_j} b_{ij}(x_i,x_j) \log \frac{b_{ij}(x_i,x_j)}{b_i(x_i) b_j(x_j)} \qquad [\mathcal{H}_{\text{bethe}}]$$

$$+ \sum_i \xi_i \Big(\sum_{x_i} b_i(x_i) - 1 \Big) \qquad [\text{norm } \forall i]$$

$$+ \sum_{(ij)} \Big[\sum_{x_i} \xi_{ij}(x_i) \Big(\sum_{x_j} b_{ij}(x_i,x_j) - b_i(x_i) \Big) + \sum_{x_j} \xi_{ji}(x_j) \Big(\sum_{x_i} b_{ij}(x_i,x_j) - b_j(x_j) \Big) \Big] \qquad [\text{marg } \forall i,j,x_i]$$

Setting derivatives wrt beliefs to 0 gives

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

$$\Rightarrow b_i(x_i) \propto f_i(x_i) \prod_{j \in \text{ne}(i)} e^{-\xi_{ij}(x_i)}$$

$$\frac{\partial \mathcal{L}}{\partial b_{ij}(x_i,x_j)} = \log f_{ij}(x_i,x_j) - \log b_{ij}(x_i,x_j) + \log b_i(x_i) b_j(x_j) + \xi_{ij}(x_i) + \xi_{ji}(x_j) + const = 0$$

$$\Rightarrow b_{ij}(x_i,x_j) \propto f_{ij}(x_i,x_j) b_i(x_i) b_j(x_j) e^{\xi_{ij}(x_i)} e^{\xi_{ji}(x_j)}$$

Bethe fixed point messages

The Bethe Lagrangian fixed point equations are:

$$b_i(x_i) \propto f_i(x_i) \prod_{j \in \text{ne}(i)} e^{-\xi_{ij}(x_i)}$$

$$b_{ij}(x_i, x_j) \propto f_{ij}(x_i, x_j) b_i(x_i) b_j(x_j) e^{\xi_{ij}(x_i)} e^{\xi_{ji}(x_j)}$$

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

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.

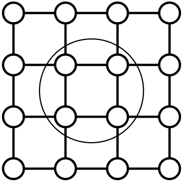
Loopy BP and Bethe free energy

- 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 enegy (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.

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 signficantly more accurate whenever it converges.

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 enegy. We can also derive algorithms that **increase** the Bethe free energy at every step, and are thus are 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.

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