Local Message Passing on Frustrated Systems

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Marginal Inference

Probabilistic Inference

Infer the state of a system $\mathcal{X} = \{x_1, \dots, x_N\}$ based on a noisy observation $\boldsymbol{y}$ and prior knowledge $p(\mathcal{X})$.

- Goal: Find the corresponding **posterior distribution** $p(\mathcal{X}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\mathcal{X}) \cdot p(\mathcal{X})}{p(\boldsymbol{y})}$
- **Marginal inference**: Infer the state of a **local** variable x_n
  - **Marginalization**: $P(x_n|\boldsymbol{y}) = \sum_{x_1} \cdots \sum_{x_{n-1}} \sum_{x_{n+1}} \cdots \sum_{x_N} P(\mathcal{X}|\boldsymbol{y}) =: \sum_{\sim\{x_n\}} P(\mathcal{X}|\boldsymbol{y})$

→ computationally complex for large systems $\mathcal{X}$

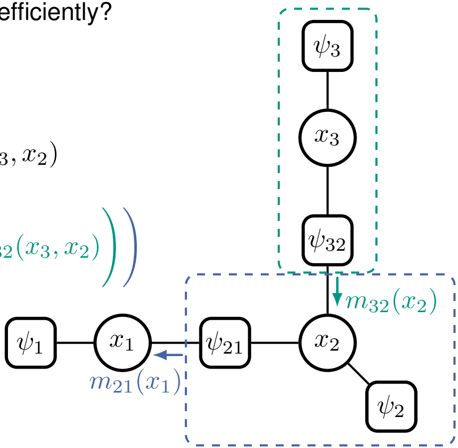
Marginal Inference on Graphical Models

- Assume structure $p(\mathcal{X}|\boldsymbol{y}) = \frac{1}{Z}\prod_{n=1}^{N}\psi_n(x_n)\prod_{n>m}\psi_{nm}(x_m, x_n)$
- Can we use this structure to perform the marginalization more efficiently?
  → **distributive law** $\widehat{=}$ **message passing on graphs**

Example:

$$p(x_1|\boldsymbol{y}) = \frac{1}{Z}\sum_{x_2}\sum_{x_3}\psi_1(x_1)\psi_2(x_2)\psi_3(x_3)\psi_{21}(x_2,x_1)\psi_{32}(x_3,x_2)$$

$$= \frac{1}{Z}\psi_1(x_1)\left(\sum_{x_2}\psi_2(x_2)\psi_{21}(x_2,x_1)\left(\sum_{x_3}\psi_3(x_3)\psi_{32}(x_3,x_2)\right)\right)$$

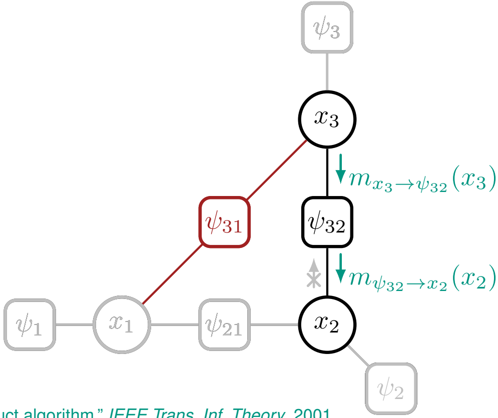


Message Passing on Graphical Models

Sum-product Algorithm (SPA) [KFL01]

$$m_{\psi \to x}(x) = \sum_{\sim\{x\}} \left(\psi(\mathcal{X}_n) \prod_{x' \in \mathcal{X}_n \setminus \{x\}} m_{x' \to \psi}(x') \right)$$

$\mathcal{X}_n \subset \mathcal{X}$: Adjacent variable nodes of factor node $\psi(\mathcal{X}_n)$



Advantages of message passing on graphs:

- Algorithm defined by **simple update rule**
- **Efficient algorithms** can be derived very intuitively
- Also **applicable to graphs with cycles**

[KFL01] F. R. Kschischang, B. J. Frey, and H.-A. Loeliger. "Factor graphs and the sum-product algorithm," *IEEE Trans. Inf. Theory*, 2001.

Message Passing on Graphs with Cycles

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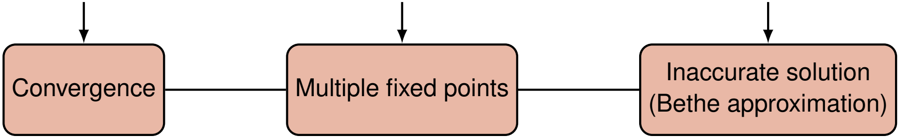
- SPA also applicable to cyclic graphs → iterative algorithm
- **But:** SPA only yields **approximation of marginals** on graphs with cycles
  - **Fixed points** of SPA correspond to **stationary points** of the **Bethe free energy** **[YFW00]**



- Alternative: Directly try to minimize the Bethe free energy, e.g., concave-convex procedure (CCCP) **[Yui02]**
- Many attemps to **mitigate this suboptimality of the SPA** on cyclic graphs: Momentum BP, Neural BP, . . .

→ Instead of fixing a mismatched algorithm, we want to
find a message update rule that is especially taylored to graphs with (many) cycles!

[YFW00] J. S. Yedidia, W. T. Freeman, and Y. Weiss. "Generalized belief propagation," *Advances in Neural Information Processing Systems*, 2000.
[Yui02] A. L. Yuille. "CCCP algorithms to minimize the Bethe and Kikuchi free energies," *Neural Computation*, 2002.

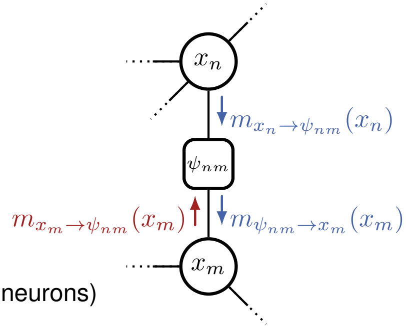
Message Passing on Graphs with Cycles

Message Update Rule

A mapping from one or multiple incident messages to one outgoing message, which is applied **locally** at a (factor) node.

Extrinsic: $\text{FN}_\text{e}(\psi_{n,m}) : m_{x_n \to \psi_{n,m}}(x_n) \mapsto m_{\psi_{n,m} \to x_m}(x_m)$

Non-extrinsic: $\text{FN}(\psi_{n,m}) : \begin{pmatrix} m_{x_n \to \psi_{n,m}}(x_n) \\ m_{x_m \to \psi_{n,m}}(x_m) \end{pmatrix} \mapsto m_{\psi_{n,m} \to x_m}(x_m)$



- Represent mapping by compact multilayer perceptron (1 hidden layer à 7 neurons)
  - **cycBP: Optimize local mapping towards good end-to-end inference performance**

Marginal Inference: Objective Functions

- Supervised Training: **Kullback-Leibler (KL) divergence** $\mathcal{L}_{\text{KL}} := D_{\text{KL}}\left(b_n(x_n) \| p(x_n)\right)$
  - $b_n(x_n), b_{n,m}(x_n, x_m)$: Single, pairwise beliefs of message passing
  - $p(x_n) = \sum_{\sim\{x_n\}} p(x_1, \dots, x_N)$: Exact marginal distributions
- Unsupervised Training: **Regularized Bethe free energy** $\mathcal{L}_{\text{Bethe}} := F_{\text{Bethe}} + \alpha \mathcal{L}_{\mathbb{L}}$ $, \alpha \in \mathbb{R}^+$
  - Bethe free energy $F_{\text{Bethe}} = \sum_{(n,m)\in\mathcal{E}} \sum_{x_n,x_m} b_{n,m}(x_n, x_m) \log\left(\frac{b_{n,m}(x_n,x_m)}{\psi_n(x_n)\psi_{n,m}(x_n,x_m)\psi_m(x_m)}\right)$

$$- \sum_{n=1}^{N} (|\mathcal{X}_n| - 1) \sum_{x_n} b_n(x_n) \log\left(\frac{b_n(x_n)}{\psi_n(x_n)}\right)$$

  - **Bethe consistency distance** (*proposed*)

$$\mathcal{L}_{\mathbb{L}} := D_{\text{KL}}\left(\sum_{x_m} b_{n,m}(x_n, x_m) \middle\| b_n(x_n)\right) + D_{\text{KL}}\left(\sum_{x_n} b_{n,m}(x_n, x_m) \middle\| b_m(x_m)\right)$$

Experiment: 2×2 Ising Model

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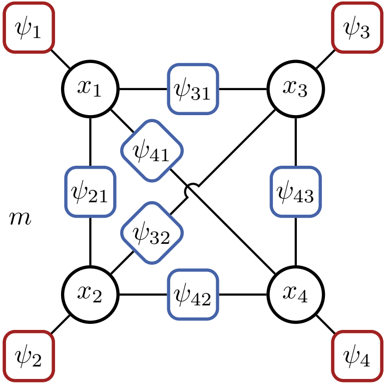
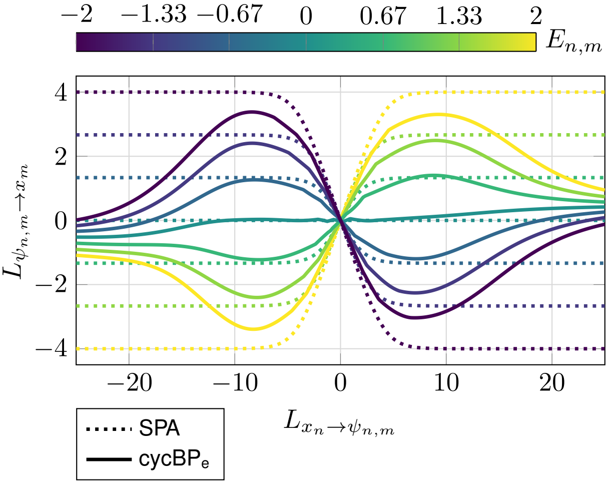
- $N = 4$ binary variables $x_n \in \{+1, -1\}$
  - Use log-likelihood ratios $L_{\psi_{nm}\to x_n} := \log\left(\frac{m_{\psi_{nm}\to x_n}(x_n=+1)}{m_{\psi_{nm}\to x_n}(x_n=-1)}\right)$
- $\psi_n(x_n) = \exp(\theta_n x_n)$ with **local fields θ_n**, $n = 1, \dots, N$
- $\psi_{n,m}(x_n, x_m) = \exp(E_{n,m} x_n x_m)$ with **local couplings $E_{n,m}$**, $n > m$
- **Spin glass**: θ_n and $E_{n,m}$ independently sampled from $\mathcal{U}[-2, +2]$
  - **Frustrated system**, e.g., for $E_{n,m} \ll 0, \forall n, m$



Experiment: 2×2 Ising Model

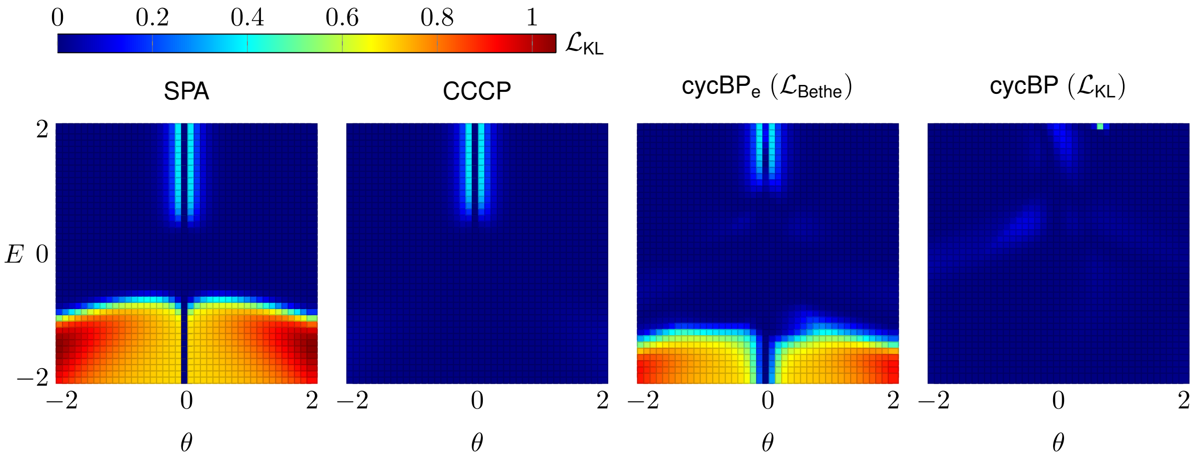
- **Training** and **evaluation** (averaged over 10^5 graphs) on samples of the Ising spin glass model

Algo.	Loss	$\mathcal{L}_{\text{KL}}$	$\mathcal{L}_{\mathbb{L}}$
SPA	-	0.087	0.30
CCCP	-	0.044	$2 \cdot 10^{-6}$
cycBP_e	$\mathcal{L}_{\text{KL}}$	0.040	0.17
cycBP_e	$\mathcal{L}_{\text{Bethe}}$	0.030	0.11
cycBP	$\mathcal{L}_{\text{KL}}$	0.014	0.48
cycBP	$\mathcal{L}_{\text{Bethe}}$	0.027	0.027



Experiment: 2×2 Ising Model

- **Training** on samples of the Ising spin glass model (as before)
- **Evaluate generalization capability** on graphs with constant parameters $E_{nm} = E$ and $\theta_n = \theta$



Conclusion & Outlook

- Alternative message update rules exist which perform especially well on cyclic graphs where the SPA fails
- **Extrinsic principle loses its objective** on graphs with many short cycles
- **Regularized Bethe free energy $\mathcal{L}_{\text{Bethe}}$** as novel objective function for unsupervised training
- Results for **symbol detection** as a practical application → **Poster session!**

- Investigate optimal message update rules for larger graphs and different topologies
- Replace NN by simple parametric function
- Make update rules a function of the node degree, the iteration number, . . .

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