New Generalizations of the Bethe Approximation via Asymptotic Expansion

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35th Symposium of Information Theory and Its Application
Beppu, Oita, Japan

13 December 2012

The Bethe approximation

- Successful approximation for low-density parity-check codes, compressed sensing, etc.
- Efficient message passing algorithm belief propagation (BP).
- A fixed point of BP is a stationary point of the Bethe free energy [Yedidia et al. 2005].

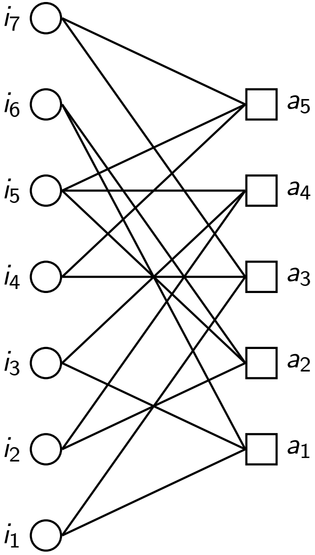
Factor graph and partition function

For a factor graph G.

- V: the set of variable nodes
- F: the set of factor nodes
- $\mathcal{X}$: the alphabet set
- N: the number of variables
- d_o: the degree of a node for $o \in V \cup F$
- f_a: a non-negative function in $\mathcal{X}^{d_a} \to \mathbb{R}_{\geq 0}$.

$$p(\mathbf{x}; G) := \frac{1}{Z(G)} \prod_{a \in F} f_a(\mathbf{x}_{\partial a})$$

$$Z(G) := \sum_{\mathbf{x} \in \mathcal{X}^N} \prod_{a \in F} f_a(\mathbf{x}_{\partial a})$$



The Legendre transformation

$$-\log Z(G) = \inf_{q \in \mathcal{P}(\mathcal{X}^N)} \left\{ -\sum_{\mathbf{x} \in \mathcal{X}^N} q(\mathbf{x}) \log \prod_{a \in F} f_a(\mathbf{x}_{\partial a}) - H(q) \right\}$$

where $H(q)$ is the Shannon entropy.

$\log Z(G)$ and $-H(q)$ are dual in the sense of Legendre transformation.

$$\log Z(G) \longleftrightarrow -H(q)$$

The Bethe free energy

$$-\log Z(G) = \inf_{q \in \mathcal{P}(\mathcal{X}^N)} \left\{ -\sum_{\mathbf{x} \in \mathcal{X}^N} q(\mathbf{x}) \log \prod_{a \in F} f_a(\mathbf{x}_{\partial a}) - H(q) \right\}$$

$$\begin{aligned} -\log Z_{\mathrm{Bethe}}(G) = \inf_{(b_i \in \mathcal{P}(\mathcal{X}))_{i \in V}, (b_a \in \mathcal{P}(\mathcal{X}^{d_a}))_{a \in F}} \Bigg\{ \\ -\sum_{a \in F} \sum_{\mathbf{x} \in \mathcal{X}^{d_a}} b_a(\mathbf{x}_{\partial a}) \log f_a(\mathbf{x}_{\partial a}) - H_{\mathrm{Bethe}}((b_i)_{i \in V}, (b_a)_{a \in F}) \Bigg\} \end{aligned}$$

where

$$H_{\mathrm{Bethe}}((b_i)_{i \in V}, (b_a)_{a \in F}) := \sum_{a \in F} H(b_a) - \sum_{i \in V} (d_i - 1) H(b_i).$$

Charactrizations of the Bethe free energy

- Loop calculus [Chertkov and Chernyak 2006, 2007]

$$Z(G) = Z_{\mathrm{Bethe}} \left(1 + \sum_{C:\,\text{generalized loop}} r(C) \right).$$

$\longrightarrow$ generalized to non-binary alphabet [This work]

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- Method of graph cover [Vontobel 2010]

$$\frac{1}{M} \log \langle Z_{\Sigma_M} \rangle \to \log Z_{\mathrm{Bethe}}$$

$\longrightarrow$ generalized to the second-order analysis [This work]

Loop calculus for the binary alphabet

Lemma (Chertkov and Chernyak 2006, Sudderth et al., 2008)

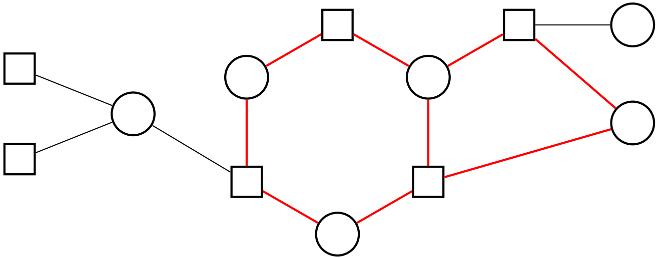
Assume that the alphabet is binary, i.e., $\mathcal{X} = \{0, 1\}$*. Let* $\eta_i := \langle X_i \rangle_{b_i} = b_i(1)$*. For any stationary point* $((b_i), (b_a))$ *of the Bethe free energy,*

$$Z(G) = Z_{\text{Bethe}}((b_i)_{i \in V}, (b_a)_{a \in F}) \sum_{E' \subseteq E} \mathcal{Z}(E')$$

where

$$\mathcal{Z}(E') := \prod_{i \in V} \left\langle \left(\frac{X_i - \eta_i}{\sqrt{\langle (X_i - \eta_i)^2 \rangle_{b_i}}} \right)^{d_i(E')} \right\rangle_{b_i} \cdot \prod_{a \in F} \left\langle \prod_{i \in \partial a,\, (i,a) \in E'} \frac{X_i - \eta_i}{\sqrt{\langle (X_i - \eta_i)^2 \rangle_{b_i}}} \right\rangle_{b_a} .$$

Generalized loop



$$\mathcal{G} := \{E' \subseteq E \mid d_o(E') \neq 1 \text{ for } o \in V \cup F\}$$

$$Z(G) = Z_{\mathrm{Bethe}}((b_i)_{i\in V}, (b_a)_{a\in F}) \left(1 + \sum_{E' \in \mathcal{G}\setminus\{\varnothing\}} \mathscr{Z}(E')\right).$$

Loop calculus for a non-binary alphabet 1/2

Theorem (This work)

For any stationary point $((b_i),(b_a))$ *of the Bethe free energy,*

$$Z(G) = Z_{\mathrm{Bethe}}((b_i)_{i \in V}, (b_a)_{a \in F}) \sum_{E' \subseteq E} \mathcal{Z}(E')$$

where

$$\mathcal{Z}(E') := \sum_{\mathbf{y} \in (\mathcal{X} \setminus \{0\})^{|E'|}} \prod_{i \in V} \left\langle \prod_{a \in \partial i, (i,a) \in E'} \frac{\partial \log b_i(X_i)}{\partial \eta_{i, y_{i,a}}} \right\rangle_{b_i} \cdot \prod_{a \in F} \left\langle \prod_{i \in \partial a, (i,a) \in E'} \frac{\partial \log b_i(X_i)}{\partial \theta_{i, y_{i,a}}} \right\rangle_{b_a}.$$

Coordinate systems the natural parameters $(\theta_{i,y})_{y \in \mathcal{X} \setminus \{0\}}$ and the expectation parameters $(\eta_{i,y})_{y \in \mathcal{X} \setminus \{0\}}$.

Loop calculus for a non-binary alphabet 2/2

The Jacobian matrix $\frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{\eta}}$ is the Fisher information matrix.

Theorem (This work)

If one chooses a sufficient statistic $\mathbf{t}_i(x_i)$ for $i \in V$ such that the Fisher information matrix is diagonal at b_i, it holds

$$\mathcal{Z}(E') = \sum_{\mathbf{y} \in (\mathcal{X} \setminus \{0\})^{|E'|}} \prod_{i \in V} \left\langle \prod_{a \in \partial i, (i,a) \in E'} \frac{t_{i,y_{i,a}}(X_i) - \eta_{i,y_{i,a}}}{\sqrt{\left\langle \left(t_{i,y_{i,a}}(X_i) - \eta_{i,y_{i,a}} \right)^2 \right\rangle_{b_i}}} \right\rangle_{b_i}$$

$$\cdot \prod_{a \in F} \left\langle \prod_{i \in \partial a, (i,a) \in E'} \frac{t_{i,y_{i,a}}(X_i) - \eta_{i,y_{i,a}}}{\sqrt{\left\langle \left(t_{i,y_{i,a}}(X_i) - \eta_{i,y_{i,a}} \right)^2 \right\rangle_{b_i}}} \right\rangle_{b_a}.$$

Acknowledgment: P. Vontobel for insightful discussion about normal factor graph.

Loop calculus for expectations

Theorem (This work; it can be simplified like the previous theorem)

Let $C \subseteq V$, $F_C := \{a \in F \mid \partial a \subseteq C\}$ and $g : \mathcal{X}^{|C|} \to \mathbb{R}$. For any $((b_i),(b_a)) \in \mathcal{A}$, it holds

$$Z\langle g(\mathbf{X}_C)\rangle_p = Z_{\text{Bethe}}((b_i)_{i\in V},(b_a)_{a\in F}) \sum_{E' \subseteq E \setminus E(F_C)} \mathcal{Z}(E')$$

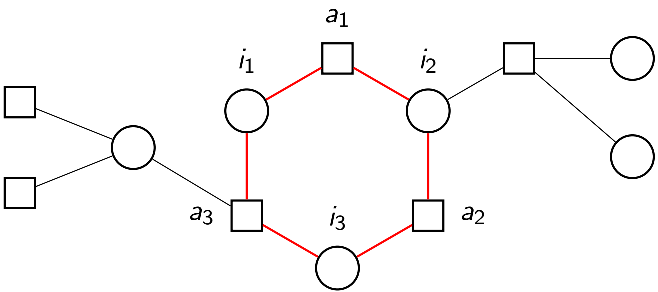
where

$$\mathcal{Z}(E') := \sum_{\mathbf{y}\in(\mathcal{X}\setminus\{0\})^{|E'|}} \prod_{i\in V\setminus C} \left\langle \prod_{a\in\partial i,(i,a)\in E'} \frac{\partial \log b_i(X_i)}{\partial \eta_{i,y_{i,a}}} \right\rangle_{b_i} \prod_{a\in F\setminus F_C} \left\langle \prod_{i\in\partial a,(i,a)\in E'} \frac{\partial \log b_i(X_i)}{\partial \theta_{i,y_{i,a}}} \right\rangle_{b_a} \cdot \left\langle g(\mathbf{X}_C) \prod_{i\in C,(i,a)\in E'} \frac{\partial \log b_i(X_i)}{\partial \eta_{i,y_{i,a}}} \right\rangle_{b_C}.$$

Here, $\langle\cdot\rangle_{b_C}$ is a pseudo expectation with respect to

$$b_C(\mathbf{x}_C) = \prod_{i\in C} b_i(x_i) \prod_{a\in F_C} \frac{b_a(\mathbf{x}_{\partial a})}{\prod_{i\in\partial a} b_i(x_i)}.$$

Loop calculus for single-cycle graph

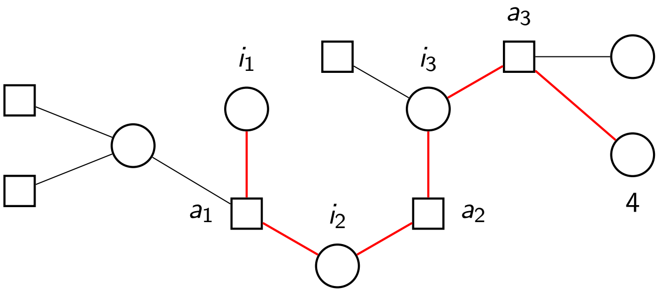


$$\mathrm{Cor}_{b_{a_k}}[\mathbf{t}_{i_k}(X_i), \mathbf{t}_{i_{k+1}}(X_{i_{k+1}})]$$
$$:= \mathrm{Var}_{b_k}[\mathbf{t}_{i_k}(X_{i_k})]^{-\frac{1}{2}} \mathrm{Cov}_{b_{a_k}}[\mathbf{t}_{i_k}(X_{i_k}), \mathbf{t}_{i_{k+1}}(X_{i_{k+1}})] \mathrm{Var}_{b_{k+1}}[\mathbf{t}_{i_{k+1}}(X_{i_{k+1}})]^{-\frac{1}{2}}.$$

Corollary (Partition function of single-cycle factor graph)

$$Z(G) = Z_{\mathrm{Bethe}}((b_i)_{i \in V}, (b_a)_{a \in F})$$
$$\cdot \left(1 + \mathrm{tr}\left(\mathrm{Cor}_{b_{a_1}}[\mathbf{t}_{i_1}(X_{i_1}), \mathbf{t}_{i_2}(X_{i_2})] \mathrm{Cor}_{b_{a_2}}[\mathbf{t}_{i_2}(X_{i_2}), \mathbf{t}_{i_3}(X_{i_3})] \cdots \mathrm{Cor}_{b_{a_n}}[\mathbf{t}_{i_n}(X_{i_n}), \mathbf{t}_{i_1}(X_{i_1})]\right)\right).$$

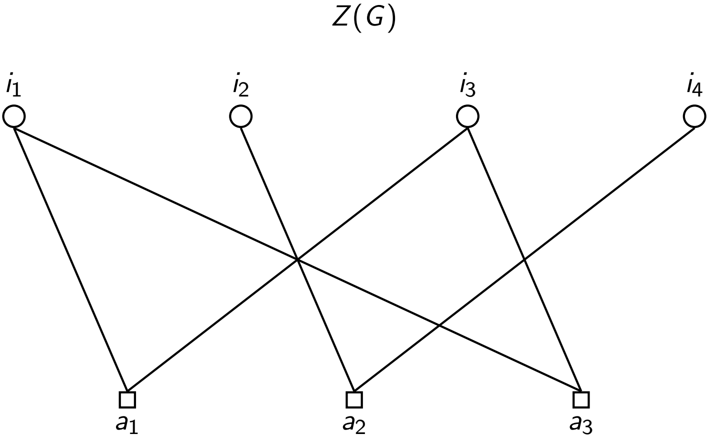
Correlation matrix on a tree factor graph



Corollary (Correlation matrix on a tree factor graph; Watanabe 2010)

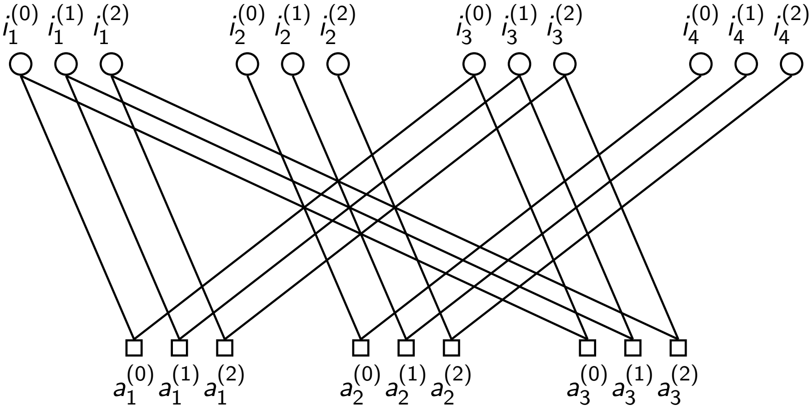
$$\mathrm{Cor}_p[X_1, X_n] \\ = \mathrm{Cor}_p[\mathbf{t}_1(X_1), \mathbf{t}_2(X_2)]\mathrm{Cor}_p[\mathbf{t}_2(X_2), \mathbf{t}_3(X_3)] \cdots \mathrm{Cor}_p[\mathbf{t}_{n-1}(X_{n-1}), \mathbf{t}_n(X_n)]$$

Graph cover



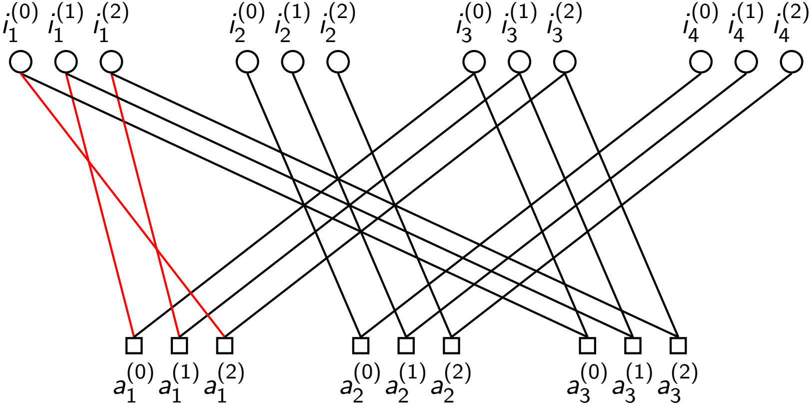
Graph cover

$Z(G)^M$



Graph cover

$$Z(G_{\boldsymbol{\sigma}}) \overset{?}{\approx} Z(G)^M$$



The method of graph cover

Lemma (Vontobel 2010)

$$\log\langle Z_{\Sigma_M}\rangle = M \log Z_{\text{Bethe}} + o(M)$$

Sketch of the proof.
The method of types and Laplace method. □

The second-order analysis for graph cover

Lemma (This work)

$$\log\langle Z_{\Sigma_M}\rangle = M \log Z_{\text{Bethe}} + \log \sqrt{\zeta(\mathbf{u})} + o(1)$$

where $\zeta(\mathbf{u})$ *is the edge zeta function and*
$u^a_{i\to j} = \mathrm{Cor}_{b_a}[\mathbf{t}_i(X_i), \mathbf{t}_j(X_j)]$.

Sketch of the proof.

Laplace method with the central approximation. □

Interpretation of Legendre transformation by large deviation

$$\log Z(G) = \frac{1}{M} \log Z(G)^M = \lim_{M\to\infty} \frac{1}{M} \log Z(G)^M$$
$$= -\inf_{p \in \mathcal{P}(\mathcal{X}^N)} \left\{ -\sum_{\mathbf{x}\in\mathcal{X}^N} p(\mathbf{x}) \log \prod_{a\in F} f_a(\mathbf{x}_{\partial a}) - H(p) \right\}$$

From more detailed analysis (asymptotic expansion)

$$\log Z(G)^M = M \log Z(G) + \underbrace{\log \sqrt{\frac{\det\left(\mathcal{J}(\boldsymbol{\theta})\right)}{\prod_{\mathbf{x}} p(\mathbf{x})}}}_{=0} + \frac{1}{M}0 + \frac{1}{M^2}0 + \cdots$$

Asymptotic expansion and asymptotic Bethe approximation

$$\log Z(G)^{M} = M \log Z(G) + \underbrace{\log \sqrt{\frac{\det(\mathcal{J}(\boldsymbol{\theta}))}{\prod_{\mathbf{x}} p(\mathbf{x})}}}_{=0} + \frac{1}{M} 0 + \frac{1}{M^2} 0 + \cdots$$

$$\log\langle Z_{\Sigma_M}\rangle = M \log Z_{\text{Bethe}} + \underbrace{\log \sqrt{\frac{\det(\nabla F_{\text{Bethe}})^{-1}}{\prod_i \prod_{x_i} b_i(x_i)^{1-d_i} \prod_{a\in F} \prod_{\mathbf{x}_{\partial a}} b_a(\mathbf{x}_{\partial a})}}}_{=\log\sqrt{\zeta(\mathbf{u})}}$$

[Watanabe and Fukumizu 2010]

$$+ \frac{1}{M} g_1 + \frac{1}{M^2} g_2 + \cdots .$$

By letting $M = 1$,

Definition (Asymptotic Bethe approximation)

For $m = 1, 2, \ldots,$

$$\log Z_{\text{AB}}^{(m)} := \log Z_{\text{Bethe}} + \log\sqrt{\zeta(\mathbf{u})} + g_1 + g_2 + \cdots + g_{m-1}.$$

Edge zeta function

Definition (Prime cycle)

A closed walk $e_1 \rightharpoonup e_2 \cdots \rightharpoonup e_n \rightharpoonup e_1$ is a prime cycle $\iff$ it is backtrackless and cannot be expressed as power of another walk.

Definition (Edge zeta function)

$$\zeta(\mathbf{u}) = \prod_{\substack{(e_1 \rightharpoonup e_2 \cdots \rightharpoonup e_n \rightharpoonup e_1) \\ \text{is a prime cycle}}} \frac{1}{\det\left(I - u_{e_1,e_2} u_{e_2,e_3} \cdots u_{e_n,e_1}\right)}.$$

Lemma (Watanabe-Fukumizu formula; 2010)

$$\zeta(\mathbf{u})^{-1} = \det(\nabla^2 F_{\text{Bethe}}((\eta_i), (\eta_{\langle a \rangle}))) \cdot \prod_{i \in V} \det(\mathrm{Var}_{b_i}[\mathbf{t}_i(X_i)])^{1-d_i} \prod_{a \in F} \det(\mathrm{Var}_{b_a}[\mathbf{t}_a(X_{\partial a})])$$

where $u^a_{i \to j} = \mathrm{Cor}_{b_a}[\mathbf{t}_i(X_i), \mathbf{t}_j(X_j)]$.

Single-cycle graph

Let

$$A := \mathrm{Cor}_{b_{a_1}}[\mathbf{t}_{i_1}(X_{i_1}), \mathbf{t}_{i_2}(X_{i_2})]\mathrm{Cor}_{b_{a_2}}[\mathbf{t}_{i_2}(X_{i_2}), \mathbf{t}_{i_3}(X_{i_3})] \cdots \mathrm{Cor}_{b_{a_n}}[\mathbf{t}_{i_n}(X_{i_n}), \mathbf{t}_{i_1}(X_{i_1})]$$

Then, the true partition function Z and the asymptotic Bethe approximation $Z^{(1)}_{\mathrm{AB}}$ are

$$Z = Z_{\mathrm{Bethe}}((b_i)_{i\in V}, (b_a)_{a\in F})\left(1 + \mathrm{tr}(A)\right).$$

$$Z^{(1)}_{\mathrm{AB}} = Z_{\mathrm{Bethe}}((b_i)_{i\in V}, (b_a)_{a\in F})\frac{1}{\det(I - A)}.$$

$$= Z_{\mathrm{Bethe}}((b_i)_{i\in V}, (b_a)_{a\in F})\left(1 + \mathrm{tr}(A) + O(\rho(A)^2)\right)$$

where $\rho(A)$ is the spectrum radius of A.

The asymptotic Bethe approximation is accurate when $A \approx 0$.

General factor graph

$$Z(G) = Z_{\mathrm{Bethe}}((b_i)_{i \in V}, (b_a)_{a \in F}) \sum_{E' \in \mathcal{G}} \mathcal{Z}(E')$$

Generalized loop

$$\mathcal{G} := \{E' \subseteq E \mid d_o(E') \neq 1 \text{ for } o \in V \cup F\}$$

(Simple) loop [Gomez et al. 2006], [Chertkov and Chernyak 2007]

$$\mathcal{L} := \{E' \subseteq E \mid d_o(E') = 0, 2 \text{ for } o \in V \cup F, \textit{connected}\}$$

For $E' \in \mathcal{L}$

$$\mathcal{Z}(E') = \mathrm{tr}(A).$$

Roughly speaking, $Z_{\mathrm{AB}}^{(m)}$ enumerates the weights of $Z(E')$ for $E' \in \mathcal{L}$.

Numerical calculation: Ising model

$$Z = \sum_{\mathbf{x} \in \{+1,-1\}^N} \exp\left\{ \beta \left(\sum_{(i,j) \in E} x_i x_j + h \sum_{i=1}^{N} x_i \right) \right\}$$

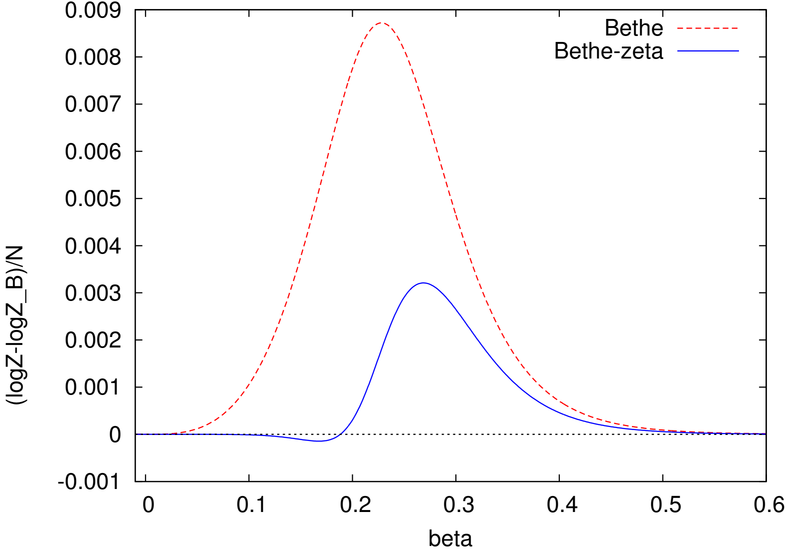
For a locally tree-like graph, if $\beta \geq 0$,
the Bethe approximation is asymptotically exact, i.e.,

$$\lim_{N \to \infty} \frac{1}{N} \log Z = \lim_{N \to \infty} \frac{1}{N} \log Z_{\text{Bethe}}$$

[Dembo and Montanari 2010].

$$|\mathrm{Cor}_{b_a}(X_i, X_j)| \leq \tanh(|\beta|) \ .$$

Results of numerical calculation: Ising model



$N = 16,\ d_{avg} = 4.375,\ h = 0.5.$

Summary and future works

Summary:

- Chertkov and Chernyak's loop calculus is generalized to non-binary alphabets by using tangent vectors for information manifold of exponential family.
- New generalization of the Bethe free energy is obtained by Vontobel's method of graph cover and Watanabe-Fukumizu formula.

Future works about asymptotic Bethe approximation:

- Rigorous proof of the accuracy for sparse factor graphs.
- Higher order approximations.
- Relationship with the Plefka expansion.