Graph Zeta Function in the Bethe Free Energy and Loopy Belief Propagation

Yusuke Watanabe
The Institute of Statistical Mathematics
10-3 Midori-cho, Tachikawa
Tokyo 190-8562, Japan
wataymath@ism.ac.jp

Kenji Fukumizu
The Institute of Statistical Mathematics
10-3 Midori-cho, Tachikawa
Tokyo 190-8562, Japan
fukumizu@ism.ac.jp

Abstract

We propose a new approach to the analysis of Loopy Belief Propagation (LBP) by establishing a formula that connects the Hessian of the Bethe free energy with the edge zeta function. The formula has a number of theoretical implications on LBP. It is applied to give a sufficient condition that the Hessian of the Bethe free energy is positive definite, which shows non-convexity for graphs with multiple cycles. The formula clarifies the relation between the local stability of a fixed point of LBP and local minima of the Bethe free energy. We also propose a new approach to the uniqueness of LBP fixed point, and show various conditions of uniqueness.

1 Introduction

Pearl's belief propagation [1] provides an efficient method for exact computation in the inference with probabilistic models associated to trees. As an extension to general graphs allowing cycles, Loopy Belief Propagation (LBP) algorithm [2] has been proposed, showing successful performance in various problems such as computer vision and error correcting codes.

One of the interesting theoretical aspects of LBP is its connection with the Bethe free energy [3]. It is known, for example, the fixed points of LBP correspond to the stationary points of the Bethe free energy. Nonetheless, many of the properties of LBP such as exactness, convergence and stability are still unclear, and further theoretical understanding is needed.

This paper theoretically analyzes LBP by establishing a formula asserting that the determinant of the Hessian of the Bethe free energy equals the reciprocal of the edge zeta function up to a positive factor. This formula derives a variety of results on the properties of LBP such as stability and uniqueness, since the zeta function has a direct link with the dynamics of LBP as we show.

The first application of the formula is the condition for the positive definiteness of the Hessian of the Bethe free energy. The Bethe free energy is not necessarily convex, which causes unfavorable behaviors of LBP such as oscillation and multiple fixed points. Thus, clarifying the region where the Hessian is positive definite is an importance problem. Unlike the previous approaches which consider the global structure of the Bethe free energy such as [4, 5], we focus the local structure. Namely, we provide a simple sufficient condition that determines the positive definite region: if all the correlation coefficients of the pseudomarginals are smaller than a value given by a characteristic of the graph, the Hessian is positive definite. Additionally, we show that the Hessian always has a negative eigenvalue around the boundary of the domain if the graph has at least two cycles.

Second, we clarify a relation between the local stability of a LBP fixed point and the local structure of the Bethe free energy. Such a relation is not necessarily obvious, since LBP is not the gradient descent of the Bethe free energy. In this line of studies, Heskes [6] shows that a locally stable fixed point of LBP is a local minimum of the Bethe free energy. It is thus interesting to ask which local minima of the Bethe free energy are stable or unstable fixed points of LBP. We answer this question by elucidating the conditions of the local stability of LBP and the positive definiteness of the Bethe free energy in terms of the eigenvalues of a matrix, which appears in the graph zeta function.

Finally, we discuss the uniqueness of LBP fixed point by developing a differential topological result on the Bethe free energy. The result shows that the determinant of the Hessian at the fixed points, which appears in the formula of zeta function, must satisfy a strong constraint. As a consequence, in addition to the known result on the one-cycle case, we show that the LBP fixed point is unique for any unattractive connected graph with two cycles without restricting the strength of interactions.

2 Loopy belief propagation algorithm and the Bethe free energy

Throughout this paper, $G = (V, E)$ is a connected undirected graph with V the vertices and E the undirected edges. The cardinality of V and E are denoted by N and M respectively.

In this article we focus on binary variables, *i.e.*, $x_i \in \{\pm 1\}$. Suppose that the probability distribution over the set of variables $\boldsymbol{x} = (x_i)_{i \in V}$ is given by the following factorization form with respect to G:

$$p(\boldsymbol{x}) = \frac{1}{Z} \prod_{ij \in E} \psi_{ij}(x_i, x_j) \prod_{i \in V} \psi_i(x_i), \tag{1}$$

where Z is a normalization constant and ψ_{ij} and ψ_i are positive functions given by $\psi_{ij}(x_i, x_j) = \exp(J_{ij} x_i x_j)$ and $\psi_i(x_i) = \exp(h_i x_i)$ without loss of generality.

In various applications, the computation of marginal distributions $p_i(x_i) := \sum_{\boldsymbol{x} \backslash \{x_i\}} p(\boldsymbol{x})$ and $p_{ij}(x_i, x_j) := \sum_{\boldsymbol{x} \backslash \{x_i x_j\}} p(\boldsymbol{x})$ is required though the exact computation is intractable for large graphs. If the graph is a tree, they are efficiently computed by Pearl's belief propagation algorithm [1]. Even if the graph has cycles, it is empirically known that the direct application of this algorithm, called Loopy Belief Propagation (LBP), often gives good approximation.

LBP is a message passing algorithm. For each directed edge, a message vector $\mu_{i \to j}(x_j)$ is assigned and initialized arbitrarily. The update rule of messages is given by

$$\mu_{i \to j}^{\text{new}}(x_j) \propto \sum_{x_i} \psi_{ji}(x_j, x_i) \psi_i(x_i) \prod_{k \in N_i \backslash j} \mu_{k \to i}(x_i), \tag{2}$$

where N_i is the neighborhood of $i \in V$. The order of edges in the update is arbitrary. In this paper we consider *parallel update*, that is, all edges are updated simultaneously. If the messages converge to a fixed point $\{\mu_{i \to j}^{\infty}\}$, the approximations of $p_i(x_i)$ and $p_{ij}(x_i, x_j)$ are calculated by the beliefs,

$$b_i(x_i) \propto \psi_i(x_i) \prod_{k \in N_i} \mu_{k \to i}^{\infty}(x_i), \quad b_{ij}(x_i, x_j) \propto \psi_{ij}(x_i, x_j) \psi_i(x_i) \psi_j(x_j) \prod_{k \in N_i \backslash j} \mu_{k \to i}^{\infty}(x_i) \prod_{k \in N_j \backslash i} \mu_{k \to j}^{\infty}(x_j), \tag{3}$$

with normalization $\sum_{x_i} b_i(x_i) = 1$ and $\sum_{x_i, x_j} b_{ij}(x_i, x_j) = 1$. From (2) and (3), the constraints $b_{ij}(x_i, x_j) > 0$ and $\sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i)$ are automatically satisfied.

We introduce the Bethe free energy as a tractable approximation of the Gibbs free energy. The exact distribution (1) is characterized by a variational problem $p(\boldsymbol{x}) = \operatorname{argmin}_{\hat{p}} F_{Gibbs}(\hat{p})$, where the minimum is taken over all probability distributions on $(x_i)_{i \in V}$ and $F_{Gibbs}(\hat{p})$ is the *Gibbs free energy* defined by $F_{Gibbs}(\hat{p}) = KL(\hat{p}||p) - \log Z$. Here $KL(\hat{p}||p) = \int \hat{p} \log(\hat{p}/p)$ is the Kullback-Leibler divergence from $\hat{p}$ to p. Note that $F_{Gibbs}(\hat{p})$ is a convex function of $\hat{p}$.

In the Bethe approximation, we confine the above minimization to the distribution of the form $b(\boldsymbol{x}) \propto \prod_{ij \in E} b_{ij}(x_i, x_j) \prod_{i \in V} b_i(x_i)^{1 - d_i}$, where $d_i := |N_i|$ is the degree and the constraints $b_{ij}(x_i, x_j) > 0$, $\sum_{x_i, x_j} b_{ij}(x_i, x_j) = 1$ and $\sum_{x_j} b_{ij}(x_i, x_j) = b_i(x_i)$ are satisfied. A set $\{b_i(x_i), b_{ij}(x_i, x_j)\}$ satisfying these constraints is called *pseudomarginals*. For computational tractability, we modify the Gibbs free energy to the objective function called *Bethe free energy*:

$$\begin{aligned} F(b) := &- \sum_{ij \in E} \sum_{x_i x_j} b_{ij}(x_i, x_j) \log \psi_{ij}(x_i, x_j) - \sum_{i \in V} \sum_{x_i} b_i(x_i) \log \psi_i(x_i) \\ &+ \sum_{ij \in E} \sum_{x_i x_j} b_{ij}(x_i, x_j) \log b_{ij}(x_i, x_j) + \sum_{i \in V} (1 - d_i) \sum_{x_i} b_i(x_i) \log b_i(x_i). \end{aligned} \tag{4}$$

The domain of the objective function F is the set of pseudomarginals. The function F does not necessarily have a unique minimum. The outcome of this modified variational problem is the same as that of LBP [3]. To put it more precisely, There is a one-to-one correspondence between the set of stationary points of the Bethe free energy and the set of fixed points of LBP.

It is more convenient if we work with minimal parameters, mean $m_i = \mathrm{E}_{b_i}[x_i]$ and correlation $\chi_{ij} = \mathrm{E}_{b_{ij}}[x_i x_j]$. Then we have an effective parametrization of pseudomarginals:

$$b_{ij}(x_i, x_j) = \frac{1}{4}(1 + m_i x_i + m_j x_j + \chi_{ij} x_i x_j), \qquad b_i(x_i) = \frac{1}{2}(1 + m_i). \tag{5}$$

The Bethe free energy (4) is rewritten as

$$F(\{m_i, \chi_{ij}\}) = -\sum_{ij \in E} J_{ij}\chi_{ij} - \sum_{i \in V} h_i m_i$$
$$+ \sum_{ij \in E} \sum_{x_i x_j} \eta\Big(\frac{1 + m_i x_i + m_j x_j + \chi_{ij} x_i x_j}{4}\Big) + \sum_{i \in V}(1 - d_i) \sum_{x_i} \eta\Big(\frac{1 + m_i x_i}{2}\Big), \tag{6}$$

where $\eta(x) := x \log x$. The domain of F is written as

$$L(G) := \Big\{\{m_i, \chi_{ij}\} \in \mathbb{R}^{N+M} | 1 + m_i x_i + m_j x_j + \chi_{ij} x_i x_j > 0 \text{ for all } ij \in E \text{ and } x_i, x_j = \pm 1\Big\}.$$

The Hessian of F, which consists of the second derivatives with respect to $\{m_i, \chi_{ij}\}$, is a square matrix of size $N + M$ and denoted by $\nabla^2 F$. This is considered to be a matrix-valued function on $L(G)$. Note that, from (6), $\nabla^2 F$ does not depend on J_{ij} and h_i.

3 Zeta function and Hessian of Bethe free energy

3.1 Zeta function and Ihara's formula

For each undirected edge of G, we make a pair of oppositely directed edges, which form a set of *directed edges* $\vec{E}$. Thus $|\vec{E}| = 2M$. For each directed edge $e \in \vec{E}$, $o(e) \in V$ is the *origin* of e and $t(e) \in V$ is the *terminus* of e. For $e \in \vec{E}$, the *inverse edge* is denoted by $\bar{e}$, and the corresponding undirected edge by $[e] = [\bar{e}] \in E$.

A *closed geodesic* in G is a sequence $(e_1, \ldots, e_k)$ of directed edges such that $t(e_i) = o(e_{i+1})$ and $e_i \neq \bar{e}_{i+1}$ for $i \in \mathbb{Z}/k\mathbb{Z}$. Two closed geodesics are said to be *equivalent* if one is obtained by cyclic permutation of the other. An equivalent class of closed geodesics is called a *prime cycle* if it is not a repeated concatenation of a shorter closed geodesic. Let P be the set of prime cycles of G. For given weights $\boldsymbol{u} = (u_e)_{e \in \vec{E}}$, the *edge zeta function* [7, 8] is defined by

$$\zeta_G(\boldsymbol{u}) := \prod_{\mathfrak{p} \in P} (1 - g(\mathfrak{p}))^{-1}, \quad g(\mathfrak{p}) := u_{e_1} \cdots u_{e_k} \quad \text{for } \mathfrak{p} = (e_1, \ldots, e_k),$$

where $u_e \in \mathbb{C}$ is assumed to be sufficiently small for convergence. This is an analogue of the Riemann zeta function which is represented by the product over all the prime numbers.

Example 1. If G is a tree, which has no prime cycles, $\zeta_G(\boldsymbol{u}) = 1$. For 1-cycle graph C_N of length N, the prime cycles are $(e_1, e_2, \ldots, e_N)$ and $(\bar{e}_N, \bar{e}_{N-1}, \ldots, \bar{e}_1)$, and thus $\zeta_{C_N}(\boldsymbol{u}) = (1 - \prod_{l=1}^N u_{e_l})^{-1}(1 - \prod_{l=1}^N u_{\bar{e}_l})^{-1}$. Except for these two types of graphs, the number of prime cycles is infinite.

It is known that the edge zeta function has the following simple determinant formula, which gives analytical continuation to the whole $\mathbb{C}^{2M}$. Let $C(\vec{E})$ be the set of functions on the directed edges. We define a matrix on $C(\vec{E})$, which is determined by the graph G, by

$$\mathcal{M}_{e,e'} := \begin{cases} 1 & \text{if } e \neq \bar{e'} \text{ and } o(e) = t(e'), \\ 0 & \text{otherwise.} \end{cases} \tag{7}$$

Theorem 1 ([8], Theorem 3)**.**

$$\zeta_G(\boldsymbol{u}) = \det(I - \mathcal{U}\mathcal{M})^{-1}, \tag{8}$$

where $\mathcal{U}$ is a diagonal matrix defined by $\mathcal{U}_{e,e'} := u_e \delta_{e,e'}$.

We need to show another determinant formula of the edge zeta function, which is used in the proof of theorem 3. We leave the proof of theorem 2 to the supplementary material.

Theorem 2 (Multivariable version of Ihara's formula)**.** *Let $C(V)$ be the set of functions on V. We define two linear operators on $C(V)$ by*

$$(\hat{\mathcal{D}}f)(i) := \Big(\sum_{\substack{e \in \vec{E} \\ t(e)=i}} \frac{u_e u_{\bar{e}}}{1-u_e u_{\bar{e}}} \Big) f(i), \quad (\hat{\mathcal{A}}f)(i) := \sum_{\substack{e \in \vec{E} \\ t(e)=i}} \frac{u_e}{1-u_e u_{\bar{e}}} f(o(e)), \quad \textit{where } f \in C(V). \tag{9}$$

Then we have

$$\Big(\zeta_G(\boldsymbol{u})^{-1} = \Big) \det(I - \mathcal{U}\mathcal{M}) = \det(I + \hat{\mathcal{D}} - \hat{\mathcal{A}}) \prod_{[e] \in E} (1 - u_e u_{\bar{e}}). \tag{10}$$

If we set $u_e = u$ for all $e \in \vec{E}$, the edge zeta function is called the *Ihara zeta function* [9] and denoted by $\zeta_G(u)$. In this single variable case, theorem 2 is reduced to Ihara's formula [10]:

$$\zeta_G(u)^{-1} = \det(I - u\mathcal{M}) = (1-u^2)^M \det(I + \frac{u^2}{1-u^2}\mathcal{D} - \frac{u}{1-u^2}\mathcal{A}), \tag{11}$$

where $\mathcal{D}$ is the *degree matrix* and $\mathcal{A}$ is the *adjacency matrix* defined by

$$(\mathcal{D}f)(i) := d_i f(i), \quad (\mathcal{A}f)(i) := \sum_{e \in \vec{E}, t(e)=i} f(o(e)), \quad f \in C(V).$$

3.2 Main formula

Theorem 3 (Main Formula)**.** *The following equality holds at any point of $L(G)$:*

$$\Big(\zeta_G(\boldsymbol{u})^{-1} = \Big) \det(I - \mathcal{U}\mathcal{M}) = \det(\nabla^2 F) \prod_{ij \in E} \prod_{x_i, x_j = \pm 1} b_{ij}(x_i, x_j) \prod_{i \in V} \prod_{x_i = \pm 1} b_i(x_i)^{1-d_i} \, 2^{2N+4M}, \tag{12}$$

where b_{ij} and b_i are given by (5) and

$$u_{i \to j} := \frac{\chi_{ij} - m_i m_j}{1 - m_j^2}. \tag{13}$$

Proof. (The detail of the computation is given in the supplementary material.)
From (6), it is easy to see that the (E,E)-block of the Hessian is a diagonal matrix given by

$$\frac{\partial^2 F}{\partial \chi_{ij} \partial \chi_{kl}} = \delta_{ij,kl} \frac{1}{4} \Big(\frac{1}{1+m_i+m_j+\chi_{ij}} + \frac{1}{1-m_i+m_j-\chi_{ij}} + \frac{1}{1+m_i-m_j-\chi_{ij}} + \frac{1}{1-m_i-m_j+\chi_{ij}} \Big).$$

Using this diagonal block, we erase (V,E)-block and (E,V)-block of the Hessian. In other words, we choose a square matrix X such that $\det X = 1$ and

$$X^T (\nabla^2 F) X = \begin{bmatrix} Y & 0 \\ 0 & \Big(\frac{\partial^2 F}{\partial \chi_{ij} \partial \chi_{kl}}\Big) \end{bmatrix}.$$

After the computation given in the supplementary material, we see that

$$(Y)_{i,j} = \begin{cases} \frac{1}{1-m_i^2} + \sum_{k \in N_i} \frac{(\chi_{ik} - m_i m_k)^2}{(1-m_i^2)(1-m_i^2-m_k^2+2m_i m_k \chi_{ik} - \chi_{ik}^2)} & \text{if } i = j, \\ -\mathcal{A}_{i,j} \frac{\chi_{ij} - m_i m_j}{1-m_i^2-m_j^2+2m_i m_j \chi_{ij} - \chi_{ij}^2} & \text{otherwise.} \end{cases} \tag{14}$$

From $u_{j \to i} = \frac{\chi_{ij} - m_i m_j}{1-m_i^2}$, it is easy to check that $I_N + \hat{\mathcal{D}} - \hat{\mathcal{A}} = YW$, where $\hat{\mathcal{A}}$ and $\hat{\mathcal{D}}$ is defined in (9) and W is a diagonal matrix defined by $W_{i,j} := \delta_{i,j}(1 - m_i^2)$. Therefore,

$$\det(I - \mathcal{U}\mathcal{M}) = \det(Y) \prod_{i \in V} (1 - m_i^2) \prod_{[e] \in E} (1 - u_e u_{\bar{e}}) = \text{ R.H.S. of (12)}$$

For the left equality, theorem 2 is used. □

Theorem 3 shows that the determinant of the Hessian of the Bethe free energy is essentially equal to $\det(I - \mathcal{U}\mathcal{M})$, the reciprocal of the edge zeta function. Since the matrix $\mathcal{U}\mathcal{M}$ has a direct connection with LBP as seen in section 5, the above formula derives many consequences shown in the rest of the paper.

4 Application to positive definiteness conditions

The convexity of the Bethe free energy is an important issue, as it guarantees uniqueness of the fixed point. Pakzad et al [11] and Heskes [5] derive sufficient conditions of convexity and show that the Bethe free energy is convex for trees and graphs with one cycle. In this section, instead of such global structure, we shall focus the local structure of the Bethe free energy as an application of the main formula.

For given square matrix X, $\mathrm{Spec}(X) \subset \mathbb{C}$ denotes the set of eigenvalues (spectra), and $\rho(X)$ the spectral radius of a matrix X, i.e., the maximum of the modulus of the eigenvalues.

Theorem 4. *Let $\mathcal{M}$ be the matrix given by (7). For given $\{m_i, \chi_{ij}\} \in L(G)$, $\mathcal{U}$ is defined by (13). Then,* $\quad \mathrm{Spec}(\mathcal{U}\mathcal{M}) \subset \mathbb{C} \setminus \mathbb{R}_{\geq 1} \quad \Longrightarrow \quad \nabla^2 F$ *is a positive definite matrix at $\{m_i, \chi_{ij}\}$.*

Proof. We define $m_i(t) := m_i$ and $\chi_{ij}(t) := t\chi_{ij} + (1-t)m_i m_j$. Then $\{m_i(t), \chi_{ij}(t)\} \in L(G)$ and $\{m_i(1), \chi_{ij}(1)\} = \{m_i, \chi_{ij}\}$. For $t \in [0,1]$, we define $\mathcal{U}(t)$ and $\nabla^2 F(t)$ in the same way by $\{m_i(t), \chi_{ij}(t)\}$. We see that $\mathcal{U}(t) = t\mathcal{U}$. Since $\mathrm{Spec}(\mathcal{U}\mathcal{M}) \subset \mathbb{C} \setminus \mathbb{R}_{\geq 1}$, we have $\det(I - t\mathcal{U}\mathcal{M}) \neq 0$ $^{\forall}t \in [0,1]$. From theorem 3, $\det(\nabla^2 F(t)) \neq 0$ holds on this interval. Using (14) and $\chi_{ij}(0) = m_i(0)m_j(0)$, we can check that $\nabla^2 F(0)$ is positive definite. Since the eigenvalues of $\nabla^2 F(t)$ are real and continuous with respect t, the eigenvalues of $\nabla^2 F(1)$ must be positive reals. □

We define the symmetrization of $u_{i\to j}$ and $u_{j \to i}$ by

$$\beta_{i\to j} = \beta_{j \to i} := \frac{\chi_{ij} - m_i m_j}{\{(1-m_i^2)(1-m_j^2)\}^{1/2}} = \frac{\mathrm{Cov}_{b_{ij}}[x_i, x_j]}{\{\mathrm{Var}_{b_i}[x_i]\mathrm{Var}_{b_j}[x_j]\}^{1/2}}. \tag{15}$$

Thus, $u_{i\to j}u_{j\to i} = \beta_{i\to j}\beta_{j\to i}$. Since $\beta_{i\to j} = \beta_{j\to i}$, we sometimes abbreviate $\beta_{i\to j}$ as β_{ij}. From the final expression, we see that $|\beta_{ij}| < 1$. Define diagonal matrices $\mathcal{Z}$ and $\mathcal{B}$ by $(\mathcal{Z})_{e,e'} := \delta_{e,e'}(1-m_{t(e)}^2)^{1/2}$ and $(\mathcal{B})_{e,e'} := \delta_{e,e'}\beta_e$ respectively. Then we have $\mathcal{Z}\mathcal{U}\mathcal{M}\mathcal{Z}^{-1} = \mathcal{B}\mathcal{M}$, because

$$(\mathcal{Z}\mathcal{U}\mathcal{M}\mathcal{Z}^{-1})_{e,e'} = (1-m_{t(e)}^2)^{1/2} u_e (\mathcal{M})_{e,e'} (1-m_{o(e)}^2)^{-1/2} = \beta_e(\mathcal{M})_{e,e'}.$$

Therefore $\mathrm{Spec}(\mathcal{U}\mathcal{M}) = \mathrm{Spec}(\mathcal{B}\mathcal{M})$.

The following corollary gives a more explicit condition of the region where the Hessian is positive definite in terms of the correlation coefficients of the pseudomarginals.

Corollary 1. *Let α be the Perron Frobenius eigenvalue of $\mathcal{M}$ and define $L_{\alpha^{-1}}(G) := \{\{m_i, \chi_{ij}\} \in L(G) | |\beta_e| < \alpha^{-1}$ for all $e \in \vec{E}\}$. Then, the Hessian $\nabla^2 F$ is positive definite on $L_{\alpha^{-1}}(G)$.*

Proof. Since $|\beta_e| < \alpha^{-1}$, we have $\rho(\mathcal{B}\mathcal{M}) < \rho(\alpha^{-1}\mathcal{M}) = 1$ ([12] Theorem 8.1.18). Therefore $\mathrm{Spec}(\mathcal{B}\mathcal{M}) \cap \mathbb{R}_{\geq 1} = \phi$. □

As is seen from (11), α^{-1} is the distance from the origin to the nearest pole of Ihara's zeta $\zeta_G(u)$. From example 1, we see that $\zeta_G(u) = 1$ for a tree G and $\zeta_{C_N}(u) = (1-u^N)^{-2}$ for a 1-cycle graph C_N. Therefore α^{-1} is ∞ and 1 respectively. In these cases, $L_{\alpha^{-1}}(G) = L(G)$ and F is a strictly convex function on $L(G)$, because $|\beta_e| < 1$ always holds. This reproduces the results shown in [11]. In general, using theorem 8.1.22 of [12], we have $\min_{i\in V} d_i - 1 \leq \alpha \leq \max_{i \in V} d_i - 1$.

Theorem 3 is also useful to show non-convexity.

Corollary 2. *Let $\{m_i(t) := 0, \chi_{ij}(t) := t\} \in L(G)$ for $t < 1$. Then we have*

$$\lim_{t\to 1} \det(\nabla^2 F(t))(1-t)^{M+N-1} = -2^{-M-N+1}(M-N)\kappa(G), \tag{16}$$

where $\kappa(G)$ is the number of spanning trees in G. In particular, F is never convex on $L(G)$ for any connected graph with at least two linearly independent cycles, i.e. $M - N \geq 1$.

Proof. The equation (16) is obtained by Hashimoto's theorem [13], which gives the $u \to 1$ limit of the Ihara zeta function. (See supplementary material for the detail.) If $M - N \geq 1$, the right hand side of (16) is negative. As approaches to $\{m_i = 0, \chi_{ij} = 1\} \in L(G)$, the determinant of the Hessian diverges to $-\infty$. Therefore the Hessian is not positive definite near the point. □

Summarizing the results in this section, we conclude that F is convex on $L(G)$ if and only if G is a tree or a graph with one cycle. To the best of our knowledge, this is the first proof of this fact.

5 Application to stability analysis

In this section we discuss the local stability of LBP and the local structure of the Bethe free energy around a LBP fixed point. Heskes [6] shows that a locally stable fixed point of sufficiently damped LBP is a local minima of the Bethe free energy. The converse is not necessarily true in general, and we will elucidate the gap between these two properties.

First, we regard the LBP update as a dynamical system. Since the model is binary, each message $\mu_{i\to j}(x_j)$ is parametrized by one parameter, say $\eta_{i\to j}$. The state of LBP algorithm is expressed by $\boldsymbol{\eta} = (\eta_e)_{e\in\vec{E}} \in C(\vec{E})$, and the update rule (2) is identified with a transform T on $C(\vec{E})$, $\boldsymbol{\eta}^{\rm new} = T(\boldsymbol{\eta})$. Then, the set of fixed points of LBP is $\{\boldsymbol{\eta}^\infty \in C(\vec{E}) | T(\boldsymbol{\eta}^\infty) = \boldsymbol{\eta}^\infty\}$.

A fixed point $\boldsymbol{\eta}^\infty$ is called *locally stable* if LBP starting with a point sufficiently close to $\boldsymbol{\eta}^\infty$ converges to $\boldsymbol{\eta}^\infty$. The local stability is determined by the linearizion T' around the fixed point. As is discussed in [14], $\boldsymbol{\eta}^\infty$ is locally stable if and only if $\mathrm{Spec}(T'(\boldsymbol{\eta}^\infty)) \subset \{\lambda \in \mathbb{C} | |\lambda| < 1\}$.

To suppress oscillatory behaviors of LBP, damping of update $T_\epsilon := (1-\epsilon)T + \epsilon I$ is sometimes useful, where $0 \le \epsilon < 1$ is a damping strength and I is the identity. A fixed point is locally stable with some damping if and only if $\mathrm{Spec}(T'(\boldsymbol{\eta}^\infty)) \subset \{\lambda \in \mathbb{C} | \mathrm{Re}\lambda < 1\}$.

There are many representations of the linearization (derivative) of LBP update (see [14, 15]), we choose a good coordinate following Furtlehner et al [16]. In section 4 of [16], they transform messages as $\mu_{i\to j} \to \mu_{i\to j}/\mu^\infty_{i\to j}$ and functions as $\psi_{ij} \to b_{ij}/(b_i b_j)$ and $\psi_i \to b_i$, where $\mu^\infty_{i\to j}$ is the message of the fixed point. This changes only the representations of messages and functions, and does not affect LBP essentially. This transformation causes $T'(\boldsymbol{\eta}^\infty) \to PT'(\boldsymbol{\eta}^\infty)P^{-1}$ with an invertible matrix P. Using this transformation, we see that the following fact holds. (See supplementary material for the detail.)

Theorem 5 ([16], Proposition 4.5)**.** *Let $u_{i\to j}$ be given by (3), (5) and (13) at a LBP fixed point $\boldsymbol{\eta}^\infty$. The derivative $T'(\boldsymbol{\eta}^\infty)$ is similar to $\mathcal{UM}$, i.e. $\mathcal{UM} = PT'(\boldsymbol{\eta}^\infty)P^{-1}$ with an invertible matrix P.*

Since $\det(I - T'(\boldsymbol{\eta}^\infty)) = \det(I - \mathcal{UM})$, the formula in theorem 3 implies a direct link between the linearization $T'(\boldsymbol{\eta}^\infty)$ and the local structure of the Bethe free energy. From theorem 4, we have that a fixed point of LBP is a local minimum of the Bethe free energy if $\mathrm{Spec}(T'(\boldsymbol{\eta}^\infty)) \subset \mathbb{C} \setminus \mathbb{R}_{\ge 1}$.

It is now clear that the condition for positive definiteness, local stability of damped LBP and local stability of undamped LBP are given in terms of the set of eigenvalues, $\mathbb{C} \setminus \mathbb{R}_{\ge 1}$, $\{\lambda \in \mathbb{C} | \mathrm{Re}\lambda < 1\}$ and $\{\lambda \in \mathbb{C} | |\lambda| < 1\}$ respectively. A locally stable fixed point of sufficiently damped LBP is a local minimum of the Bethe free energy, because $\{\lambda \in \mathbb{C} | \mathrm{Re}\lambda < 1\}$ is included in $\mathbb{C} \setminus \mathbb{R}_{\ge 1}$. This reproduces Heskes's result [6]. Moreover, we see the gap between the locally stable fixed points with some damping and the local minima of the Bethe free energy: if $\mathrm{Spec}(T'(\boldsymbol{\eta}^\infty))$ is included in $\mathbb{C} \setminus \mathbb{R}_{\ge 1}$ but not in $\{\lambda \in \mathbb{C} | \mathrm{Re}\lambda < 1\}$, the fixed point is a local minimum of the Bethe free energy though it is not a locally stable fixed point of LBP with any damping.

It is interesting to ask under which condition a local minimum of the Bethe free energy is a stable fixed point of (damped) LBP. While we do not know a complete answer, for an attractive model, which is defined by $J_{ij} \ge 0$, the following theorem implies that if a stable fixed point becomes unstable by changing J_{ij} and h_i, the corresponding local minimum also disappears.

Theorem 6. *Let us consider continuously parametrized attractive models $\{\psi_{ij}(t), \psi_i(t)\}$, e.g. t is a temperature: $\psi_{ij}(t) = \exp(t^{-1} J_{ij} x_i x_j)$ and $\psi_i(t) = \exp(t^{-1} h_i x_i)$. For given t, run LBP algorithm and find a (stable) fixed point. If we continuously change t and see the LBP fixed point becomes unstable across $t = t_0$, then the corresponding local minimum of the Bethe free energy becomes a saddle point across $t = t_0$.*

Proof. From (3), we see $b_{ij}(x_i, x_j) \propto \exp(J_{ij} x_i x_j + \theta_i x_i + \theta_j x_j)$ for some θ_i and θ_j. From $J_{ij} \ge 0$, we have $\mathrm{Cov}_{b_{ij}}[x_i, x_j] = \chi_{ij} - m_i m_j \ge 0$, and thus $u_{i\to j} \ge 0$. When the LBP fixed point becomes unstable, the Perron Frobenius eigenvalue of $\mathcal{UM}$ goes over 1, which means $\det(I - \mathcal{UM})$ crosses 0. From theorem 3 we see that $\det(\nabla^2 F)$ becomes positive to negative at $t = t_0$. □

Theorem 6 extends theorem 2 of [14], which discusses only the case of vanishing local fields $h_i = 0$ and the trivial fixed point (i.e. $m_i = 0$).

6 Application to uniqueness of LBP fixed point

The uniqueness of LBP fixed point is a concern of many studies, because the property guarantees that LBP finds the global minimum of the Bethe free energy if it converges. The major approaches to the uniqueness is to consider equivalent minimax problem [5], contraction property of LBP dynamics [17, 18], and to use the theory of Gibbs measure [19]. We will propose a different, differential topological approach to this problem.

In our approach, in combination with theorem 3, the following theorem is the basic apparatus.

Theorem 7. *If* $\det \nabla^2 F(q) \neq 0$ *for all* $q \in (\nabla F)^{-1}(0)$ *then*

$$\sum_{q:\nabla F(q)=0} \operatorname{sgn}\left(\det \nabla^2 F(q)\right) = 1, \quad \textit{where } \operatorname{sgn}(x) := \begin{cases} 1 & \textit{if } x > 0, \\ -1 & \textit{if } x < 0. \end{cases}$$

We call each summand, which is $+1$ *or* -1*, the index of* F *at* q.

Note that the set $(\nabla F)^{-1}(0)$, which is the stationary points of the Bethe free energy, coincides with the fixed points of LBP. The above theorem asserts that the sum of indexes of all the fixed points must be one. As a consequence, the number of the fixed points of LBP is always odd. Note also that the index is a local quantity, while the assertion expresses the global structure of the function F.

For the proof of theorem 7, we prepare two lemmas. The proof of lemma 1 is shown in the supplementary material. Lemma 2 is a standard result in differential topology, and we refer [20] theorem 13.1.2 and comments in p.104 for the proof.

Lemma 1. *If a sequence* $\{q_n\} \subset L(G)$ *converges to a point* $q_* \in \partial L(G)$*, then* $\|\nabla F(q_n)\| \to \infty$*, where* $\partial L(G)$ *is the boundary of* $L(G) \subset \mathbb{R}^{N+M}$.

Lemma 2. *Let* M_1 *and* M_2 *be compact, connected and orientable manifolds with boundaries. Assume that the dimensions of* M_1 *and* M_2 *are the same. Let* $f : M_1 \to M_2$ *be a smooth map satisfying* $f(\partial M_1) \subset \partial M_2$*. For a regular value of* $p \in M_2$*, i.e.* $\det(\nabla f(q)) \neq 0$ *for all* $q \in f^{-1}(p)$*, we define the degree of the map* f *by* $\deg f := \sum_{q \in f^{-1}(p)} \operatorname{sgn}(\det \nabla f(q))$*. Then* $\deg f$ *does not depend on the choice of a regular value* $p \in M_2$.

Sketch of proof. Define a map $\Phi : L(G) \to \mathbb{R}^{N+M}$ by $\Phi := \nabla F + \binom{\boldsymbol{h}}{\boldsymbol{J}}$. Note that Φ does not depend on $\boldsymbol{h}$ and $\boldsymbol{J}$ as seen from (6). Then it is enough to prove

$$\sum_{q \in \Phi^{-1}(\binom{\boldsymbol{h}}{\boldsymbol{J}})} \operatorname{sgn}(\det \nabla \Phi(q)) = \sum_{q \in \Phi^{-1}(0)} \operatorname{sgn}(\det \nabla \Phi(q)), \tag{17}$$

because $\Phi^{-1}(0)$ has a unique element $\{m_i = 0, \chi_{ij} = 0\}$, at which $\nabla^2 F$ is positive definite, and the right hand side of (17) is equal to one. Define a sequence of manifolds $\{C_n\}$ by $C_n := \{q \in L(G) | \sum_{ij \in E} \sum_{x_i,x_j} -\log b_{ij} \leq n\}$, which increasingly converges to $L(G)$. Take $K > 0$ and $\epsilon > 0$ to satisfy $K - \epsilon > \|\binom{\boldsymbol{h}}{\boldsymbol{J}}\|$. From lemma 1, for sufficiently large n_0, we have $\Phi^{-1}(0), \Phi^{-1}\binom{\boldsymbol{h}}{\boldsymbol{J}} \subset C_{n_0}$ and $\Phi(\partial C_{n_0}) \cap B_0(K) = \phi$, where $B_0(K)$ is the closed ball of radius K at the origin. Let $\Pi_\epsilon : \mathbb{R}^{N+M} \to B_0(K)$ be a smooth map that is the identity on $B_0(K-\epsilon)$, monotonically increasing on $\|x\|$, and $\Pi_\epsilon(x) = \frac{K}{\|x\|}x$ for $\|x\| \geq K$. We obtain a map $\tilde{\Phi} := \Pi_\epsilon \circ \Phi : C_{n_0} \to B_0(K)$ such that $\tilde{\Phi}(\partial C_{n_0}) \subset \partial B_0(K)$. Applying lemma 2 yields (17). □

If we can guarantee that the index of every fixed point is $+1$ in advance of running LBP, we conclude that fixed point of LBP is unique. We have the following a priori information for β.

Lemma 3. *Let* β_{ij} *be given by (15) at any fixed point of LBP. Then* $|\beta_{ij}| \leq \tanh(|J_{ij}|)$ *and* $\operatorname{sgn}(\beta_{ij}) = \operatorname{sgn}(J_{ij})$ *hold.*

Proof. From (3), we see that $b_{ij}(x_i, x_j) \propto \exp(J_{ij}x_ix_j + \theta_i x_i + \theta_j x_j)$ for some θ_i and θ_j. With (15) and straightforward computation, we obtain $\beta_{ij} = \sinh(2J_{ij})(\cosh(2\theta_i) + \cosh(2J_{ij}))^{-1/2}(\cosh(2\theta_j) + \cosh(2J_{ij}))^{-1/2}$. The bound is attained when $\theta_i = 0$ and $\theta_j = 0$. □

From theorem 7 and lemma 3, we can immediately obtain the uniqueness condition in [18], though the stronger contractive property is proved under the same condition in [18].

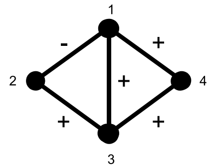

Figure 1: Graph of Example 2.

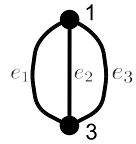

Figure 2: Graph $\hat{G}$.

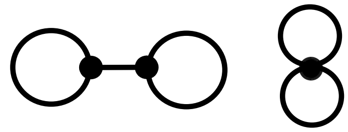

Figure 3: Two other types.

Corollary 3 ([18]). *If $\rho(\mathcal{J}\mathcal{M}) < 1$, then the fixed point of LBP is unique, where $\mathcal{J}$ is a diagonal matrix defined by $\mathcal{J}_{e,e'} = \tanh(|J_e|)\delta_{e,e'}$.*

Proof. Since $|\beta_{ij}| \leq \tanh(|J_{ij}|)$, we have $\rho(\mathcal{B}\mathcal{M}) \leq \rho(\mathcal{J}\mathcal{M}) < 1$. ([12] Theorem 8.1.18.) Then $\det(I - \mathcal{B}\mathcal{M}) = \det(I - \mathcal{U}\mathcal{M}) > 0$ implies that the index of any LBP fixed point must be $+1$. $\square$

In the proof of the above corollary, we only used the bound of modulus. In the following case of corollary 4, we can utilize the information of signs. To state the corollary, we need a terminology. The interactions $\{J_{ij}, h_i\}$ and $\{J'_{ij}, h'_i\}$ are said to be *equivalent* if there exists $(s_i) \in \{\pm 1\}^V$ such that $J'_{ij} = J_{ij} s_i s_j$ and $h'_i = h_i s_i$. Since an equivalent model is obtained by gauge transformation $x_i \to x_i s_i$, the uniqueness property of LBP for equivalent models is unchanged.

Corollary 4. *If the number of linearly independent cycle of G is two (i.e. $M - N + 1 = 2$), and the interaction is not equivalent to attractive model, then the LBP fixed point is unique.*

The proof is shown in the supplementary material. We give an example to illustrate the outline.

Example 2. Let $V := \{1, 2, 3, 4\}$ and $E := \{12, 13, 14, 23, 34\}$. The interactions are given by arbitrary $\{h_i\}$ and $\{-J_{12}, J_{13}, J_{14}, J_{23}, J_{34}\}$ with $J_{ij} \geq 0$. See figure 1. It is enough to check that $\det(I - \mathcal{B}\mathcal{M}) > 0$ for arbitrary $0 \leq \beta_{13}, \beta_{23}, \beta_{14}, \beta_{34} < 1$ and $-1 < \beta_{12} \leq 0$. Since the prime cycles of G bijectively correspond to those of $\hat{G}$ (in figure 2), we have $\det(I - \mathcal{B}\mathcal{M}) = \det(I - \hat{\mathcal{B}}\hat{\mathcal{M}})$, where $\hat{\beta}_{e_1} = \beta_{12}\beta_{23}$, $\hat{\beta}_{e_2} = \beta_{13}$, and $\hat{\beta}_{e_3} = \beta_{34}$. We see that $\det(I - \hat{\mathcal{B}}\hat{\mathcal{M}}) = (1 - \hat{\beta}_{e_1}\hat{\beta}_{e_2} - \hat{\beta}_{e_1}\hat{\beta}_{e_3} - \hat{\beta}_{e_2}\hat{\beta}_{e_3} - 2\hat{\beta}_{e_1}\hat{\beta}_{e_2}\hat{\beta}_{e_3})(1 - \hat{\beta}_{e_1}\hat{\beta}_{e_2} - \hat{\beta}_{e_1}\hat{\beta}_{e_3} - \hat{\beta}_{e_2}\hat{\beta}_{e_3} + 2\hat{\beta}_{e_1}\hat{\beta}_{e_2}\hat{\beta}_{e_3}) > 0$. In other cases, we can reduce to the graph $\hat{G}$ or the graphs in figure 3 similarly (see the supplementary material).

For attractive models, the fixed point of the LBP is not necessarily unique.

For graphs with multiple cycles, all the existing results on uniqueness make assumptions that upperbound $|J_{ij}|$ essentially. In contrast, corollary 4 applies to arbitrary strength of interactions if the graph has two cycles and the interactions are not attractive. It is noteworthy that, from corollary 2, the Bethe free energy is non-convex in the situation of corollary 4, while the fixed point is unique.

7 Concluding remarks

For binary pairwise models, we show the connection between the edge zeta function and the Bethe free energy in theorem 3, in the proof of which the multi-variable version of Ihara's formula (theorem 2) is essential. After the initial submission of this paper, we found that theorem 3 is extended to a more general class of models including multinomial models and Gaussian models represented by arbitrary factor graphs. We will discuss the extended formula and its applications in a future paper.

Some recent researches on LBP have suggested the importance of zeta function. In the context of the LDPC code, which is an important application of LBP, Koetter et al [21, 22] show the connection between pseudo-codewords and the edge zeta function. On the LBP for the Gaussian graphical model, Johnson et al [23] give zeta-like product formula of the partition function. While these are not directly related to our work, pursuing covered connections is an interesting future research topic.

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References

[1] J. Pearl. *Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference*. Morgan Kaufmann Publishers, San Mateo, CA, 1988.

[2] K. Murphy, Y. Weiss, and M.I. Jordan. Loopy belief propagation for approximate inference: An empirical study. *Proc. of Uncertainty in AI*, 15:467–475, 1999.

[3] J.S. Yedidia, W.T. Freeman, and Y. Weiss. Generalized belief propagation. *Adv. in Neural Information Processing Systems*, 13:689–95, 2001.

[4] Y. Weiss. Correctness of Local Probability Propagation in Graphical Models with Loops. *Neural Computation*, 12(1):1–41, 2000.

[5] T. Heskes. On the uniqueness of loopy belief propagation fixed points. *Neural Computation*, 16(11):2379–2413, 2004.

[6] T. Heskes. Stable fixed points of loopy belief propagation are minima of the Bethe free energy. *Adv. in Neural Information Processing Systems, 15*, pages 343–350, 2002.

[7] K. Hashimoto. Zeta functions of finite graphs and representations of p-adic groups. *Automorphic forms and geometry of arithmetic varieties*, 15:211–280, 1989.

[8] H.M. Stark and A.A. Terras. Zeta functions of finite graphs and coverings. *Advances in Mathematics*, 121(1):124–165, 1996.

[9] Y. Ihara. On discrete subgroups of the two by two projective linear group over p-adic fields. *Journal of the Mathematical Society of Japan*, 18(3):219–235, 1966.

[10] H. Bass. The Ihara-Selberg zeta function of a tree lattice. *Internat. J. Math*, 3(6):717–797, 1992.

[11] P. Pakzad and V. Anantharam. Belief propagation and statistical physics. *Conference on Information Sciences and Systems*, (225), 2002.

[12] R.A. Horn and C.R. Johnson. *Matrix analysis*. Cambridge University Press, 1990.

[13] K. Hashimoto. On zeta and L-functions of finite graphs. *Internat. J. Math*, 1(4):381–396, 1990.

[14] JM Mooij and HJ Kappen. On the properties of the Bethe approximation and loopy belief propagation on binary networks. *Journal of Statistical Mechanics: Theory and Experiment*, (11):P11012, 2005.

[15] S. Ikeda, T. Tanaka, and S. Amari. Information geometry of turbo and low-density parity-check codes. *IEEE Transactions on Information Theory*, 50(6):1097–1114, 2004.

[16] C. Furtlehner, J.M. Lasgouttes, and A. De La Fortelle. Belief propagation and Bethe approximation for traffic prediction. *INRIA RR-6144, Arxiv preprint physics/0703159*, 2007.

[17] A.T. Ihler, JW Fisher, and A.S. Willsky. Loopy belief propagation: Convergence and effects of message errors. *Journal of Machine Learning Research*, 6(1):905–936, 2006.

[18] J. M. Mooij and H. J. Kappen. Sufficient Conditions for Convergence of the Sum-Product Algorithm. *IEEE Transactions on Information Theory*, 53(12):4422–4437, 2007.

[19] S. Tatikonda and M.I. Jordan. Loopy belief propagation and Gibbs measures. *Uncertainty in AI*, 18:493–500, 2002.

[20] B.A. Dubrovin, A.T. Fomenko, S.P. Novikov, and Burns R.G. *Modern Geometry: Methods and Applications: Part 2: the Geometry and Topology of Manifolds* . Springer-Verlag, 1985.

[21] R. Koetter, W.C.W. Li, PO Vontobel, and JL Walker. Pseudo-codewords of cycle codes via zeta functions. *IEEE Information Theory Workshop*, pages 6–12, 2004.

[22] R. Koetter, W.C.W. Li, P.O. Vontobel, and J.L. Walker. Characterizations of pseudo-codewords of (low-density) parity-check codes. *Advances in Mathematics*, 213(1):205–229, 2007.

[23] J.K. Johnson, V.Y. Chernyak, and M. Chertkov. Orbit-Product Representation and Correction of Gaussian Belief Propagation. *Proceedings of the 26th International Conference on Machine Learning*, (543), 2009.