Graph polynomials and approximation of partition functions with Loopy Belief Propagation

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Abstract: The Bethe approximation, or loopy belief propagation algorithm, is a successful method for approximating partition functions of probabilistic models associated with graphs. Chertkov and Chernyak derived an interesting formula called “Loop Series Expansion”, which is an expansion of the partition function. The main term of the series is the Bethe approximation while the other terms are labeled by subgraphs called generalized loops.

In our recent paper, we derive the loop series expansion in form of a polynomial with coefficients positive integers, and extend the result to the expansion of marginals. In this paper, we give more clear derivation of the results and discuss the properties of newly introduced polynomials.

1 Introduction

A Markov random field (MRF) associated with a graph is given by a joint probability distribution over a set of variables. In the associated graph, the nodes represent variables and the edges represent probabilistic dependence between variables. The joint distribution is often given in an unnormalized form, and the normalization factor of a MRF is called a partition function.

Computation of the partition function and the marginal distributions of a MRF with discrete variables is in general computationally intractable for a large number of variables, and some approximation method is required. Among many approximation methods, the Bethe approximation has attracted renewed interest of computer scientists; it is equivalent to Loopy Belief Propagation (LBP) algorithm [2, 3], which has been successfully used for many applications such as error correcting codes, inference on graphs, image processing, and so on [4, 5, 6]. If the associated graph is a tree, the algorithm computes the exact value, not an approximation [9].

The performance of this approximation is surprisingly well for many applications even if the graph has many cycles. If the graph has one cycle, the behavior of the algorithm is well understood, and maximum marginal assignment of the approximation is known to be exact [10]. On the other hand, if the graph has many cycles, little analysis have done in the connection with the topological structure of the underlying graph. Theoretical analysis of the approximation is important both for improving the algorithm and extending it to wide range of applications.

Chertkov and Chernyak [7, 8] give a formula called loop series expansion, which expresses the partition function in terms of a finite series. The first term is the Bethe approximation, and the others are labeled by so-called generalized loops. The Bethe approximation can be corrected with this formula. This expansion highlights the connection between the accuracy of the approximation and the topology of the graph.

In our recent paper [1], we derive the formula in terms of message passing scheme with diagrams based on the method called propagation diagrams. We also showed that the true marginals can be also expanded around the approximated marginals.

In this paper we give a simple and easy derivation of the expansion of the partition function and the marginal distributions. Similar but a different approach is found in [11]. We also discuss the properties of the bivariate polynomial which is introduced in [1]. Since this polynomial represents the ratio of the true partition function and the Bethe approximated partition function, investigation of it is important for understanding the relation between the graph topology and the approximation performance.

2 Bethe approximation and LBP algorithm

In this section, we review the definitions and notations of Markov Random Field (MRF) and loopy belief propagation algorithm.

2.1 Pairwise Markov random field

We introduce a probabilistic model considered in this paper, MRF of binary states with pairwise interactions. Let \( G := (V, E) \) be a connected undirected graph, where \( V = \{1, \ldots, N\} \) is a set of nodes and \( E \subset \{(i,j) : 1 \leq i < j \leq N\} \) is a set of undirected edges. We abbreviate undirected edges \((i,j)\) to \(ij = ji\). Each node \(i \in V\) is associated with a binary space \(\chi_i = \{\pm1\}\). We make a set of directed edges from \(E\): \(\hat{E} = \{(i,j), (j,i) : (i,j) \in E\}\). The neighbors of \(i\) is denoted by \(N(i) \subset V\), and \(d_i = |N(i)|\) is called the
degree of \( i \). A joint probability distribution on the graph \( G \) is given by the form:

\[
p(x) = \frac{1}{Z} \prod_{ij \in E} \psi_{ij}(x_i, x_j) \prod_{i \in V} \phi_i(x_i), \quad (1)
\]

where \( \psi_{ij}(x_i, x_j) : \chi_i \times \chi_j \rightarrow \mathbb{R}_{>0} \) and \( \phi_i : \chi_i \rightarrow \mathbb{R}_{>0} \) are positive functions called compatibility functions. The normalization factor \( Z \) is called the partition function. A set of random variables which has a probability distribution in the form of (1) is called a Markov random field (MRF) or an undirected graphical model on the graph \( G \).

Without loss of generality, univariate compatibility functions \( \phi_i \) can be neglected because they can be included in bivariate compatibility functions \( \psi_{ij} \). This operation does not affect the Bethe approximation and the LBP algorithm given below; we assume it as per the following.

### 2.2 Loopy belief propagation algorithm

The LBP algorithm computes the Bethe approximation of the partition function and the marginal distribution of each node with the message passing method \[9, 2, 3\]. This algorithm is summarized as follows.

1. Initialization:
   For all \((j, i) \in E\), the message from \( i \) to \( j \) is a vector \( m_{0,(j,i)} \in \mathbb{R}^2 \). Initialize as
   \[
m_{0,(j,i)}(x_j) = 1 \quad \forall x_j \in \chi_j,
   \]
   (2)

2. Message Passing:
   For each \( t = 0, 1, \ldots \), update the messages by
   \[
m^{t+1}_{(j,i)}(x_j) = \omega \sum_{x_i \in \chi_i} \psi_{ji}(x_j, x_i) \prod_{k \in N(i) \setminus \{j\}} m^t_{(i,k)}(x_i),
   \]
   (3)
   until it converges. Finally we obtain \( \{m^*_{(j,i)}\} \).

3. Approximated marginals and the partition function are computed by the following formulas:
   \[
   b_i(x_i) := \omega \prod_{j \in N(i)} m^*_{(i,j)}(x_i),
   \]
   (4)
   \[
   b_{ji}(x_j, x_i) := \omega \psi_{ji}(x_j, x_i) \prod_{k \in N(j) \setminus \{i\}} m^*_{(k,j)}(x_j) \prod_{k' \in N(i) \setminus \{j\}} m^*_{(i,k')}(x_i),
   \]
   (5)
   \[
   \log Z_B := \sum_{j \in E} b_{ji}(x_j, x_i) \log \psi_{ji}(x_j, x_i)
   \]
   \[
   - \sum_{j \in E} b_{ji}(x_j, x_i) \log b_{ji}(x_j, x_i)
   \]
   \[
   + \sum_{i \in V} (d_i - 1) b_i(x_i) \log b_i(x_i),
   \]
   where \( \omega \) are appropriate normalization constants, \( b_i \) are called beliefs, and \( Z_B \) is called the Bethe approximation of the partition function.

In step 2, there is ambiguity as to the order of updating the messages. We do not specify the order, because the fixed points of LBP algorithm do not depend on its choice.

We normalize as

\[
\sum_{x_j, x_i} b_{ji}(x_j, x_i) = \sum_{x_i} b_i(x_i) = 1,
\]

so that the relation \( \sum_{x_j} b_{ji}(x_j, x_i) = b_j(x_j) \) is always satisfied for all \( ij \in E \).

### 3 Derivation of the Loop Series Expansion

In this section, we prove the loop series expansion formula of the partition function and marginals.

#### 3.1 Expansion of partition functions

First, we prove the following identity which plays a key role in our derivation. We define a set of polynomials \( \{f_n(x)\} \) inductively by the relations \( f_0(x) = 1, f_1(x) = 0 \), and \( f_{n+1}(x) = x f_n(x) + f_{n-1}(x) \). This polynomials are transformations of the Chebyshev polynomials of the second kind.

**Theorem 1.** Let \( \{\xi_i\}_{i \in V} \) and \( \{\beta_{ij}\}_{ij \in E} \) be sets of free variables associated to nodes and edges. Then,

\[
\sum_{x_1, \ldots, x_N = \pm 1} \prod_{ij \in E} \left( 1 + x_i x_j \beta_{ij} \xi_i^{-x_i} \xi_j^{-x_j} \right) \prod_{i \in V} \frac{\xi_i^{x_i}}{\xi_i + \xi_i^{-1}} = \sum_{s \subseteq E} \prod_{ij \in s} \beta_{ij} \prod_{i \in V} f_{d_i(s)}(\xi_i - \xi_i^{-1}),
\]

(6)

where \( d_i(s) \) is the degree of node \( i \) in the subgraph induced by an edge set \( s \).

**Proof.**

\[
\text{(L.H.S.)} = \sum_{s \subseteq E} \prod_{ij \in s} x_i x_j \beta_{ij} \xi_i^{-x_i} \xi_j^{-x_j} \prod_{i \in V} \frac{\xi_i^{x_i}}{\xi_i + \xi_i^{-1}}
\]

\[
= \sum_{s \subseteq E} \prod_{ij \in s} \beta_{ij} \prod_{i \in V} \sum_{x_i = \pm 1} (-x_i \xi_i^{-x_i})^d(s) \frac{\xi_i^{x_i}}{\xi_i + \xi_i^{-1}}
\]

\[
= \sum_{s \subseteq E} \prod_{ij \in s} \prod_{i \in V} \frac{(-\xi_i)^{-d(s)+1} + \xi_i^{d(s)-1}}{\xi_i + \xi_i^{-1}}.
\]

On the other hand, by the definition of \( f_n \)

\[
f_n(\xi - \xi^{-1}) = \frac{\xi^{n-1} - (-\xi)^{-n+1}}{\xi + \xi^{-1}}.
\]

(7)

Secondly, we give a relation between the true partition function and the Bethe approximation.

**Lemma 1.**

\[
\frac{Z}{Z_B} = \sum_{\{x_i\} \in E} \frac{b_{ji}(x_i, x_j)}{b_{ji}(x_i)} \prod_{i \in V} b_i(x_i)
\]

(8)
Proof. If we write the normalization terms explicitly, (1) and (2) are rewritten as
\[ b_i(x_i) = c_i^{-1} \prod_{j \in N(i)} m^*_i(x_i, x_j), \]
\[ b_{ij}(x_j, x_i) = c_{ij}^{-1} \psi_{ji}(x_j, x_i) \prod_{k \in N(j) \setminus i} m^*_j(x_j) \prod_{k' \in N(i) \setminus j} m^*_i(x_i, k'). \]

By the definition of the Bethe approximation of partition function, it is easy to see that
\[ Z_B = \prod_{ij \in E} \frac{c_{ij}}{c_i c_j} \prod_{i \in V} c_i. \]  

Then, we use (9) again, the right hand side of (8) is equal to \( \frac{Z_B}{Z} \).

Finally, we give the loop series expansion formula of the partition function (11) [8].

**Theorem 2.** Let
\[ \gamma_i := \frac{b_i(1) - b_i(-1)}{\sqrt{b_i(1)b_i(-1)}}. \] (11)
and
\[ \beta_{ij} := \frac{b_{ij}(1,1)b_{ij}(-1,1) - b_{ij}(-1,1)b_{ij}(-1,1)}{\sqrt{b_i(1)b_i(-1)} \sqrt{b_j(1)b_j(-1)}}. \] (12)

Then, the following formula holds.
\[ Z = Z_B \sum_{s \subseteq E} r(s), \] (13)
\[ r(s) := \prod_{ij \in s} \beta_{ij} \prod_{i \in V} f_{d_i}(\gamma_i). \] (14)

Before accomplishing the proof, let us consider the meaning of the theorem. Equation (11) states that \( \gamma_i \) is related to the bias of the approximated marginal \( b_i(x_i) \), and \( \gamma_i = 0 \) if and only if \( b_i(1) = b_i(-1) \). Equation (12) states that \( \beta_{ij} \) is related to the correlation by \( b_{ij} \). It is easy to see that \( |\beta_{ij}| \leq 1 \) and \( \beta_{ij} = 0 \) if and only if \( b_{ij}(x_i, x_j) = b_i(x_i)b_j(x_j) \).

The definitions and properties of these quantities \( \beta_{ij} \) and \( \gamma_i \), in the context of message passing procedures, are found in [1].

In (13), the summation runs over all subsets of \( E \) including \( s = \emptyset \). As \( f_1(x) = 0 \), \( s \) makes a contribution to the sum only if \( s \) does not have a node of degree one in \( s \). Such a subgraph \( s \) is called a generalized loop [7] [8] or a closed graph [12] [13]. In the case that \( G \) is a tree, there is no generalized loops, therefore \( Z = Z_B \).

If \( \beta_{ij} \) and \( \gamma_i \) are sufficiently small, the first term \( r(\emptyset) = 1 \) is mainly contribute to the sum, and \( Z_B \) is close to \( Z \).

**Proof of theorem 3.** For a given \( b_{ij}(x_i, x_j) \) which satisfies the normalization condition \( \sum_{x_i, x_j} b_{ij}(x_i, x_j) = 1 \), we can always choose \( \xi_i, \xi_j, \beta_{ij}' \) to satisfy
\[ b_{ij}(x_i, x_j) = \frac{1}{(\xi_i + \xi^{-1}_i)(\xi_j + \xi^{-1}_j)} (\xi_i^{x_i} \xi_j^{x_j} + \beta_{ij}' x_i x_j). \] (15)

From (12), we see that \( \beta_{ij}' = \beta_{ij} \). Using
\[ b_i(x_i) = \sum_{x_j} b_{ij}(x_i, x_j) = \frac{\xi_i^{x_i}}{\xi_i + \xi^{-1}_i} \] (16)
and (11), we have \( \gamma_i = \xi_i - \xi_i^{-1} \). Notice that
\[ \frac{b_{ij}(x_i, x_j)}{b_i(x_i)b_j(x_j)} = 1 + x_i x_j \beta_{ij} \xi_i^{-x_i} \xi_j^{-x_j}. \] (17)
the left hand side of (16) is equal to the right hand side of (8) and the assertion is proved.

**Example 1**

![Figure 1: Original graph](image)

![Figure 2: List of generalized loops](image)

**3.2 Expansion of marginals**

In this subsection, we head for proving theorem 3. We define a set of polynomials \( \{g_n(x)\}_{n=0}^{\infty} \) inductively by the relations \( g_0(x) = x, g_1(x) = -2 \) and \( g_{n+1}(x) = x g_n(x) + g_{n-1}(x) \). This set of polynomials is a transformation of the Chebyshev polynomials of the first kind. We introduce the following lemma which is a modification of theorem 1.
Lemma 2.

\[
\sum_{x_1, \ldots, x_N = \pm 1} x_1 \prod_{i \in E} (1 + x_i x_j \beta_{ij} \xi_i^{x_i} \xi_j^{x_j}) \prod_{i \in V} \frac{\xi_i^{x_i}}{\xi_i + \xi_i} = \sum_{s \subseteq E} \beta_{ij} \prod_{i \in s} f_{d_i(s)}(\xi_i - \xi_i^{-1}) \prod_{i \notin V \setminus \{1\}} \frac{\xi_i^{x_i}}{\xi_i + \xi_i^{-1}}.
\]

(19)

Proof. Check that

\[
\sum_{x_1 = \pm 1} x_1 (-x_1 \xi_1^{x_1})^n \frac{\xi_1^{x_1}}{\xi_1 + \xi_1^{-1}} = g_n(\xi_1 - \xi_1^{-1}).
\]

(20)

Theorem 3. Let \( p_1(x_1) \) be the true marginal distribution defined by the joint probability distribution [4]. Then,

\[
\frac{Z_B}{Z} \frac{Z_B(p_1(-1) - p_1(1))}{b_1(1)b_1(-1)} = \sum_{s \subseteq E} \beta_{ij} \prod_{i \in s} f_{d_i(s)}(\gamma_1) \prod_{i \notin V \setminus \{1\}} \frac{\xi_i^{x_i}}{\xi_i + \xi_i^{-1}}.
\]

(21)

Proof. The key fact is

\[
\frac{Z}{Z_B}(p_1(1) - p_1(-1)) = \sum_{\{x_i\}} x_1 \prod_{i \in E} b_i(x_i, x_j) \prod_{i \in V} b_i(x_i),
\]

which is a modification of lemma 1. Follow the proof of theorem 2.

Corollary 1. Let \( G \) be a graph with a single cycle and the node 1 on it. See figure 3 for example. Then, \( p_1(x_1) - p_1(-1) \) and \( b_1(1) - b_1(-1) \) have the same sign.

Proof. In the right hand side of (21), only two subgraphs \( s \) are contribute to the sum. From \( g_0(\gamma_1) = \gamma_1 \) , \( g_2(\gamma_1) = -\gamma_1 \) and \( |\beta_{ij}| \leq 1 \), we see that the sum is positively proportional to \( \gamma_1 \).

4 Bound on the number of generalized loops

In the loop series expansion formula [13], the summation runs over all generalized loops. To know the computational cost for summing up the terms, the number of generalized loops is of interest.

Definition 1.

\[
\theta_G(\beta, \xi) := \sum_{s \subseteq E} \beta_{ij} \prod_{i \in s} f_{d_i(s)}(\xi - \xi^{-1}).
\]

(22)

This is a bivariate (Laurent) polynomial with respect to \( \beta \) and \( \xi \). The coefficients are all integers. Let \( n(G) := |E| - |V| + 1 \) be the number of linearly independent cycles. The next lemma shows that the value of \( \theta_G \) on \( \beta = 1 \) is determined by \( n(G) \).

Lemma 3.

\[
\theta_G(1, \xi) = \sum_{k=0}^{n(G)} \left( \frac{n(G)}{k} \right) f_{2k}(\xi - \xi^{-1})
\]

(23)

Proof. The left hand side of theorem 1 gives an alternative representation of \( \theta_G \). If \( x_i \neq x_j \), then \( 1 + x_i x_j \beta^{-x_i, x_j} = 0 \). As we assumed the graph \( G \) is connected, only two terms of \( x_1 = \cdots = x_N = 1 \) and \( x_1 = \cdots = x_N = -1 \) contribute to the sum. Therefore,

\[
\theta_G(1, \xi) = (1 + \xi^{-2}) |E| \left( \frac{\xi}{\xi + \xi^{-1}} \right)^{|V|} + (1 + \xi^{-2}) |E| \left( \frac{\xi^{-1}}{\xi + \xi^{-1}} \right)^{|V|}.
\]

(24)

From (17), the right hand side of (23) is equal to (24).

If \( \xi = \frac{1 + \sqrt{5}}{2} \), then \( \xi - \xi^{-1} = 1 \). From (23) or (24), we see that

\[
\theta_G(1, \frac{1 + \sqrt{5}}{2}) = \left( \frac{5 - \sqrt{5}}{2} \right)^{n(G)-1} + \left( \frac{5 + \sqrt{5}}{2} \right)^{n(G)-1}.
\]

This fact can be used to bound the number of generalized loops [4].

Theorem 4. Let \( G_0 \) be the set of all generalized loops of \( G \) including empty set. Then,

\[
|G_0| \leq \left( \frac{5 - \sqrt{5}}{2} \right)^{n(G)-1} + \left( \frac{5 + \sqrt{5}}{2} \right)^{n(G)-1}.
\]

(25)

This bound is attained if and only if every node of a generalized loop has the degree at most three.

Proof. If we set \( \beta = 1 \) and \( \xi = \frac{1 + \sqrt{5}}{2} \),

\[
\theta_G(1, \frac{1 + \sqrt{5}}{2}) = \sum_{s \in G_0} r(s),
\]

(26)
where \( r(s) = \prod_{i \in V} f_{d_i(s)}(1) \). As \( f_n(1) > 1 \) for all \( n > 4 \) and \( f_2(1) = f_3(1) = 1 \), we have \( r(s) \geq 1 \) for all \( s \in \mathcal{G}_0 \), and the equality holds if and only if \( d_i(C) \leq 3 \) for all \( i \in V \). This shows \( |\mathcal{G}_0| \leq \theta(1, \frac{1 + \sqrt{5}}{2}) \) and the equality condition. \( \square \)

5 Generalization to factor graph model

In this section we briefly introduce the factor graph model, which is more general than the pairwise model in section 1. We generalize the result of theorem 4 and Theorem 3 is also generalized straightforwardly.

5.1 Factor graph model

Let \( H = (V, F) \) be a hypergraph, that is, \( V = \{1, \ldots, N\} \) is a set of nodes and \( F \subset 2^V \) is a set of hyperedges. A hypergraph \( H \) is represented by a bipartite graph \( G_H = (V_H, E_H) \). Each type of node corresponds to elements of \( V \) and \( F \); the first type is called variable node and the second type is called factor node. For example, see figure 4. In this example, the hypergraph \( H = (V, F) \) is given by \( V = \{1, 2, 3\} \) and \( F = \{\lambda_1, \lambda_2, \lambda_3\} \), where \( \lambda_1 = \{1, 2\}, \lambda_2 = \{1, 2, 3\} \) and \( \lambda_3 = \{2\} \).

![Figure 4: Example of \( G_H \)](image)

The joint probability distribution is given by the following form:

\[
p(x) = \frac{1}{Z} \prod_{\lambda \in F} \psi_\lambda(x_\lambda),
\]

where \( x_\lambda = \{x_i\}_{i \in \lambda} \). If each hyperedge \( \lambda \in F \) consists of a pair of nodes, this class of probability distributions reduces to the pairwise MRF model.

5.2 Loopy belief propagation algorithm

For a node \( i \in V \) and a hyperedge \( \lambda \in F \) which satisfy \( i \in \lambda \), messages \( m_{(i,\lambda)}^t(x_i) \) and \( m_{(\lambda,i)}^t(x_i) \) are defined and updated by the following rules:

\[
m_{(i,\lambda)}^t(x_i) = \omega \sum_{x_\lambda \setminus \{i\}} \psi_\lambda(x_\lambda) \prod_{j \in \lambda \setminus i} m_{(j,\lambda)}^t(x_j),
\]

\[
m_{(\lambda,i)}^t(x_i) = \omega \prod_{\mu \ni i, \mu \neq \lambda} m_{(i,\mu)}^t(x_i).
\]

Beliefs are defined by

\[
b_t(x_i) := \omega \prod_{\mu \ni i} m_{(i,\mu)}^t(x_i)
\]

and

\[
b_\lambda(x_\lambda) := \omega \psi_\lambda(x_\lambda) \prod_{j \in \lambda} m_{(i,j)}^t(x_\lambda).
\]

The Bethe approximation of the partition function is given by

\[
\log Z_B := \sum_{\lambda \in F} b_\lambda(x_\lambda) \log \psi_\lambda(x_\lambda)
- \sum_{\lambda \in F} b_\lambda(x_\lambda) \log b_\lambda(x_\lambda)
+ \sum_{i \in V} (d_i - 1) b_i(x_i) \log b_i(x_i).
\]

5.3 Expansion of partition functions

To state factor graph version of theorem 2 we need a little complicated notations. For each hyperedge \( \lambda \in F \) and \( I \subset \lambda \), we introduce a variable \( \beta^I_\lambda \). We use convention that \( \beta^{\emptyset}_\lambda = 1 \) and \( \beta^I_\emptyset = 0 \) if \(|I| = 1\).

Theorem 1 is modified to the following identity:

\[
\sum_{\{s\}} \prod_{\lambda \in F, I \subset \lambda} \sum_{I \lambda} \prod_{s \in E_H, \lambda \in F, I \subset \lambda} (-1)^{|I\lambda(s)|} \beta^I_\lambda \prod_{s \in I\lambda(s)} f_{d_s}(\xi_s - \xi_s^{-1}),
\]

where \( I = \{i_1, \ldots, i_k\} \) and \( I\lambda(s) \) is a set of variable nodes which connect to \( \lambda \) by edges in \( s \).

Lemma 1 is modified to

\[
\frac{Z}{Z_B} = \sum_{\{s\}} \prod_{\lambda \in F} \prod_{i \in \lambda} \frac{b_\lambda(x_\lambda)}{b_i(x_i)} \prod_{i \in V} b_i(x_i).
\]

Theorem 5. For a factor graph model on \( H \), we have

\[
Z = Z_B \sum_{s \subset E_H} r(s)
\]

\[
r(s) := (-1)^{|s|} \prod_{\lambda \in F} \beta^I_\lambda \prod_{s \in I\lambda(s)} f_{d_s}(\gamma_s).
\]

Sketch of proof. For a given \( b_\lambda(x_\lambda) \), we can choose \( \{\xi_s\}_{i \in \lambda} \) and \( \{\beta^I_\lambda\}_{I \subset \lambda, |I| \geq 2} \) to satisfy

\[
b_\lambda(x_\lambda) = \frac{1}{\prod_{i \in \lambda} (\xi_i + \xi_i^{-1})} \sum_{I \subset \lambda} \beta^I_\lambda \prod_{s \in I} \prod_{j \in \lambda \setminus I} \xi_{ij}.
\]

The definition of \( \gamma_i \) is the same as \( (11) \). \( \square \)

In the summation (32), only generalized loops in \( G_H \) contribute to the sum. Therefore, this expansion is again called loop series expansion.
5.4 Expansion of marginals

In the same way as section 3.2 we have the following theorem.

**Theorem 6.**

\[
Z_B \left[ \frac{c_1(1)}{b_1(1)b_1(-1)} \right] = \sum_{s \in E_B} (-1)^{|s|} \prod_{e \in F} b_g(s) \prod_{i \in V \setminus \{1\}} f_g(s)(\gamma_i) g_d(s)(\gamma_i) . \tag{33}
\]

6 Properties of \( \theta_G \)

In the rest of this article, we will focus on the (Laurent) polynomial of \( \theta_G \). The accuracy of the Bethe approximation depends both on the graph topology and strength of the interactions; the formula in theorem 2 displays this fact. To exploit the graph topology for the analysis of the performance of the LBP algorithm, we need sophisticated techniques. One of the techniques is graph polynomials. Graph polynomials have long history since Birkhoff introduced the chromatic polynomial \([14]\) and Tutte generalized it to the Tutte polynomial \([15]\).

6.1 Contraction-Deletion relation

In this subsection we explain that the function \( \theta_G \) admits the contraction-deletion relation. If a function from graph satisfies the contraction-deletion relation and multiplicativity for disjoint unions of graphs, such a function is called the Tutte’s V-function. Though the Tutte polynomial is the most famous example of the V-functions, \( \theta_G \) is another interesting example of the V-functions.

The graph which is obtained by deleting an edge \( e \in E \) is denoted by \( G/e \). The graph which is obtained by contracting \( e \) is denoted by \( G/e \). In this article, the operations of the contraction and the deletion are only applied to the non loop edges. Note that an edge \( e \in E \) is called a loop if both ends of \( e \) are connected to the same node.

The formula of \( f_n(x) \) is essential in the proof of the contraction-deletion relation.

**Lemma 4.** \( \forall n, m \in \mathbb{N}, f_{n+m-2}(x) = f_n(x)f_m(x) + f_{n-1}(x)f_{m-1}(x) \)

**Theorem 7.** For a non loop edge \( e \in E \)

\[
\theta_G(\beta, \xi) = (1 - \beta) \theta_G(\beta, \xi) + \beta \theta_G(\beta, \xi). \tag{34}
\]

**Sketch of proof.** Classify \( s \in \{0, 1\} \) if \( s \) include edge or not. Then apply lemma 4 for \( s \supseteq e \).

6.2 The case of \( \xi = \sqrt{1} \)

At the point of \( \xi = \sqrt{1} \), \( \theta_G \) has special and interesting properties. From \([24]\), \( \theta_G(1, \sqrt{1}) = 0 \). The following theorem asserts that \( \theta(\beta, \sqrt{-1}) \) can be divided by \( (1 - \beta) \) at \( |E| - |V| \) times.

**Theorem 8.**

\[
\omega_G(\beta) := \frac{\theta_G(\beta, \sqrt{-1})}{(1 - \beta)^{|E| - |V|}} \in \mathbb{Z}[\beta] \tag{35}
\]

**Proof.** Theorem 7 and definition of \( \omega_G \) imply that

\[
\omega_G(\beta) = \omega_G(\beta) + \beta \omega_G(\beta) . \tag{36}
\]

For a bouquet graph \( B_L \), which has a single node and \( L \) loops, we can easily check that

\[
\omega_{B_L}(\beta) = 1 + (2L - 1)\beta . \tag{37}
\]

We can show the assertion inductively by \([20]\) and \([21]\).

The value of \( \omega_G \) at \( \beta = 1 \) has a combinatorial interpretation.

**Theorem 9.** If the graph \( G \) does not have loop edge, \( \omega_G(1) = \#\{ \psi : V \rightarrow E; \psi \text{ satisfies } (c1), (c2) \} \).

The condition \( (c1) \) is that \( \psi \) is injective and \( (c2) \) is that for all \( i \in V \) \( \psi(i) \) is one of a connecting edges to \( i \).

We omit the proof of this theorem. The assumption that the graph is loop-less is not essential.

6.3 Relation between \( \omega_G \) and matching polynomials

The polynomial \( \omega_G(\beta) \), introduced in the previous section, is closely related to the matching polynomial.

A matching of \( G \) is a set of edges in which any edges does not occupy a same node. If a matching consists of \( k \) edges, it is called \( k \)-matching. Let \( p_G(k) \) be the number of \( k \)-matchings of \( G \). The matching polynomial \( \alpha_G \) is defined by

\[
\alpha_G(x) = \sum_{k=0}^{[\frac{n}{2}]} (-1)^k T_G(k)x^{n-2k} . \tag{38}
\]

We introduce two square matrices indexed by \( V \). Let \( A \) be a adjacency matrix of the graph \( G \) and let \( D \) be a diagonal matrix called degree matrix. In other words, for a function \( \phi : V \rightarrow \mathbb{R} \),

\[
(A\phi)(i) = \sum_{j \neq i} \phi(j), \quad (D\phi)(i) = \deg(i) \phi(i) . \tag{39}
\]

**Theorem 10.**

\[
\omega_G(u^2) = \sum_{C: \text{cycles}} 2^{|C|} \det[I + u^2(D - I) - uA] \big|_{G \setminus C} u^{|C|} , \tag{40}
\]

where \( \big|_{G \setminus C} \) denotes a restriction to the principal minor of \( G \setminus C \). The summation runs over all node disjoint cycles, i.e. 2-regular edge induced subgraphs. The number of connected components of \( C \) is denoted by \( k(C) \).
We omit the proof of theorem 10. The following corollary shows that $\omega_G$ is a matching polynomial if $G$ is a regular graph.

**Corollary 2.** If $G$ is a $(q + 1)$-regular graph, then
\[
\omega_G(u^2) = \alpha_G(1/u + qu)u^n. \tag{41}
\]

**Proof.** In [16], it is shown that
\[
\alpha_G(x) = \sum_{C: \text{cycles}} 2^k(C) \det[xI - A_G\setminus C]. \tag{42}
\]

If $G$ is a $(q + 1)$-regular graph, then $D = (q + 1)I$. From theorem 10 and (42), the assertion follows. \qed

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