Estimation of quenched random fields in the inverse Ising problem using a diagonal matching method

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We consider a method for the accurate estimation of quenched random fields in the inverse Ising problem. Approximations such as the mean-field or Bethe methods are applied to estimate quenched random coupling parameters and external fields. A diagonal matching method is introduced to ensure consistency of the diagonal part of the susceptibility, and the method yields an accurate estimation of the external fields. We introduce the diagonal matching method into the mean-field, Thouless-Anderson-Palmer, and Bethe approximations, and we investigate the effect of the diagonal matching method on the accuracy of estimation of the external fields.

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I. INTRODUCTION

Statistical physics has been deeply connected with computer science in recent years [1]. Techniques developed in statistical physics have been applied to various problems in computer science. The Monte Carlo method is one such technique, and the popularly used Monte Carlo method relies significantly on computing power. Two other techniques applicable to problems in computer science include the mean-field and Bethe approximations in statistical physics. These approximations are useful to estimate the marginals of a probability distribution with many random variables. Obtaining the average over a probability distribution with many variables is a laborious task even if we utilize an advanced computer. However, expectations can be easily evaluated using the marginals. Consequently, researchers have attempted to discover an accurate approximate method to estimate marginals. Invoking the Bayes formula, we can infer a cause from results, and the posterior probability in the Bayes formula is evaluated using the marginals. In the field of statistical physics, the mean-field and Bethe approximations have been developed to estimate expectations averaged over the Boltzmann distribution. In the field of computer science, the belief-propagation algorithm, which is the same as the Bethe approximation, has been discovered independently. The belief propagation consists of recursive procedures in which a message is passed from one vertex to another.

The inverse Ising problem, which is a typical problem common to fields ranging from statistical physics to computer science, has attracted considerable attention in recent years [2–6]. The inverse Ising problem originates from Boltzmann machine learning. In the conventional Ising model, magnetizations and correlation functions are estimated by averaging over the Boltzmann distribution, and these expectations are functions of coupling parameters between spins and external fields applied to spins. The inverse Ising problem consists of obtaining the inference of the coupling parameters and external fields from magnetizations and correlation functions. It has been pointed out that the inverse Ising problem has a close connection with inference in biological problems [7–11].

Provided that magnetizations and correlation functions are given, obtaining the inference of the coupling parameters and external fields is a computationally difficult problem. In this light, approximate methods have been proposed for obtaining the inference within feasible computational times. The mean-field method is useful to infer coupling parameters and external fields [12]. However, estimations made via the mean-field method lack accuracy and, therefore, advanced approximations such as the Thouless-Anderson-Palmer (TAP) method, Sessak–Monasson expansion, and Bethe approximation have been developed [13–17]. Since the mean-field approximation does not provide the correlation function between spins, we have to resort to the linear response theory [12]. The linear response theory provides the inference equations for the coupling parameters. When we solve the inference equations for the coupling parameters, the use of the diagonal matching method yields good estimations. Recently, it has been shown that the adaptive TAP equation [18,19] yields accurate estimations of the external fields [20]. It has also been shown that the adaptive TAP equation is similar to the mean-field approximation with the use of the diagonal matching method [21]. Raymond and Ricci-Tersenghi have expanded the matching method into off-diagonal constraint [22,23]. Thus, the diagonal matching method has drawn revived interest.

In this paper, we concentrate on accurate estimations of the external fields. The external fields are estimated more accurately by the diagonal matching method than by any conventional method. Although almost all of the existing studies have been performed by numerical methods, we focus on analytic elucidation of the diagonal matching method. We introduce the diagonal matching method into the mean-field, TAP, and Bethe approximations. The effect of the diagonal matching method is investigated analytically. The mean-field and TAP methods correspond to Gibbs free energy approximated up to the first and second order of the coupling parameters, respectively [24–26]. Therefore, the external fields are expressed as expansions up to the first and second orders of the coupling parameters. The introduction of the diagonal parameter into the mean-field and TAP approximations leads to the introduction of infinite-order terms of the coupling parameters into the external fields. The Bethe approximation is exact for treelike graphs. We find that the diagonal matching method introduces the effect of loops into the external fields.

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Recently, susceptibility propagation has been considered as an efficient approach to estimate a correlation function between spins [27–29]. Susceptibility propagation is an iterative algorithm for solving recursive equations. In addition, susceptibility propagation incorporating the diagonal matching method has been proposed and shown to provide good results. We show that the susceptibility propagation incorporating the diagonal matching method is identical to the Bethe approximation with the use of the diagonal matching method.

II. MODEL

Let us consider a graph $\mathcal{G}=(\mathcal{V},\mathcal{E})$, where $\mathcal{V}$ denotes a set of vertices labeled by $\{1,2,\ldots,N\}$, and $\mathcal{E}$ denotes a set of edges connecting vertices. On each vertex $i\in\mathcal{V}$, there is an Ising spin $S_i\in\{+1,-1\}$, and an external field h_i is randomly applied to the Ising spin. The system is completed by the following energy function:

$$H=-\sum_{i\in\mathcal{V}}h_iS_i-\sum_{(i,j)\in\mathcal{E}}J_{ij}S_iS_j, \tag{1}$$

wherein the second summation for (i,j) runs over all of the edges. The quantity J_{ij} represents the weight of a random coupling parameter between Ising spins S_i and S_j. For simplicity, we assume that the coupling parameter J_{ij} is symmetric with respect to i and j. If there is no edge between a vertex i and j, the value of J_{ij} is zero. The probability for the system to be found in the state $\{S_i\}$ is given by the following Boltzmann distribution:

$$P(\{S_i\})=\frac{1}{Z(\{h_i\},\{J_{ij}\})}\exp(-\beta H)$$
$$\text{with}\quad Z(\{h_i\},\{J_{ij}\})=\prod_{i\in\mathcal{V}}\sum_{S_i=\pm1}\exp(-\beta H), \tag{2}$$

where β denotes the inverse temperature. Denoting the expectation value with respect to the above Boltzmann distribution by angle brackets $\langle\cdots\rangle$, we obtain the magnetization on a vertex i and the correlation function between S_i and S_j as $\langle S_i\rangle$ and $\langle S_iS_j\rangle$, respectively. The magnetizations and correlation functions are functions of $\{h_i\}$ and $\{J_{ij}\}$. Given $\{h_i\}$ and $\{J_{ij}\}$, we can evaluate the magnetizations $\langle S_i\rangle$ and correlation functions $\langle S_iS_j\rangle$. However, an inverse Ising problem is formulated by evaluation of a set of $\{h_i\}$ and $\{J_{ij}\}$ from a given set of $\langle S_i\rangle$ and $\langle S_iS_j\rangle$. Given $\langle S_i\rangle$ and $\langle S_iS_j\rangle$, it is possible to evaluate the exact values of $\{h_i\}$ and $\{J_{ij}\}$ by adjusting them at the expense of an enormous amount of computation. In order to avoid such expensive computation, approximate methods have been developed.

It is useful to introduce the Gibbs free energy for the formulation of approximate methods. The Gibbs free energy is defined as

$$G(\{m_i\},\{J_{ij}\})=\max_{\{h_i\}}\left[\sum_{i\in\mathcal{V}}h_im_i-\frac{1}{\beta}\ln Z(\{h_i\},\{J_{ij}\})\right]. \tag{3}$$

The magnetization is derived from $\langle S_i\rangle=\mathrm{argmin}_{m_i}G(\{m_i\},\{J_{ij}\})$. Although it is impossible to evaluate Eq. (3) exactly, the Plefka expansion is a useful approximate method to evaluate $G(\{m_i\},\{J_{ij}\})$, and it is an expansion with respect to the coupling parameters $\{J_{ij}\}$ [25]. The Plefka expansion of $G(\{m_i\},\{J_{ij}\})$ is given by

$$G(\{m_i\},\{J_{ij}\})=\sum_{k=0}^{\infty}G^{(k)}(\{m_i\},\{J_{ij}\}), \tag{4}$$

wherein the superscript represents the order of the coupling parameters $\{J_{ij}\}$, and the values of $G^{(k)}(\{m_i\},\{J_{ij}\})$ up to the third-order term are [26]

$$G^{(0)}(\{m_i\},\{J_{ij}\})=\frac{1}{\beta}\sum_{i\in\mathcal{V}}\left(\frac{1+m_i}{2}\ln\frac{1+m_i}{2}+\frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right), \tag{5}$$

$$G^{(1)}(\{m_i\},\{J_{ij}\})=-\sum_{(i,j)\in\mathcal{E}}J_{ij}m_im_j, \tag{6}$$

$$G^{(2)}(\{m_i\},\{J_{ij}\})=-\frac{1}{2}\beta\sum_{(i,j)\in\mathcal{E}}J_{ij}^2\left(1-m_i^2\right)\left(1-m_j^2\right), \tag{7}$$

$$G^{(3)}(\{m_i\},\{J_{ij}\})=-\frac{2}{3}\beta^2\sum_{(i,j)\in\mathcal{E}}J_{ij}^3m_im_j\left(1-m_i^2\right)\left(1-m_j^2\right)-\beta^2\sum_{(i,j,k)}J_{ij}J_{jk}J_{ki}\left(1-m_i^2\right)\left(1-m_j^2\right)\left(1-m_k^2\right). \tag{8}$$

The symbol $\sum_{(i,j,k)}$ in Eq. (8) denotes summation over all three distinct vertices. The Gibbs free energy up to the first-order approximation in Eq. (4), i.e., $G\simeq G^{(0)}+G^{(1)}$, corresponds to the mean-field approximation, and the Gibbs free energy up to the second-order approximation, i.e., $G\simeq G^{(0)}+G^{(1)}+G^{(2)}$, corresponds to the TAP approximation [24].

By the property of the Legendre transformation, we obtain the external field h_i conjugated with m_i as follows:

$$h_i=\frac{\partial G(\{m_i\},\{J_{ij}\})}{\partial m_i}=\frac{1}{\beta}\tanh^{-1}m_i+\sum_{k=1}^{\infty}\frac{\partial G^{(k)}(\{m_i\},\{J_{ij}\})}{\partial m_i}. \tag{9}$$

As for the nth-order approximation, the external field yields

$$h_i=\frac{1}{\beta}\tanh^{-1}m_i+\sum_{k=1}^{n}\frac{\partial G^{(k)}(\{m_i\},\{J_{ij}\})}{\partial m_i}. \tag{10}$$

The right-hand side (rhs) of Eqs. (9) and (10) are functions of $\{m_i\}$ and $\{J_{ij}\}$. Consequently, if $\{m_i\}$ and $\{J_{ij}\}$ are given, the external field $\{h_i\}$ is approximately evaluated by Eq. (10). In order to estimate the coupling parameters $\{J_{ij}\}$, the linear response theory is utilized [12,13]. In the case of Eq. (1), the susceptibility between spins on the vertices i and j is defined by $\chi_{ij}=\langle S_iS_j\rangle-\langle S_i\rangle\langle S_j\rangle$ and is also expressed as $\beta\bar{\chi}_{ij}=\partial m_i/\partial h_j$. We distinguish χ_{ij} from $\bar{\chi}_{ij}$ because χ_{ij} is a given quantity in the inverse Ising problem and $\bar{\chi}_{ij}$ is derived from Eq. (9) or (10). We introduce two matrices $\boldsymbol{X}$ and $\boldsymbol{G}$ whose ijth elements are given by $(\boldsymbol{X})_{ij}=\chi_{ij}$ and $(\boldsymbol{G})_{ij}=\partial^2G/\partial m_i\partial m_j$, respectively. The coupling parameters $\{J_{ij}\}$ are evaluated from the relations

$$\beta \frac{\partial^2 G(\{m_i\},\{J_{ij}\})}{\partial m_i \partial m_j} = (X^{-1})_{ij}, \tag{11}$$

where $i \neq j$, and X^{-1} is an inverse matrix of X. Within the nth-order approximation, we approximate the Gibbs free energy at $G = \sum_{k=0}^{n} G^{(k)}$. In the case of $i \neq j$, the coupling parameter J_{ij} is estimated by the ijth element of Eq. (11). In the case of $i = j$, the left-hand side (lhs) of Eq. (11) does not equal the rhs when we use the approximate methods. In order to equalize the lhs of Eq. (11) with the rhs, the diagonal matching method has been proposed [12,13]. The diagonal matching method introduces additional parameters $\{\Lambda_i\}$ into the Gibbs free energy as follows:

$$G_{\rm DM}(\{m_i\},\{J_{ij}\}) = G(\{m_i\},\{J_{ij}\}) - \frac{1}{2}\sum_{i\in\mathcal{V}} \Lambda_i \left(1 - m_i^2\right), \tag{12}$$

where the subscript DM denotes the Gibbs free energy obtained using the diagonal matching method. The quantities $\{\Lambda_i\}$ are determined to satisfy the diagonal element of Eq. (11) or the following relation:

$$\beta\left(1 - m_i^2\right) = \left(G_{\rm DM}^{-1}\right)_{ii}, \tag{13}$$

where $(G_{\rm DM})_{ii} = \partial^2 G_{\rm DM}/\partial m_i^2 = \partial^2 G/\partial m_i^2 + \Lambda_i$ and $(G_{\rm DM})_{ij} = \partial^2 G_{\rm DM}/\partial m_i \partial m_j = \partial^2 G/\partial m_i \partial m_j$, provided $i \neq j$. Equation (13) is derived from the diagonal elements of $\beta X = G_{\rm DM}^{-1}$ by using the relation $\chi_{ii} = \langle S_i S_j\rangle - \langle S_i\rangle\langle S_j\rangle = 1 - m_i^2$. By considering Eq. (11) and the relation $\partial^2 G_{\rm DM}/\partial m_i \partial m_j = \partial^2 G/\partial m_i \partial m_j$ for $i \neq j$, we conclude that the use of the diagonal matching method does not influence the evaluation of J_{ij}. Substituting Eq. (12) into Eq. (9), we can derive the external field by the diagonal matching method as follows:

$$h_i = \frac{\partial G_{\rm DM}(\{m_i\},\{J_{ij}\})}{\partial m_i} = \frac{\partial G(\{m_i\},\{J_{ij}\})}{\partial m_i} + \Lambda_i m_i. \tag{14}$$

Upon comparing Eqs. (9) and (14), the external fields $\{h_i\}$ are found to be modified by the diagonal matching method, and they significantly depend on the values of $\{\Lambda_i\}$. We evaluate Λ_i using various approximate methods and compare them from the viewpoint of accuracy of approximations.

III. RESULTS

A. Mean-field theory with diagonal matching method

In this section, we consider the mean-field theory with the diagonal matching method. The Gibbs free energy of the mean-field theory with the diagonal matching method becomes

$$G_{\rm DM}^{\rm (mf)}(\{m_i\},\{J_{ij}\}) = G^{(0)}(\{m_i\},\{J_{ij}\}) + G^{(1)}(\{m_i\},\{J_{ij}\}) - \frac{1}{2}\sum_{i\in\mathcal{V}} \Lambda_i \left(1 - m_i^2\right), \tag{15}$$

where $G^{(0)}$ and $G^{(1)}$ are given by Eqs. (5) and (6), respectively. The second derivatives with respect to m_i and m_j yield

$$\frac{\partial^2 G_{\rm DM}^{\rm (mf)}(\{m_i\},\{J_{ij}\})}{\partial m_i \partial m_j} = -J_{ij} \quad (i \neq j), \tag{16}$$

$$\frac{\partial^2 G_{\rm DM}^{\rm (mf)}(\{m_i\},\{J_{ij}\})}{\partial m_i^2} = \frac{1}{\beta}\frac{1}{1 - m_i^2} + \Lambda_i, \tag{17}$$

where Eq. (16) corresponds to the off-diagonal element of $G_{\rm DM}$ and Eq. (17) corresponds to the diagonal element of $G_{\rm DM}$. Substituting Eqs. (16) and (17) into Eq. (13), we obtain the relation that determines Λ_i. Equation (13) is the adaptive TAP equation first introduced in Refs. [18,19]. In order to derive an implicit relation for Λ_i, we utilize the following formula given in Appendix A: upon dividing the matrix $G_{\rm DM}$ into the diagonal elements and off-diagonal elements, the diagonal elements and off-diagonal elements correspond to A and B, respectively. The formula (A3) can be applied to the derivation of $(G_{\rm DM}^{-1})_{ii}$ as follows:

$$\begin{aligned}
&\beta\left(1 - m_i^2\right) \\
&= \frac{\beta\left(1 - m_i^2\right)}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} + \frac{\beta\left(1 - m_i^2\right)}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} \\
&\quad \times \sum_{j\in\partial i} J_{ij} \frac{\beta\left(1 - m_j^2\right)}{1 + \Lambda_j\beta\left(1 - m_j^2\right)} J_{ji} \frac{\beta\left(1 - m_i^2\right)}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} \\
&\quad + \frac{\beta\left(1 - m_i^2\right)}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} \sum_{j\in\partial i}\sum_{k\in\partial i(k\neq j)} J_{ij} \frac{\beta\left(1 - m_j^2\right)}{1 + \Lambda_j\beta\left(1 - m_j^2\right)} \\
&\quad \times J_{jk} \frac{\beta\left(1 - m_k^2\right)}{1 + \Lambda_k\beta\left(1 - m_k^2\right)} J_{ki} \frac{\beta\left(1 - m_i^2\right)}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} + \cdots,
\end{aligned} \tag{18}$$

where $\sum_{j\in\partial i}$ denotes the summation with respect to all of the vertices connecting to a vertex i. Upon dividing both sides of Eq. (18) by $\beta(1 - m_i^2)/[1 + \Lambda_i\beta(1 - m_i^2)]$, we have

$$\begin{aligned}
&1 + \Lambda_i\beta\left(1 - m_i^2\right) \\
&= 1 + \sum_{j\in\partial i} \frac{\beta\left(1 - m_j^2\right)}{1 + \Lambda_j\beta\left(1 - m_j^2\right)} J_{ij}^2 \frac{\beta\left(1 - m_i^2\right)}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} \\
&\quad + \sum_{j\in\partial i}\sum_{k\in\partial i(k\neq j)} \frac{\beta\left(1 - m_j^2\right)}{1 + \Lambda_j\beta\left(1 - m_j^2\right)} \frac{\beta\left(1 - m_k^2\right)}{1 + \Lambda_k\beta\left(1 - m_k^2\right)} \\
&\quad \times J_{ij}J_{jk}J_{ki} \frac{\beta\left(1 - m_i^2\right)}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} + \cdots.
\end{aligned} \tag{19}$$

After rearrangement of the expression, we obtain the following implicit relation for Λ_i:

$$\begin{aligned}
\Lambda_i &= \frac{1}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} \sum_{j\in\partial i} \frac{\beta\left(1 - m_j^2\right)}{1 + \Lambda_j\beta\left(1 - m_j^2\right)} J_{ij}^2 \\
&\quad + \frac{1}{1 + \Lambda_i\beta\left(1 - m_i^2\right)} \sum_{j\in\partial i}\sum_{k\in\partial i(k\neq j)} \frac{\beta\left(1 - m_j^2\right)}{1 + \Lambda_j\beta\left(1 - m_j^2\right)} \\
&\quad \times \frac{\beta\left(1 - m_k^2\right)}{1 + \Lambda_k\beta\left(1 - m_k^2\right)} J_{ij}J_{jk}J_{ki} + \cdots.
\end{aligned} \tag{20}$$

We evaluate Λ_i using an iterative method. Substituting $\Lambda_i = 0$ into the rhs of Eq. (20), Λ_i, which is up to the third-order terms of $\{J_{ij}\}$, is obtained as

$$\Lambda_i = \beta \sum_{j\in\partial i} J_{ij}^2 (1-m_j^2) + \beta^2 \sum_{j\in\partial i} \sum_{k\in\partial i (k\neq j)} J_{ij} \times J_{jk} J_{ki} (1-m_j^2)(1-m_k^2) + O(J_{ij}^4). \quad (21)$$

Correction for higher-order terms of $\{J_{ij}\}$ in Λ_i is obtained by considering the higher-order terms in Eq. (18) and substitution of Eq. (21) into the rhs of Eq. (20). The first term in Eq. (21) corresponds to the Onsager reaction term. Substituting Eqs. (15) and (21) into Eq. (14), we obtain

$$h_i = \frac{1}{\beta} \tanh^{-1} m_i - \sum_{j\in\partial i} J_{ij} m_j + \beta \sum_{j\in\partial i} J_{ij}^2 m_i (1-m_j^2) + 2\beta^2 \sum_{(j,k)\in\mathcal{E}} J_{ij} J_{jk} J_{ki} m_i (1-m_j^2)(1-m_k^2) + O(J_{ij}^4). \quad (22)$$

The third and fourth terms in Eq. (22) stem from the diagonal matching method, i.e., Λ_i in Eq. (14). Substituting Eqs. (6)–(8) into Eq. (9), we obtain an exact formula of the external field as follows:

$$h_i = \frac{1}{\beta} \tanh^{-1} m_i - \sum_{j\in\partial i} J_{ij} m_j + \beta \sum_{j\in\partial i} J_{ij}^2 m_i (1-m_j^2) \underline{- \frac{2}{3}\beta^2 \sum_{j\in\partial i} J_{ij}^3 (1-3m_i^2) m_j (1-m_j^2)} + 2\beta^2 \sum_{(j,k)\in\mathcal{E}} J_{ij} J_{jk} J_{ki} m_i (1-m_j^2)(1-m_k^2) + O(J_{ij}^4). \quad (23)$$

The mean-field method is an approximation up to the first order of $\{J_{ij}\}$. By the use of the diagonal matching method, the external field is correct up to the second order of $\{J_{ij}\}$, and it is partially correct up to the third order of $\{J_{ij}\}$. The second-order term of $\{J_{ij}\}$ in Eq. (22) corresponds to the Onsager reaction term. Although the mean-field method does not contain the Onsager reaction term in the approximated Gibbs free energy, the term $\{\Lambda_i\}$ in Eq. (15) includes the Onsager reaction term. The term Λ_i partially reproduces the third-order term of $\{J_{ij}\}$, but the underlined term in Eq. (23) is not included in Eq. (22). We consider that the term Λ_i of the diagonal matching method partially reproduces the higher-order terms of $\{J_{ij}\}$ in the external field. General-order terms of $\{J_{ij}\}$ are discussed later.

B. TAP theory with diagonal matching method

Within the TAP approximation, the Gibbs free energy is expressed by an expansion up to the second order of $\{J_{ij}\}$ as follows:

$$G_{\rm DM}^{\rm (TAP)}(\{m_i\},\{J_{ij}\}) = G^{(0)}(\{m_i\},\{J_{ij}\}) + G^{(1)}(\{m_i\},\{J_{ij}\}) + G^{(2)}(\{m_i\},\{J_{ij}\}) - \frac{1}{2}\sum_{i\in\mathcal{V}} \Lambda_i (1-m_i^2). \quad (24)$$

The second derivatives with respect to m_i and m_j yield

$$\frac{\partial^2 G_{\rm DM}^{\rm (TAP)}(\{m_i\},\{J_{ij}\})}{\partial m_i \partial m_j} = -J_{ij} - 2\beta m_i m_j J_{ij}^2 \quad (i\neq j), \quad (25)$$

$$\frac{\partial^2 G_{\rm DM}^{\rm (TAP)}(\{m_i\},\{J_{ij}\})}{\partial m_i^2} = \frac{1}{\beta}\frac{1}{1-m_i^2} + \beta \sum_{j\in\partial i} J_{ij}^2 (1-m_j^2) + \Lambda_i. \quad (26)$$

Equation (25) corresponds to the off-diagonal element of $\boldsymbol{G}_{\rm DM}$, and Eq. (26) corresponds to the diagonal element. Using Eq. (A3), we can evaluate an inverse matrix of $\boldsymbol{G}_{\rm DM}$. Substituting the inverse matrix into Eq. (13), we obtain the relation that determines Λ_i as follows:

$$\beta(1-m_i^2) = \frac{\beta(1-m_i^2)}{1+\beta(1-m_i^2)[\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2 + \Lambda_i]} + \frac{\beta(1-m_i^2)}{1+\beta(1-m_i^2)[\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2 + \Lambda_i]} \times \sum_{j\in\partial i}(J_{ij} + 2\beta m_i m_j J_{ij}^2) \times \frac{\beta(1-m_j^2)}{1+\beta(1-m_j^2)[\sum_{k\in\partial j}\beta(1-m_k^2)J_{jk}^2 + \Lambda_j]} \times (J_{ij} + 2\beta m_i m_j J_{ij}^2) \times \frac{\beta(1-m_i^2)}{1+\beta(1-m_i^2)[\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2 + \Lambda_i]} \times + \cdots. \quad (27)$$

Multiplication of $\{1+\beta(1-m_i^2)[\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2 + \Lambda_i]\}/\beta(1-m_i^2)$ to both sides of Eq. (27) yields

$$1+\beta(1-m_i^2)\left[\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2 + \Lambda_i\right] = 1 + \sum_{j\in\partial i}\frac{\beta(1-m_j^2)}{1+\beta(1-m_j^2)[\sum_{k\in\partial j}\beta(1-m_k^2)J_{jk}^2 + \Lambda_j]} \times \frac{\beta(1-m_i^2)}{1+\beta(1-m_i^2)[\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2 + \Lambda_i]} \times (J_{ij} + 2\beta m_i m_j J_{ij}^2)^2 + \cdots. \quad (28)$$

After rearrangement of the expression, we obtain

$$\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2 + \Lambda_i = \sum_{j\in\partial i}\frac{\beta(1-m_j^2)}{1+\beta(1-m_j^2)[\sum_{k\in\partial j}\beta(1-m_k^2)J_{jk}^2 + \Lambda_j]} \times \frac{(J_{ij} + 2\beta m_i m_j J_{ij}^2)^2}{1+\beta(1-m_i^2)[\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2 + \Lambda_i]} + \cdots. \quad (29)$$

Equation (29) determines Λ_i implicitly. Before evaluation of Λ_i, we estimate $\sum_{k\in\partial i}\beta(1-m_k^2)J_{ik}^2+\Lambda_i$ iteratively. Substituting $\sum_{k\in\partial l}\beta(1-m_k^2)J_{lk}^2+\Lambda_l=0$, where $l=i$ or j, into the rhs of Eq. (29), we obtain

$$\sum_{k\in\partial i}\beta\left(1-m_k^2\right)J_{ik}^2+\Lambda_i = \sum_{j\in\partial i}\beta\left(1-m_j^2\right)\left(J_{ij}+2\beta m_i m_j J_{ij}^2\right)^2+\cdots. \quad (30)$$

As a result, Λ_i becomes

$$\Lambda_i = 4\beta^2\sum_{j\in\partial i}J_{ij}^3 m_i m_j\left(1-m_j^2\right)+2\beta^2\sum_{(j,k)\in\mathcal{E}}J_{ij}J_{jk} \times J_{ki}\left(1-m_j^2\right)\left(1-m_k^2\right)+O\left(J_{ij}^4\right). \quad (31)$$

The second term in Eq. (31) is evaluated by considering the next-order term in Eq. (27). Substituting Eqs. (24) and (31) into Eq. (14), we derive the external field as

$$h_i = \frac{1}{\beta}\tanh^{-1}m_i-\sum_{j\in\partial i}J_{ij}m_j+\beta\sum_{j\in\partial i}J_{ij}^2 m_i\left(1-m_j^2\right) + 4\beta^2\sum_{j\in\partial i}J_{ij}^3 m_i^2 m_j\left(1-m_j^2\right)+2\beta^2\sum_{(j,k)\in\mathcal{E}}J_{ij}J_{jk} \times J_{ki}m_i\left(1-m_j^2\right)\left(1-m_k^2\right)+O\left(J_{ij}^4\right). \quad (32)$$

Equation (32) represents the external field evaluated by the TAP approximation with the diagonal matching method. A comparison of Eqs. (23) and (32) indicates that the TAP approximation with the diagonal matching method does not correctly yield the underlined term in Eq. (23). Although the TAP approximation is exact up to the second-order term of $\{J_{ij}\}$, the diagonal matching method yields a part of correct terms, which are of a higher order than the second-order term.

C. Arbitrary-order theory with diagonal matching method

In this section, we consider the effect of the diagonal matching method on inference about the external field in the case that the Gibbs free energy is composed of arbitrary-order terms of the coupling parameter. The Gibbs free energy up to nth order of the coupling parameter is given by

$$G_{\rm DM}^{(n{\rm th})}(\{m_i\},\{J_{ij}\}) = \sum_{k=0}^{n}G^{(k)}(\{m_i\},\{J_{ij}\})-\frac{1}{2}\sum_{i\in\mathcal{V}}\Lambda_i\left(1-m_i^2\right). \quad (33)$$

The above Gibbs free energy with $n=1$ corresponds to the Gibbs free energy of the mean-field approximation and that with $n=2$ corresponds to that of the TAP approximation. The diagonal matching parameter Λ_i is determined by the diagonal element of Eq. (11) or Eq. (13). Substituting Eq. (33) into the diagonal element of Eq. (11), we obtain the following relation for Λ_i:

$$\beta\frac{\partial^2 G_{\rm DM}^{(n{\rm th})}}{\partial m_i^2} = \beta\sum_{k=0}^{n}\frac{\partial^2 G^{(k)}}{\partial m_i^2}+\beta\Lambda_i = (\boldsymbol{X}^{-1})_{ii}. \quad (34)$$

The rhs of Eq. (34) is given by the inverse matrix of the susceptibility matrix $\boldsymbol{X}$, which is composed of the susceptibilities. Since the susceptibilities are evaluated by the Boltzmann distribution, the inverse matrix of the susceptibility matrix is given by the exact Gibbs free energy. Substituting the exact Gibbs free energy, i.e., Eq. (4), into the rhs of Eq. (34), we obtain Λ_i as follows:

$$\Lambda_i = \sum_{k=n+1}^{\infty}\frac{\partial^2 G^{(k)}}{\partial m_i^2}. \quad (35)$$

By substitution of Eq. (35) into Eq. (14), we formulate the external field given by the diagonal matching method as follows:

$$h_i = \frac{\partial G_{\rm DM}^{(n{\rm th})}}{\partial m_i} = \sum_{k=0}^{n}\frac{\partial G^{(k)}}{\partial m_i}+\sum_{k=n+1}^{\infty}\frac{\partial^2 G^{(k)}}{\partial m_i^2}m_i. \quad (36)$$

Equation (36) provides the approximate external field evaluated by the nth-order Gibbs free energy with the diagonal matching method. The exact external field is given by Eq. (9). A comparison of Eqs. (9) and (36) indicates that the diagonal matching method yields exact terms up to nth order of the coupling parameter and approximates $\partial G^{(k)}/\partial m_i$ at $\partial^2 G^{(k)}/\partial m_i^2\times m_i$ for $n<k$. When the dependence of $G^{(k)}$ on m_i is $G^{(k)}=a+bm_i^2$ (a and b are independent of m_i), the relation $\partial G^{(k)}/\partial m_i=\partial^2 G^{(k)}/\partial m_i^2\times m_i$ is satisfied, and the diagonal matching method yields the correct terms. Since the m_i dependence of the term in Eq. (7) and the second term in Eq. (8) are proportional to $(1-m_i^2)$, these terms are correctly reproduced by the diagonal matching method. We conclude that the higher-order terms, whose m_i dependence is $(1-m_i^2)$, are correctly reproduced by the diagonal matching method. Since the first term in Eq. (8) is not proportional to $(1-m_i^2)$, it is not correctly reproduced by the diagonal matching method. Substituting the first term in Eq. (8) into the formula $\partial^2 G^{(k)}/\partial m_i^2\times m_i$, we obtain the fourth term in Eq. (32) in the case of the TAP approximation. Although we investigate the validity of the diagonal matching method by using the relation (34), the diagonal matching parameter Λ_i is determined by the relation (13). As for the mean-field approximation, since the off-diagonal elements of Eq. (16) are given by $\partial^2 G_{\rm DM}^{(\rm mf)}/\partial m_i\partial m_j=-J_{ij}$, the diagonal matching method does not yield the fourth term in Eq. (32). Taking into consideration the higher-order terms of the coupling parameter, we can reproduce the fourth term in Eq. (32) by using the mean-field approximation with the diagonal matching method.

D. Bethe approximation with diagonal matching method

In this section, we consider inference about the external field by the Bethe approximation with the diagonal matching method. The Gibbs free energy of the Bethe approximation is formulated by [15–17]

$$G^{(\mathrm{Bethe})}(\{m_i\},\{J_{ij}\}) = -\sum_{(i,j)\in\mathcal{E}} J_{ij}\xi_{ij} + \frac{1}{\beta}\sum_{i\in\mathcal{V}}(1-|\partial i|)\sum_{S_i=\pm1}\rho_1(S_i|m_i)\ln\rho_1(S_i|m_i) + \frac{1}{\beta}\sum_{(i,j)\in\mathcal{E}}\sum_{S_i=\pm1}\sum_{S_j=\pm1}\rho_2(S_i,S_j|m_i,m_j,\xi_{ij})\ln\rho_2(S_i,S_j|m_i,m_j,\xi_{ij}), \tag{37}$$

where

$$\rho_1(S_i|m_i) = \frac{1+S_i m_i}{2}, \tag{38}$$

$$\rho_2(S_i,S_j|m_i,m_j,\xi_{ij}) = \frac{1+S_i m_i + S_j m_j + S_i S_j \xi_{ij}}{4}, \tag{39}$$

$$\xi_{ij} = \cosh(2\beta J_{ij})\left[1-\sqrt{1-\left(1-m_i^2-m_j^2\right)\tanh^2(2\beta J_{ij}) - 2m_i m_j\tanh(2\beta J_{ij})}\right]. \tag{40}$$

The mean-field approximation adopts an approach to account for the effect of the other spins with an external field. In the Bethe approximation, the effect of two spins is considered in the approximation, and the effect of the other spins is considered as an external field. Equations (38) and (39) correspond to the one-spin and two-spin marginal probabilities, respectively. From the viewpoint of the expansion with respect to the order of the coupling parameter, the Bethe approximation corresponds to resumming for all of the orders of the coupling parameters between two spins in the Plefka expansion [30]. Another advantage of the Bethe approximation is that it is formulated by the message-passing rule of belief propagations [31]. The Gibbs free energy by the Bethe approximation with the diagonal matching method is given by

$$G_{\mathrm{DM}}^{(\mathrm{Bethe})}(\{m_i\},\{J_{ij}\}) = G^{(\mathrm{Bethe})}(\{m_i\},\{J_{ij}\}) - \frac{1}{2}\sum_{i\in\mathcal{V}}\Lambda_i\left(1-m_i^2\right). \tag{41}$$

By differentiating Eq. (41) with respect to m_i, the external field is obtained as

$$h_i = \frac{\partial G_{\mathrm{DM}}^{(\mathrm{Bethe})}}{\partial m_i} = \frac{1}{\beta}\tanh^{-1}m_i - \frac{1}{\beta}\sum_{j\in\partial i}M_{j\to i} + \Lambda_i m_i, \tag{42}$$

where $M_{j\to i}$ denotes a message that propagates from vertex j to vertex i. The quantity $M_{j\to i}$ is defined as

$$M_{j\to i} = -\frac{1}{2}\tanh^{-1}\left(\frac{m_i+\xi_{ij}}{1+m_j}\right) - \frac{1}{2}\tanh^{-1}\left(\frac{m_i-\xi_{ij}}{1-m_j}\right) + \tanh^{-1}m_i, \tag{43}$$

or expressed by an iterative relation. The second derivatives of $G_{\mathrm{DM}}^{(\mathrm{Bethe})}$ with respect to m_i and m_j are derived as

$$\frac{\partial^2 G_{\mathrm{DM}}^{(\mathrm{Bethe})}(\{m_i\},\{J_{ij}\})}{\partial m_i\partial m_j} = -\frac{1}{\beta}\frac{\partial M_{j\to i}}{\partial m_j}, \tag{44}$$

$$\frac{\partial^2 G_{\mathrm{DM}}^{(\mathrm{Bethe})}(\{m_i\},\{J_{ij}\})}{\partial m_i^2} = \frac{1}{\beta}\frac{1}{1-m_i^2} - \frac{1}{\beta}\sum_{j\in\partial i}\frac{\partial M_{j\to i}}{\partial m_i} + \Lambda_i. \tag{45}$$

Substituting Eqs. (44) and (45) into the rhs of Eq. (13), we obtain the relation that determines Λ_i. By using the same derivation as those used in the mean-field and TAP approximations, the implicit equation for Λ_i is obtained as follows:

$$\begin{aligned}\beta\Lambda_i - \sum_{x\in\partial i}\frac{\partial M_{x\to i}}{\partial m_i} &= \sum_{j\in\partial i}\frac{\beta}{1+\left(1-m_i^2\right)\left[\beta\Lambda_i - \sum_{x\in\partial i}\frac{\partial M_{x\to i}}{\partial m_i}\right]}\frac{\beta\left(1-m_j^2\right)}{1+\left(1-m_j^2\right)\left[\beta\Lambda_j - \sum_{y\in\partial j}\frac{\partial M_{y\to j}}{\partial m_j}\right]}\left(-\frac{1}{\beta}\frac{\partial M_{j\to i}}{\partial m_j}\right)^2\\ &\quad - \sum_{j\in\partial i}\sum_{k\in\partial i(k\neq j)}\frac{\beta}{1+\left(1-m_i^2\right)\left[\beta\Lambda_i - \sum_{x\in\partial i}\frac{\partial M_{x\to i}}{\partial m_i}\right]}\frac{\beta\left(1-m_j^2\right)}{1+\left(1-m_j^2\right)\left[\beta\Lambda_j - \sum_{y\in\partial j}\frac{\partial M_{y\to j}}{\partial m_j}\right]}\\ &\quad\times\frac{\beta\left(1-m_k^2\right)}{1+\left(1-m_k^2\right)\left[\beta\Lambda_k - \sum_{z\in\partial k}\frac{\partial M_{z\to k}}{\partial m_k}\right]}\left(-\frac{1}{\beta}\frac{\partial M_{j\to i}}{\partial m_j}\right)\left(-\frac{1}{\beta}\frac{\partial M_{k\to j}}{\partial m_k}\right)\left(-\frac{1}{\beta}\frac{\partial M_{i\to k}}{\partial m_i}\right)\\ &\quad+\cdots.\end{aligned} \tag{46}$$

Substituting $\beta\Lambda_l - \sum_{x\in\partial l}\frac{\partial M_{x\to l}}{\partial m_l} = 0$ with $l = i,j,k$ into the rhs of Eq. (46), we obtain Λ_i up to the third-order terms of $\frac{\partial M_{j\to i}}{\partial m_j}$ as follows:

$$\beta\Lambda_i = \sum_{j\in\partial i}\frac{\partial M_{j\to i}}{\partial m_i} + \sum_{j\in\partial i}(1-m_i^2)\left(\frac{\partial M_{j\to i}}{\partial m_j}\right)^2 + \sum_{j\in\partial i}\sum_{k\in\partial i(k\neq j)}(1-m_j^2)(1-m_k^2)\frac{\partial M_{j\to i}}{\partial m_j}\frac{\partial M_{k\to j}}{\partial m_k}\frac{\partial M_{i\to k}}{\partial m_i} + \cdots. \tag{47}$$

By substitution of Eqs. (B2) and (B3) into Eq. (47), we obtain the diagonal matching parameter Λ_i, which is expanded with respect to J_{ij}, as follows:

$$\Lambda_i = \beta^2\sum_{j\in\partial i}\sum_{k\in\partial i(k\neq j)} J_{ij}J_{jk}J_{ki}(1-m_j^2)(1-m_k^2) + O(J_{ij}^4). \tag{48}$$

Substituting Eq. (48) into Eq. (42) and expanding Eq. (42) with respect to the coupling parameters, we obtain

$$\begin{aligned} h_i =& \frac{1}{\beta}\tanh^{-1} m_i - \sum_{j\in\partial i} J_{ij}m_j + \beta\sum_{j\in\partial i} J_{ij}^2 m_i(1-m_j^2) - \frac{2}{3}\beta^2\sum_{j\in\partial i} J_{ij}^3(1-3m_i^2)m_j(1-m_j^2) \\ &+ 2\beta^2\sum_{(j,k)\in\mathcal{E}} J_{ij}J_{jk}J_{ki}m_i(1-m_j^2)(1-m_k^2) + O(J_{ij}^4). \end{aligned} \tag{49}$$

Equation (49) is in accord with Eq. (23) up to the third-order terms of the coupling parameters. The above term Λ_i includes the fifth term in Eq. (23). Since the Bethe approximation includes the contribution of clusters composed of two vertices, the Bethe-approximated Gibbs free energy includes all of the terms of $(J_{ij})^n$ in the Plefka expansion given by Eqs. (6)–(8). The Bethe approximation is exact for the system that does not include loops consisting of more than three edges. Equation (48) indicates that the contribution of the loops is included in the Bethe-approximated Gibbs free energy by the introduction of the diagonal matching method. By the diagonal matching method, the arbitrary-order terms that satisfy the relation $\partial G^{(k)}/\partial m_i = \partial^2 G^{(k)}/\partial m_i^2 \times m_i$ are included in the inferred external field.

E. Equivalence between Bethe approximation and susceptibility propagation

Susceptibility is required to infer the coupling parameter in the inverse Ising problem. In order to estimate the susceptibility, the susceptibility propagation algorithm has recently been introduced to address the inverse Ising problem [27–29]. In this section, we show the equivalence between the Bethe approximation with the diagonal matching method and susceptibility propagation with the diagonal matching method [21]. Differentiating both sides of Eq. (42) by h_j and rearranging the expression, we obtain the susceptibility as follows:

$$\beta\bar{\chi}_{ij} = \frac{1-m_i^2}{1+\beta\Lambda_i(1-m_i^2)}\left(\beta\delta_{ij} + \sum_{k\in\partial i}\eta_{k\to i}^{(j)}\right), \tag{50}$$

where δ_{ij} represents the Kronecker's delta and $\eta_{k\to i}^{(j)} = \partial M_{k\to i}/\partial h_j$. The formula $\eta_{k\to i}^{(j)}$ is also expressed by a recursive equation. Substituting the iterative solution $\eta_{k\to i}^{(j)}$ of the recursive equation into Eq. (50), we can evaluate the susceptibility. The adjustment of Λ_i for $\bar{\chi}_{ii} = 1-m_i^2$ leads to

$$\bar{\Lambda}_i = \frac{1}{\beta^2}\frac{1}{1-m_i^2}\sum_{j\in\partial i}\eta_{j\to i}^{(i)}. \tag{51}$$

In order to distinguish Eq. (51) from Λ_i derived by Eq. (11), we attach a bar to Λ_i.

To begin with, we show the equivalence of the inferred coupling parameter between the Bethe approximation with the diagonal matching method and the susceptibility propagation with the diagonal matching method. By multiplication of both sides of Eq. (50) by $[1+\beta\Lambda_i(1-m_i^2)]/[\beta(1-m_i^2)]$, we obtain

$$\beta\bar{\chi}_{ij}\left(\frac{1}{\beta}\frac{1}{1-m_i^2} + \Lambda_i\right) = \delta_{ij} + \frac{1}{\beta}\sum_{k\in\partial i}\eta_{k\to i}^{(j)}. \tag{52}$$

From the definition of $M_{k\to i}$ in Eq. (43), $\eta_{k\to i}^{(j)}$ is transformed into

$$\begin{aligned} \eta_{k\to i}^{(j)} &= \frac{\partial M_{k\to i}}{\partial h_j} = \frac{\partial M_{k\to i}}{\partial m_k}\frac{\partial m_k}{\partial h_j} + \frac{\partial M_{k\to i}}{\partial m_i}\frac{\partial m_i}{\partial h_j} \\ &= \frac{\partial M_{k\to i}}{\partial m_k}\beta\bar{\chi}_{kj} + \frac{\partial M_{k\to i}}{\partial m_i}\beta\bar{\chi}_{ij}, \end{aligned} \tag{53}$$

where we use the property that $M_{k\to i}$ is a function of m_k and m_i. Substituting Eq. (53) into Eq. (52), we obtain the following formula:

$$\begin{aligned} &\beta\bar{\chi}_{ij}\left(\frac{1}{\beta}\frac{1}{1-m_i^2} + \Lambda_i\right) \\ &\quad = \delta_{ij} + \frac{1}{\beta}\sum_{k\in\partial i}\left(\frac{\partial M_{k\to i}}{\partial m_k}\beta\bar{\chi}_{kj} + \frac{\partial M_{k\to i}}{\partial m_i}\beta\bar{\chi}_{ij}\right). \end{aligned} \tag{54}$$

Equation (54) is transformed into

$$\begin{aligned} &\beta\bar{\chi}_{ij}\left(\frac{1}{\beta}\frac{1}{1-m_i^2} - \frac{1}{\beta}\sum_{k\in\partial i}\frac{\partial M_{k\to i}}{\partial m_i} + \Lambda_i\right) \\ &\quad - \frac{1}{\beta}\sum_{k\in\partial i}\frac{\partial M_{k\to i}}{\partial m_k}\beta\bar{\chi}_{kj} = \delta_{ij}, \end{aligned} \tag{55}$$

and, subsequently, taking Eqs. (44) and (45) into consideration, we obtain the following formula:

$$\frac{\partial^2 G_{\rm DM}^{(\rm Bethe)}}{\partial m_i^2}\beta\bar{\chi}_{ij} + \sum_{k\in\partial i}\frac{\partial^2 G_{\rm DM}^{(\rm Bethe)}}{\partial m_i\partial m_k}\beta\bar{\chi}_{kj} = \delta_{ij}. \tag{56}$$

Equation (56) is rewritten as

$$\beta\big(\boldsymbol{G}_{\rm DM}^{\rm (Bethe)}\bar{\boldsymbol{X}}\big)_{ij} = \delta_{ij}, \tag{57}$$

where $(\bar{\boldsymbol{X}})_{ij} = \bar{\chi}_{ij}$. Equation (57) indicates the equivalence between the Bethe approximation with the diagonal matching method and susceptibility propagation with the diagonal matching method.

We next show the equivalence between Λ_i evaluated by Eq. (11) and $\bar{\Lambda}_i$ in Eq. (51). Invoking Eq. (53), we transform Eq. (51) into the following formula:

$$\begin{aligned}\bar{\Lambda}_i =& \frac{1}{\beta^2}\frac{1}{1-m_i^2}\sum_{j\in\partial i}\left(\frac{\partial M_{j\to i}}{\partial m_j}\beta\bar{\chi}_{ji} + \frac{\partial M_{j\to i}}{\partial m_i}\beta\bar{\chi}_{ii}\right)\\ =& \frac{1}{\beta}\frac{1}{1-m_i^2}\sum_{j\in\partial i}\frac{\partial M_{j\to i}}{\partial m_j}\bar{\chi}_{ji} + \frac{1}{\beta}\sum_{j\in\partial i}\frac{\partial M_{j\to i}}{\partial m_i},\end{aligned} \tag{58}$$

where we use the formula $\bar{\chi}_{ii} = 1 - m_i^2$. On the other hand, Λ_i is determined by the diagonal element of $\beta(\boldsymbol{G}_{\rm DM}^{\rm (Bethe)})_{ij} = (\bar{\boldsymbol{X}}^{-1})_{ij}$, which is derived from Eq. (57), as follows:

$$\beta\frac{\partial^2 G_{\rm DM}^{\rm (Bethe)}}{\partial m_i^2} = \beta\left(\frac{\partial^2 G^{\rm (Bethe)}}{\partial m_i^2} + \Lambda_i\right) = (\bar{\boldsymbol{X}}^{-1})_{ii}, \tag{59}$$

and, subsequently, we obtain

$$\begin{aligned}\Lambda_i =& -\frac{\partial^2 G^{\rm (Bethe)}}{\partial m_i^2} + \frac{1}{\beta}(\bar{\boldsymbol{X}}^{-1})_{ii}\\ =& -\frac{1}{\beta}\frac{1}{1-m_i^2} + \frac{1}{\beta}\sum_{j\in\partial i}\frac{\partial M_{j\to i}}{\partial m_i} + \frac{1}{\beta}(\bar{\boldsymbol{X}}^{-1})_{ii},\end{aligned} \tag{60}$$

where we use Eq. (45). The expression $(\bar{\boldsymbol{X}}^{-1})_{ii}$ is derived from the following relation:

$$\begin{aligned}1 =& \sum_j(\bar{\boldsymbol{X}}^{-1})_{ij}(\bar{\boldsymbol{X}})_{ji}\\ =& \sum_{j\in\partial i}(\bar{\boldsymbol{X}}^{-1})_{ij}(\bar{\boldsymbol{X}})_{ji} + (\bar{\boldsymbol{X}}^{-1})_{ii}(\bar{\boldsymbol{X}})_{ii}\\ =& \sum_{j\in\partial i}(\bar{\boldsymbol{X}}^{-1})_{ij}(\bar{\boldsymbol{X}})_{ji} + (\bar{\boldsymbol{X}}^{-1})_{ii}\big(1-m_i^2\big),\end{aligned} \tag{61}$$

and, subsequently, from the final line in Eq. (61), we obtain

$$\begin{aligned}(\bar{\boldsymbol{X}}^{-1})_{ii} =& \frac{1}{1-m_i^2} - \frac{1}{1-m_i^2}\sum_{j\in\partial i}(\bar{\boldsymbol{X}}^{-1})_{ij}(\bar{\boldsymbol{X}})_{ji}\\ =& \frac{1}{1-m_i^2} - \frac{\beta}{1-m_i^2}\sum_{j\in\partial i}\frac{\partial^2 G_{\rm DM}^{\rm (Bethe)}}{\partial m_i\partial m_j}\bar{\chi}_{ji}\\ =& \frac{1}{1-m_i^2} + \frac{1}{1-m_i^2}\sum_{j\in\partial i}\frac{\partial M_{j\to i}}{\partial m_j}\bar{\chi}_{ji}.\end{aligned} \tag{62}$$

Substituting Eq. (62) into $(\bar{\boldsymbol{X}}^{-1})_{ii}$ in Eq. (60), we obtain

$$\Lambda_i = \frac{1}{\beta}\sum_{j\in\partial i}\frac{\partial M_{j\to i}}{\partial m_i} + \frac{1}{\beta}\frac{1}{1-m_i^2}\sum_{j\in\partial i}\frac{\partial M_{j\to i}}{\partial m_j}\bar{\chi}_{ji} = \bar{\Lambda}_i. \tag{63}$$

From Eqs. (57) and (63), we observe the equivalence between the Bethe approximation with the diagonal matching method and susceptibility propagation with the diagonal matching method. The quantity $\bar{\Lambda}_i$, therefore, is obtained as Eq. (47) or (48). These two methods yield the same values of $\{J_{ij}\}$ and $\{h_i\}$ in the inverse Ising problem.

IV. SUMMARY AND DISCUSSION

We considered inference about the coupling parameters and external fields in the inverse Ising problem by the use of approximations. Some conventional approximations are classified by the order of the coupling parameters. The Gibbs free energy approximated up to the first-order term of the coupling parameters and the second-order term correspond to Gibbs free energies of the mean-field method and the TAP method, respectively. The Gibbs free energy that includes all of the $(J_{ij})^n$ terms corresponds to the Bethe approximation. The higher is the order of terms that the approximation contains in the Gibbs free energy, the more accurate is the estimation of the coupling parameters and the external fields it gives. Although the number of the unknown coupling parameters $\{J_{ij}\}$ is $N(N-1)/2$, the number of the derivatives of the Gibbs free energy with respect to m_i and m_j is $N(N+1)/2$. The number of the unknown parameters is smaller than the number of conditions. In order to utilize redundant conditions, the diagonal matching method is introduced. The diagonal matching method has been numerically shown to provide an accurate estimation of the external fields. We analytically evaluated the diagonal parameters Λ_i for the mean-field, TAP, and Bethe approximations, and we investigated the effect of the diagonal matching method on inference of the external fields. As for the naive mean-field approximation and TAP approximation, the estimated external fields are given by expansions of the finite-order terms of the coupling parameters. By introduction of the diagonal matching method, we can include the infinite-order terms of the coupling parameters in the external fields. The diagonal parameter Λ_i is evaluated by means of two distinct approaches using Eqs. (13) and (34), and Λ_i evaluated by Eq. (13) differs from that by Eq. (34). In the case of the mean-field approximation with the diagonal matching method, it has already been numerically shown that the external fields evaluated through Λ_i by Eq. (13) differ from those evaluated using Eq. (34). The derivation through Eq. (13) corresponds to the adaptive TAP equation. In this paper, we extended the adaptive TAP equation to the case of the Gibbs free energy that contains the higher-order terms of the coupling parameters, and we clarified the relationship between the external fields obtained by Eq. (13) and those obtained using Eq. (34).

The Bethe approximation is known to be identical to the belief-propagation algorithm. In order to estimate susceptibility efficiently, susceptibility propagation was introduced. Susceptibility propagation combined with the diagonal matching method has been numerically shown to provide an accurate estimation of magnetizations and correlation functions. We showed that susceptibility propagation with the diagonal matching method is the same as the Bethe approximation with the diagonal matching method.

Although we can estimate the external fields accurately by means of the diagonal matching method, the estimation of the coupling parameters is not affected by it. The coupling

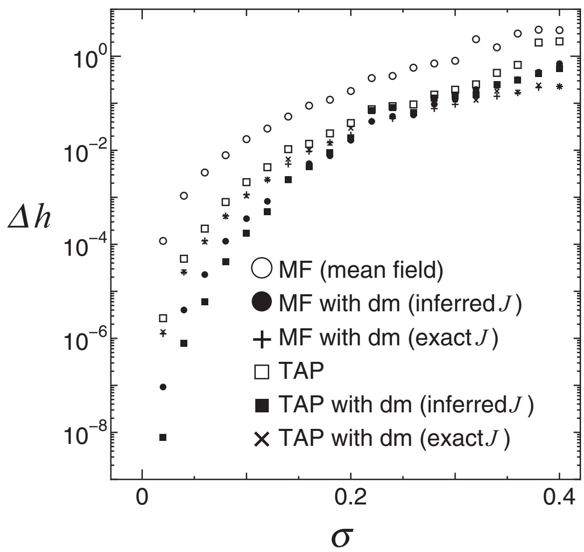

FIG. 1. Inference performance of naive approximations and those with diagonal matching method (dm) on the Sherrington-Kirkpatrick model. Magnetizations and correlations used to infer coupling parameters and external fields are calculated through exact exhaustive enumeration. The coupling parameters and external fields are generated as $J_{ij} \sim$ Normal $(0,\sigma^2)$ and $h_i \sim$ Normal $(0,\sigma^2)$, respectively. The inference error is defined as $\Delta h = [\sum_i (h_i^* - h_i)^2/N]^{1/2}$, where h_i^* is the inferred external field. The number of vertices is $N = 16$, and β is fixed at unity.

parameters are estimated by the naive approximations. Since the external fields are estimated by using the inferred coupling parameters, the accuracy of the inferred external fields seems to depend on the accuracy of the inferred coupling parameters. We investigate the effect of errors of the inferred coupling parameters on the inference of the external fields. Figure 1 shows a comparison between the external fields estimated by using the exact coupling parameters and those by using the inferred coupling parameters. The external fields by using the exact coupling parameters are less accurate than those by using the inferred coupling parameters. Within the diagonal matching method, the exact coupling parameters do not increase the accuracy of the inference of the external fields. The accurate estimation of both of the coupling parameters and the external fields is a problem for future research. We discussed the approximations based on the expansion with respect to the order of the coupling parameters, and these are applicable to the case that the coupling parameters are small. The development of a method that is applicable to large coupling parameters is also a problem for future research.

APPENDIX A: INVERSE MATRIX

In this Appendix, we present the formula of an inverse matrix by perturbation. Let us consider two $n \times n$ matrices, $\boldsymbol{A}$ and $\boldsymbol{B}$. We can easily derive the following formula for an inverse matrix of $(\boldsymbol{A} + \boldsymbol{B})$:

$$\frac{1}{\boldsymbol{A}+\boldsymbol{B}} - \frac{1}{\boldsymbol{A}} = -\frac{1}{\boldsymbol{A}+\boldsymbol{B}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}. \tag{A1}$$

Using the above formula iteratively, we obtain the inverse matrix of $(\boldsymbol{A} + \boldsymbol{B})$ as follows:

$$\begin{aligned}\frac{1}{\boldsymbol{A}+\boldsymbol{B}} &= \frac{1}{\boldsymbol{A}} - \frac{1}{\boldsymbol{A}+\boldsymbol{B}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}\\ &= \frac{1}{\boldsymbol{A}} - \left(\frac{1}{\boldsymbol{A}} - \frac{1}{\boldsymbol{A}+\boldsymbol{B}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}\right)\boldsymbol{B}\frac{1}{\boldsymbol{A}}\\ &= \frac{1}{\boldsymbol{A}} - \frac{1}{\boldsymbol{A}}\boldsymbol{B}\frac{1}{\boldsymbol{A}} + \frac{1}{\boldsymbol{A}+\boldsymbol{B}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}\\ &\;\vdots\\ &= \frac{1}{\boldsymbol{A}} - \frac{1}{\boldsymbol{A}}\boldsymbol{B}\frac{1}{\boldsymbol{A}} + \frac{1}{\boldsymbol{A}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}\boldsymbol{B}\frac{1}{\boldsymbol{A}} - \frac{1}{\boldsymbol{A}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}\boldsymbol{B}\frac{1}{\boldsymbol{A}}\cdots\\ &= \sum_{n=0}^{\infty}\frac{1}{\boldsymbol{A}}\left\{(-\boldsymbol{B})\frac{1}{\boldsymbol{A}}\right\}^n.\end{aligned} \tag{A2}$$

In order to evaluate the inverse matrix $\boldsymbol{G}_{\mathrm{DM}}^{-1}$ in Eq. (13), we divide $\boldsymbol{G}_{\mathrm{DM}}$ into two matrices, the diagonal part and the off-diagonal one. By setting $\boldsymbol{A}$ as the diagonal part of $\boldsymbol{G}_{\mathrm{DM}}$ and $\boldsymbol{B}$ as the off-diagonal part, Eq. (A2) is applicable to evaluation of the inverse matrix. The diagonal element $(\boldsymbol{G}_{\mathrm{DM}}^{-1})_{ii}$ becomes

$$\begin{aligned}(\boldsymbol{G}_{\mathrm{DM}}^{-1})_{ii} =& \frac{1}{(\boldsymbol{G}_{\mathrm{DM}})_{ii}} + \frac{1}{(\boldsymbol{G}_{\mathrm{DM}})_{ii}}\sum_{j\in\partial i}(\boldsymbol{G}_{\mathrm{DM}})_{ij}\frac{1}{(\boldsymbol{G}_{\mathrm{DM}})_{jj}}(\boldsymbol{G}_{\mathrm{DM}})_{ji}\frac{1}{(\boldsymbol{G}_{\mathrm{DM}})_{ii}}\\ &- \frac{1}{(\boldsymbol{G}_{\mathrm{DM}})_{ii}}\sum_{j\in\partial i}\sum_{k\in\partial i}(\boldsymbol{G}_{\mathrm{DM}})_{ij}\frac{1}{(\boldsymbol{G}_{\mathrm{DM}})_{jj}}(\boldsymbol{G}_{\mathrm{DM}})_{jk}\frac{1}{(\boldsymbol{G}_{\mathrm{DM}})_{kk}}(\boldsymbol{G}_{\mathrm{DM}})_{ki}\frac{1}{(\boldsymbol{G}_{\mathrm{DM}})_{ii}} + \cdots .\end{aligned} \tag{A3}$$

APPENDIX B: BETHE-APPROXIMATED GIBBS FREE ENERGY EXPANDED WITH RESPECT TO COUPLING PARAMETER

An expansion with respect to the coupling parameter for the Bethe-approximated Gibbs free energy given by Eq. (37) is obtained as follows:

$$\begin{aligned}G^{(\mathrm{Bethe})}(\{m_i\},\{J_{ij}\}) =& \frac{1}{\beta}\sum_{i\in\mathcal{V}}\left(\frac{1+m_i}{2}\ln\frac{1+m_i}{2} + \frac{1-m_i}{2}\ln\frac{1-m_i}{2}\right) - \sum_{(i,j)\in\mathcal{E}}J_{ij}m_im_j\\ &- \frac{1}{2}\beta\sum_{(i,j)\in\mathcal{E}}J_{ij}^2\left(1-m_i^2\right)\left(1-m_j^2\right) - \frac{2}{3}\beta^2\sum_{(i,j)\in\mathcal{E}}J_{ij}^3m_im_j\left(1-m_i^2\right)\left(1-m_j^2\right) + O\left(J_{ij}^4\right).\end{aligned} \tag{B1}$$

The expansion (B1) shows that the Bethe approximation includes all of the $(J_{ij})^n$ terms in the formula (37). By substitution of Eq. (B1) into Eqs. (44) or (45), the differentiations of $M_{j\to i}$ with respect to m_j or m_i are, respectively, derived as follows:

$$\frac{\partial M_{j\to i}}{\partial m_j} = \beta J_{ij} + 2\beta^2 J_{ij}^2 m_i m_j + O\left(J_{ij}^3\right), \tag{B2}$$

$$\frac{\partial M_{j\to i}}{\partial m_i} = -\beta^2 J_{ij}^2\left(1 - m_j^2\right) - 4\beta^3 J_{ij}^3 m_i m_j\left(1 - m_j^2\right) + O\left(J_{ij}^4\right). \tag{B3}$$

[1] M. Mezard and A. Montanari, *Information, Physics, and Computation* (Oxford University Press, Oxford, 2009).
[2] M. Welling and Y. W. Teh, Artif. Intell. **143**, 19 (2003).
[3] Y. Roudi, E. Aurell, and J. A. Hertz, Front. Comput. Neurosci. **3**, 22 (2009).
[4] Y. Roudi, J. Tyrcha, and J. Hertz, Phys. Rev. E **79**, 051915 (2009).
[5] S. Cocco and R. Monasson, Phys. Rev. Lett. **106**, 090601 (2011).
[6] S. Cocco and R. Monasson, J. Stat. Phys. **147**, 252 (2012).
[7] E. Schneidman, M. J. Berry, R. Segev, and W. Bialek, Nature (London) **440**, 1007 (2006).
[8] M. Weigt, R. A. White, H. Szurmant, J. A. Hoch, and T. Hwa, Proc. Natl. Acad. Sci. USA **106**, 67 (2008).
[9] Y. Roudi, S. Nirenberg, and P. E. Latham, PLoS Comput. Biol. **5**, e1000380 (2009).
[10] M. Bailly-Bechet, A. Braunstein, A. Pagnani, M. Weigt, and R. Zecchina, BMC Bioinf. **11**, 355 (2010).
[11] D. S. Marks., L. J. Colwell, R. Sheridan, T. A. Hopf, A. Pagnani, R. Zecchina, and C. Sander, PLoS ONE **6**, e28766 (2011).
[12] H. J. Kappen and F. B. Rodriguez, Neural Comput. **10**, 1137 (1998).
[13] T. Tanaka, Phys. Rev. E **58**, 2302 (1998).
[14] V. Sessak and R. Monasson, J. Phys. A: Math. Theor. **42**, 055001 (2009).
[15] M. Yasuda and K. Tanaka, Neural Comput. **21**, 3130 (2009).
[16] H. C. Nguyen and J. Berg, J. Stat. Mech. (2012) P03004.
[17] F. Ricci-Tersenghi, J. Stat. Mech. (2012) P08015.
[18] M. Opper and O. Winther, Phys. Rev. Lett. **86**, 3695 (2001).
[19] M. Opper and O. Winther, Phys. Rev. E **64**, 056131 (2001).
[20] H. Huang and Y. Kabashima, Phys. Rev. E **87**, 062129 (2013).
[21] M. Yasuda and K. Tanaka, Phys. Rev. E **87**, 012134 (2013).
[22] J. Raymond and F. Ricci-Tersenghi, Phys. Rev. E **87**, 052111 (2013).
[23] J. Raymond and F. Ricci-Tersenghi, in *IEEE International Conference on Communications Workshops (ICC)* (IEEE, New York, NY, 2013), pp. 1429–1433.
[24] D. J. Thouless, P. W. Anderson, and R. G. Palmer, Philos. Mag. **35**, 593 (1977).
[25] T. Plefka, J. Phys. A **15**, 1971 (1982).
[26] A. Georges and J. S. Yedidia, J. Phys. A **24**, 2173 (1991).
[27] M. Mézard and T. Mora, J. Physiol. (Paris) **103**, 107 (2009).
[28] E. Marinari and V. Van Kerrebroeck, J. Stat. Mech. (2010) P02008.
[29] E. Aurell, C. Ollion, and Y. Roudi, Eur. Phys. J. B **77**, 587 (2010).
[30] M. Yasuda and K. Tanaka, J. Phys. Soc. Jpn. **75**, 084006 (2006).
[31] T. Horiguchi, Physica A **107**, 360 (1981).