Interdisciplinary Information Sciences, Vol. 13, No. 1, pp. 25–31 (2007)

Boltzmann Machines with Bounded Continuous Random Variables

Muneki YASUDA* and Kazuyuki TANAKA†

Graduate School of Information Sciences, Tohoku University, 6-3-09 Aramaki-aza-aoba, Aoba-ku, Sendai 980-8579, Japan

Received October 26, 2006; final version accepted December 26, 2006

We propose a Boltzmann machine formulated as a probabilistic model where every random variable takes bounded continuous values, and we derive the Thouless–Anderson–Palmer equation for the model. The proposed model includes the non-negative Boltzmann machine and the Sherrington–Kirkpatrick model with spin-S at $S \to \infty$ as a special case. It is known that the Sherrington–Kirkpatrick model with spin-S has a spin glass phase. Thus, the proposed Boltzmann machine is expected to be able to learn practical complex data.

KEYWORDS: machine learning, non-negative boltzmann machine, Plefka expansion, TAP equation, SK model

1. Introduction

For the case of binary data, the maximum entropy distribution matches the first- and the second-order statistics of the data are given by the binary Boltzmann machine [1]. The Boltzmann machine is one of the most important probabilistic models used in neural computations [2]. The distribution of the Boltzmann machine is identified as a *Gibbs-Boltzmann distribution* with spin variables in statistical mechanics, and the distribution is both complex and intractable. Thus, the Boltzmann machine is expected to be able to learn complex structures of data.

In some practical cases, data are not always binary. For instance, in image processing, image data usually take integer values from 0 to 255 as a gray-level. Problems with multiple-valued data, like the case of image processing, may be able to formulated, assuming that data are generated by a probability density function with continuous random variables. Downs *et al.* proposed the *non-negative Boltzmann machine* (NNBM), for which every random variable takes continuous non-negative values [3]. The probability density function of the NNBM is given as a multivariate Gaussian distribution in which the lower bounds of every random variable is limited to zero. Since the random variables of the normal multivariate Gaussian take any real number within the interval $(-\infty, \infty)$, the probability density function of the NNBM differs from that of the normal multivariate Gaussian. The normal multivariate Gaussian is a uni-modal distribution, so it is not expected to fit probability density functions which generate complex data. On the other hand, the probability density function of the NNBM, which is called a *rectified Gaussian distribution* [4], can express multi-modal distributions, and can be expected to fit probability density functions which generate practical complex data. The NNBM has been applied to orientation tuning in the visual cortex, the decomposition of a database of the handwritten digits, and so on [3, 7]. In general, the rectified Gaussian distribution is an intractable distribution, and, consequently, Downs formulated the Thouless–Anderson–Palmer (TAP) equation [5, 6] to enable the NNBM to calculate some important statistical quantities [7]. The TAP equation is an approximation method developed in statistical mechanics, and is extended from the naive mean-field approximation. No random variable of the probability density function of the NNBM has an upper bound; however, in practical cases data usually have finite upper bounds. Therefore, it is expected that a probability density function with bounded continuous random variables is better fitted to some probability density functions which generate practical data than the NNBM.

Katayama and Horiguchi have proposed the Sherrington–Kirkpatrick (SK) model with spin-S, and they have investigated some of its statistical properties [8]. In the model, every random variable takes $2S + 1$ states belonging to the set $\{-1, -1 + 1/S, \dots, 1\}$. Thus, in the case $S \to \infty$, each random variable takes any real number within the interval $[-1, 1]$. They concluded that the SK model with spin-S, including $S \to \infty$, has a spin glass phase where the system presents complex and rich structures. Therefore, the Boltzmann machine with bounded continuous values at each random variable can be expected to learn a probability density function for complex data.

In the present paper, we propose a Boltzmann machine with bounded continuous random variables, and we derive a TAP equation for it. The present model includes the SK model with spin-S at $S \to \infty$ and the NNBM as special cases. In Section 2, we introduce the Boltzmann machine with bounded continuous random variables and then derive the naive mean-field equation and the TAP equation using *Plefka's expansion* [9]. In Section 3, we outline our numerical experiments and, Section 4 includes our concluding remarks.

* E-mail: muneki@smapip.is.tohoku.ac.jp
† E-mail: kazu@smapip.is.tohoku.ac.jp

2. Boltzmann Machine with Bounded Continuous Random Variables and Its Approximations

We consider a Boltzmann machine on a complete graph with N nodes labeled by i ($i = 1, 2, \ldots, N$). A random variable S_i is assigned at each node i and takes any real value within a specified interval $[a, b]$. The Boltzmann machine is described by the following energy function:

$$\mathcal{E}(\boldsymbol{S}) \equiv -\sum_{i=1}^{N} \theta_i S_i - \sum_{i \le j} w_{ij} S_i S_j, \tag{1}$$

where $\boldsymbol{S} = \{S_1, S_2, \ldots, S_N\}$ is a set of all random variables. θ_i is a bias which acts on node i. w_{ij} is a weight which expresses the intensity of the interaction between each pair of nodes i and j, and satisfies $w_{ij} = w_{ji}$. The summation of the second term of the energy function takes over all the pairs of nodes, *i.e.*, $\sum_{i \le j} \equiv \sum_{i=1}^{N} \sum_{j=i}^{N}$. In the simplest case, every weight w_{ii} is set to zero. However, to formulate the Boltzmann machine for data with complicated correlations, we consider the case that every weight w_{ii} is generally non-zero. The parameter w_{ii} is called the self-connection, or the anisotropic parameter in statistical mechanics. If $a = 0$ and $b \to \infty$, this model corresponds to the NNBM.

A state of the present Boltzmann machine is expressed by the following probabilistic model:

$$p(\boldsymbol{S}) \equiv \frac{\exp(-\beta \mathcal{E}(\boldsymbol{S}))}{\displaystyle\int_a^b \int_a^b \cdots \int_a^b \exp(-\beta \mathcal{E}(\boldsymbol{S})) dS_1 dS_2 \cdots dS_N}, \tag{2}$$

where β is the inverse temperature and, is usually set to 1 in the conventional Boltzmann machine. The probability density function $p(\boldsymbol{S})$ is called the Gibbs-Boltzmann distribution in statistical mechanics. Some statistical quantities of the probability density function (2) need to be calculated in the forward and backward problems of the Boltzmann machine. However, the probability density function (2) is intractable and we generally need computational complexity proportional to 2^N to calculate them. Thus, we have to employ some approximations to calculate the statistical quantities of the probability density function (2).

In the present section, we derive a TAP equation for the proposed model by employing Plefka's expansion [9]. The TAP equation is one of the extensions of the naive mean-field approximation and is one of the most important methods of the mean-field theory. Using this method, it is possible to obtain a perturbation from a naive mean-filed approximation systematically and obtain some important statistical quantities with any order approximation.

Following Ref. 9, we introduce a parameter α in the energy function (1) as follows:

$$\widehat{\mathcal{E}}(\boldsymbol{S}) \equiv -\sum_{i=1}^{N} \theta_i S_i - \alpha \sum_{i \le j} w_{ij} S_i S_j, \tag{3}$$

and consider the following probability density function:

$$\widehat{p}(\boldsymbol{S}) \equiv \frac{\exp(-\beta \widehat{\mathcal{E}}(\boldsymbol{S}))}{\displaystyle\int_a^b \int_a^b \cdots \int_a^b \exp(-\beta \widehat{\mathcal{E}}(\boldsymbol{S})) dS_1 dS_2 \cdots dS_N}. \tag{4}$$

If $\alpha = 1$, the energy function $\widehat{\mathcal{E}}(\boldsymbol{S})$ is equivalent to $\mathcal{E}(\boldsymbol{S})$, thus the probability density function $\widehat{p}(\boldsymbol{S})$ is equivalent to $p(\boldsymbol{S})$. On the other hand, if $\alpha = 0$, the random variables $\{S_i\}$ become independent of each other since the contribution of interactions in energy function (3) vanishes. Therefore, in the case of $\alpha = 0$, the probability density function (4) leads to a factorable distribution and becomes tractable.

For the energy function (3), we define the Helmholtz free energy as follows:

$$F\big(\{\theta_i\}, \{w_{ij}\}, \beta, \alpha\big) \equiv -\frac{1}{\beta} \ln\bigg(\int_a^b \int_a^b \cdots \int_a^b \exp\Big(-\beta \widehat{\mathcal{E}}(\boldsymbol{S})\Big) dS_1 dS_2 \cdots dS_N\bigg). \tag{5}$$

The Helmholtz free energy is one of the most important quantities in statistical mechanics and can be regarded as a cumulant generating function. We define the Gibbs free energy as follows:

$$G\big(\{m_i\}, \{w_{ij}\}, \beta, \alpha\big) \equiv -\frac{1}{\beta} \ln\bigg(\int_a^b \int_a^b \cdots \int_a^b \exp\Big(-\beta \widehat{\mathcal{E}}(\boldsymbol{S})\Big) dS_1 dS_2 \cdots dS_N\bigg) + \sum_{i=1}^{N} \theta_i(\alpha) m_i, \tag{6}$$

where m_i is defined as follows:

$$m_i \equiv \int_a^b \int_a^b \cdots \int_a^b S_i \widehat{p}(\boldsymbol{S}) dS_1 dS_2 \cdots dS_N. \tag{7}$$

Because $\partial F/\partial h_i = -m_i$, the Gibbs free energy is regarded as the Legendre transform of the Helmholtz free energy. From the definition (7), we find that m_i refers the moment of the random variable S_i with respect to the probability density function $\widehat{p}(\boldsymbol{S})$. Note that, in Eq. (6), $\{m_i\}$ can be regarded as independent variables and $\{\theta_i\}$ are functions of $\{m_i\}$, $\{w_{ij}\}$, β and α, *i.e.*, $\theta_i = \theta_i(\{m_i\}, \{w_{ij}\}, \beta, \alpha)$. Since m_i is an independent variable, a value of m_i does not depend on α. Note that, in the case of $\alpha = 1$, Eqs. (5) and (6) become the Helmholtz and Gibbs free energies corresponding to the system described by the energy function (1), respectively, since $\mathcal{E}(\boldsymbol{S}) = \widehat{\mathcal{E}}(\boldsymbol{S})$ in this case. From the definition (7), we have

$$m_i = \frac{\int_a^b S_i \exp\big(\beta\theta_i(0)S_i\big)dS_i}{\int_a^b \exp\big(\beta\theta_i(0)S_i\big)dS_i} = -\frac{1}{\beta\theta_i(0)} + \frac{b-a}{2}\coth\frac{\beta\theta_i(0)(b-a)}{2} + \frac{b+a}{2}, \tag{8}$$

for $\alpha = 0$, where the notation $\theta_i(0)$ means $\theta_i(\{m_i\}, \{w_{ij}\}, \beta, \alpha = 0)$. This equation can be regarded as the relationship between m_i and $\theta_i(0)$. One can see that $\theta_i(0)$ acts as an *effective field* on node i in Eq. (8), so that this quantity is important in the present method. Hence forth in this paper, to mark them as special, we use the notation μ_i instead of $\beta\theta_i(0)$, *i.e.*, $\mu_i \equiv \beta\theta_i(0)$. Note that μ_i can be regarded as a function of only m_i (See Eq. (8)).

For the expanding the Gibbs free energy (6) with respect to α, we have the following series:

$$G(\alpha) = G(0) + \alpha \frac{\partial G(\alpha)}{\partial \alpha}\bigg|_{\alpha=0} + \frac{\alpha^2}{2}\frac{\partial^2 G(\alpha)}{\partial \alpha^2}\bigg|_{\alpha=0} + \cdots. \tag{9}$$

For convenience, we omit the explicit description for the dependence of $\{m_i\}$, $\{w_{ij}\}$ and β, *i.e.*, $G(\{m_i\}, \{w_{ij}\}, \beta, \alpha) \equiv G(\alpha)$. By truncating the right-hand side of Eq. (9) to a finite term and letting $\alpha = 1$, one obtains any order approximation of the Gibbs free energy corresponding to the system described by the energy function (1). If one truncates the right-hand side of Eq. (9) up to the first order term, Eq. (9) is reduced to the naive mean-field Gibbs free energy and, if one truncates it up to the second order term, Eq. (9) is reduced to the TAP Gibbs free energy. By applying the relationship $\partial G(1)/\partial m_i = \theta_i$, the property of the Legendre transform, to the naive mean-field Gibbs free energy and the TAP Gibbs free energy, one can obtain the naive mean-field equation and the TAP equation, respectively. By using these equations, one can calculate moments of random variables $\{S_i\}$ with respect to the probability density function $p(\boldsymbol{S})$ with corresponding order approximations (See Sec. 2.1 and Sec. 2.2).

We now give the coefficients of Eq. (9) up to the second order. The coefficient of the first term of Eq. (9) is

$$\begin{aligned} G(0) &= \frac{1}{\beta}\sum_{i=1}^{N}\left(\mu_i m_i - \ln\int_a^b e^{\mu_i S_i} dS_i\right) \\ &= \frac{1}{\beta}\sum_{i=1}^{N}\left\{\mu_i m_i - \frac{1}{2}\mu_i(b+a) - \ln\left(\frac{2}{\mu_i}\sinh\frac{\mu_i(b-a)}{2}\right)\right\}. \end{aligned} \tag{10}$$

The coefficient of the second term of Eq. (9) is

$$\frac{\partial G(\alpha)}{\partial \alpha}\bigg|_{\alpha=0} = -\sum_{i<j} w_{ij} m_i m_j - \sum_{i=1}^{N} w_{ii} m_i^{(2)}, \tag{11}$$

where the summation of the first term of Eq. (11) takes over all distinct pairs of nodes, *i.e.*, $\sum_{i<j} \equiv \sum_{i=1}^{N}\sum_{j=i+1}^{N}$, and $m_i^{(2)}$ is defined as follows:

$$m_i^{(2)} \equiv \frac{\int_a^b S_i^2 \exp(\mu_i S_i) dS_i}{\int_a^b \exp(\mu_i S_i) dS_i} = -\frac{2m_i - b - a}{\mu_i} + (b+a)m_i - ab. \tag{12}$$

The coefficient of the third term of Eq. (9) is

$$\begin{aligned} \frac{\partial^2 G(\alpha)}{\partial \alpha^2}\bigg|_{\alpha=0} &= -\beta\sum_{i<j} w_{ij}^2\big(m_i^{(2)} - m_i^2\big)\Big(m_j^{(2)} - m_j^2\Big) \\ &\quad - \beta\sum_{i=1}^{N} w_{ii}^2\Big(m_i^{(4)} - \big(m_i^{(2)}\big)^2\Big) - \beta\sum_{i=1}^{N} w_{ii}^2\big(m_i^{(2)} - m_i^2\big)\big(\phi_i^{(2)}\big)^2 \\ &\quad + 2\beta\sum_{i=1}^{N} w_{ii}^2\big(m_i^{(3)} - m_i m_i^{(2)}\big)\phi_i^{(2)}, \end{aligned} \tag{13}$$

Here $m_i^{(3)}$, $m_i^{(4)}$ and $\phi_i^{(2)}$ are defined as follows:

$$m_i^{(3)} \equiv \frac{\displaystyle\int_a^b S_i^3 \exp(\mu_i S_i) dS_i}{\displaystyle\int_a^b \exp(\mu_i S_i) dS_i} = -\frac{3m_i^{(2)}}{\mu_i} + (b^2 + a^2 + ab)\left(m_i + \frac{1}{\mu_i}\right) - ab(b+a), \tag{14}$$

$$m_i^{(4)} \equiv \frac{\displaystyle\int_a^b S_i^4 \exp(\mu_i S_i) dS_i}{\displaystyle\int_a^b \exp(\mu_i S_i) dS_i} = -\frac{4m_i^{(3)}}{\mu_i} + (b+a)(b^2 + a^2)\left(m_i + \frac{1}{\mu_i}\right) - ab(b^2 + a^2 + ab) \tag{15}$$

and

$$\phi_i^{(2)} \equiv \frac{\partial m_i^{(2)}}{\partial m_i} = -\frac{2}{\mu_i} + \left(\frac{2m_i - b - a}{\mu_i^2}\right)\xi_i + b + a, \tag{16}$$

where ξ_i is defined by

$$\xi_i \equiv \frac{\partial \mu_i}{\partial m_i} = \left(\frac{1}{\mu_i^2} - \frac{(b-a)^2}{4}\sinh^{-2}\frac{\mu_i(b-a)}{2}\right)^{-1}. \tag{17}$$

Equation (17) can be obtained by using Eq. (8). Note that, from Eq. (8), we have $\partial\mu_i/\partial m_j = 0$ for $i \neq j$. Therefore, for $i \neq j$

$$\frac{\partial m_i^{(2)}}{\partial m_j} = \frac{2m_i - b - a}{\mu_i^2}\frac{\partial \mu_i}{\partial m_j} = 0. \tag{18}$$

We use Eq. (18) in the derivation of Eq. (13). Since we have $m_i m_i^{(2)} - m_i^{(3)} = (m_i^2 - m_i^{(2)})\phi_i^{(2)}$, Eq. (13) is reduced to

$$\begin{aligned}\left.\frac{\partial^2 G(\alpha)}{\partial \alpha^2}\right|_{\alpha=0} &= -\beta \sum_{i<j} w_{ij}^2 \left(m_i^{(2)} - m_i^2\right)\left(m_j^{(2)} - m_j^2\right) \\ &\quad - \beta \sum_{i=1}^N w_{ii}^2 \left(m_i^{(4)} - \left(m_i^{(2)}\right)^2\right) + \beta \sum_{i=1}^N w_{ii}^2 \left(m_i^{(3)} - m_i m_i^{(2)}\right)\phi_i^{(2)}.\end{aligned} \tag{19}$$

2.1 Naive mean-field equation

From the above argument, the naive mean-field Gibbs free energy for the proposed model is expressed as follows:

$$\begin{aligned}G(1) \approx G_{\text{MF}} &= \frac{1}{\beta}\sum_{i=1}^N \left\{\mu_i m_i - \frac{1}{2}\mu_i(b+a) - \ln\left(\frac{2}{\mu_i}\sinh\frac{\mu_i(b-a)}{2}\right)\right\} \\ &\quad - \sum_{i<j} w_{ij} m_i m_j - \sum_{i=1}^N w_{ii} m_i^{(2)}.\end{aligned} \tag{20}$$

By applying the relationship $\partial G(1)/\partial m_i = \theta_i$ to the naive mean-field Gibbs free energy G_{MF}, we obtain

$$\mu_i = \beta\theta_i + \beta w_{ii}\phi_i^{(2)} + \beta \sum_{j=1}^N w_{ij} m_j. \tag{21}$$

Since m_i is expressed by only μ_i in Eq. (8), Eq. (21) can be regarded as a self-consistent equation of $\{\mu_i\}$. Therefore, we find that Eq. (21) is the naive mean-field equation for the proposed model. By solving Eq. (21) numerically, we can obtain approximate values of moments $\{m_i\}$ and effective fields $\{\mu_i\}$ for the proposed model within the naive mean-field approximation. By substituting those values to Eq. (20), the naive mean-field Gibbs free energy for the proposed model can be given numerically.

In the case of $w_{ii} = 0$ for all i, by using Eqs. (8) and (21), the self-consistent equation of $\{m_i\}$ can be derived as follows:

$$m_i = -\left(\beta\theta_i + \beta\sum_{j=1}^N w_{ij} m_j\right)^{-1} + \frac{b-a}{2}\coth\left\{\frac{b-a}{2}\left(\beta\theta_i + \beta\sum_{j=1}^N w_{ij} m_j\right)\right\} + \frac{b+a}{2}. \tag{22}$$

2.2 TAP equation

The TAP Gibbs free energy for the proposed model is expressed as follows:

$$G(1) \approx G_{\mathrm{TAP}} = \frac{1}{\beta}\sum_{i=1}^{N}\left\{\mu_i m_i - \frac{1}{2}\mu_i(b+a) - \ln\left(\frac{2}{\mu_i}\sinh\frac{\mu_i(b-a)}{2}\right)\right\}$$
$$- \sum_{i<j} w_{ij}m_i m_j - \sum_{i=1}^{N} w_{ii}m_i^{(2)} - \frac{\beta}{2}\sum_{i<j} w_{ij}^2\left(m_i^{(2)} - m_i^2\right)\left(m_j^{(2)} - m_j^2\right)$$
$$- \frac{\beta}{2}\sum_{i=1}^{N} w_{ii}^2\left(m_i^{(4)} - \left(m_i^{(2)}\right)^2\right) + \frac{\beta}{2}\sum_{i=1}^{N} w_{ii}^2\left(m_i^{(3)} - m_i m_i^{(2)}\right)\phi_i^{(2)}. \tag{23}$$

By applying the relationship $\partial G(1)/\partial m_i = \theta_i$ to the TAP Gibbs free energy G_{TAP} in a similar way to Sec. 2.1, we derive the TAP equation for the proposed model as follows:

$$\mu_i = \beta\theta_i + \beta w_{ii}\phi_i + \beta\sum_{j=1}^{N} w_{ij}m_j + \frac{\beta^2}{2}\left(\phi_i^{(2)} - 2m_i\right)\sum_{j=1}^{N} w_{ij}^2\left(m_j^{(2)} - m_j^2\right)$$
$$+ \frac{\beta^2 w_{ii}^2}{2}\left(\phi_i^{(4)} - \phi_i^{(2)}\phi_i^{(3)} - m_i^{(2)}\phi_i^{(2)} + m_i\left(\phi_i^{(2)}\right)^2 - m_i^{(3)}\zeta_i^{(2)} + m_i m_i^{(2)}\zeta_i^{(2)}\right), \tag{24}$$

where $\phi_i^{(3)}$, $\phi_i^{(4)}$ and $\zeta_i^{(2)}$ are defined as follows:

$$\phi_i^{(3)} \equiv \frac{\partial m_i^{(3)}}{\partial m_i} = -\frac{3\phi_i^{(2)}}{\mu_i} + \frac{(3m_i^{(2)} - b^2 - a^2 - ab)\xi_i}{\mu_i^2} + b^2 + a^2 + ab, \tag{25}$$

$$\phi_i^{(4)} \equiv \frac{\partial m_i^{(4)}}{\partial m_i} = -\frac{4\phi_i^{(3)}}{\mu_i} + \frac{\{4m_i^{(3)} - (b+a)(b^2+a^2)\}\xi_i}{\mu_i^2} + (b+a)(b^2+a^2) \tag{26}$$

and

$$\zeta_i^{(2)} \equiv \frac{\partial \phi_i^{(2)}}{\partial m_i} = \frac{1}{\mu_i^2}\left\{(2m_i - b - a)\eta_i + 2\xi_i\left(2 - \frac{2m_i - b - a}{\mu}\right)\right\}, \tag{27}$$

where η_i is defined by

$$\eta_i \equiv \frac{\partial \xi_i}{\partial m_i} = \left(\frac{2}{\mu_i^3} + \frac{(b-a)^3}{4}\coth\frac{\mu_i(b-a)}{2}\sinh^{-2}\frac{\mu_i(b-a)}{2}\right)\xi_i^3. \tag{28}$$

By solving Eq. (24) numerically, we can obtain the values of the moments $\{m_i\}$ and effective fields $\{\mu_i\}$ for the proposed model within the TAP equation, and then, by substituting those values to Eq. (23), we can obtain the TAP Gibbs free energy for the proposed model numerically.

2.3 Case of $a = 0$ and $b \to \infty$

The TAP equation in Eq. (24) yields to Downs' TAP equation for the NNBM in the case of $a = 0$ and $b \to \infty$. We now assume that the independent variable m_i takes any real positive value, *i.e.*, $0 < m_i < \infty$. Since all random variables take any positive value in this case, the assumption is consistent. The assumption leads to $\mu_i < 0$ from the definition (8). In this case, from Eq. (8), we obtain $m_i = -1/\mu_i$. Therefore, $G(0)$ in Eq. (10) yields

$$G(0) = \frac{1}{\beta}\sum_{i=1}^{N}\left\{\mu_i m_i - \ln\left(-\frac{1}{\mu_i}\right)\right\} = -\frac{1}{\beta}(N + \ln m_i). \tag{29}$$

From Eq. (12), we have $m_i^{(2)} = 2m_i^2$ in the present case. Thus, Eq. (11) yields

$$\left.\frac{\partial G(\alpha)}{\partial \alpha}\right|_{\alpha=0} = -\sum_{i\le j}(1+\delta_{ij})w_{ij}m_i m_j, \tag{30}$$

where δ_{ij} is Kronecker's delta. From Eqs. (14), (15) and (16), we obtain equalities $m_i^{(3)} = 6m_i^3$, $m_i^{(4)} = 24m_i^4$ and $\phi_i^{(2)} = 4m_i$, respectively. Thus, Eq. (19) yields

$$\left.\frac{\partial^2 G(\alpha)}{\partial \alpha^2}\right|_{\alpha=0} = -\beta\sum_{i\le j}(1+4\delta_{ij})w_{ij}^2 m_i^2 m_j^2. \tag{31}$$

Therefore, the TAP Gibbs free energy is reduced to

$$G_{\mathrm{TAP}} = -\frac{1}{\beta}(N + \ln m_i) - \sum_{i\le j}(1+\delta_{ij})w_{ij}m_i m_j - \frac{\beta}{2}\sum_{i\le j}(1+4\delta_{ij})w_{ij}^2 m_i^2 m_j^2. \tag{32}$$

This is identified as Downs' TAP Gibbs free energy for the NNBM [7]. Thus, our formulation can be regarded as a generalization of Downs' TAP equation for the NNBM.

3. Numerical Experiments

In this section, we check the accuracy of the naive mean-field equation in Eq. (21) and the TAP equation in Eq. (24). We consider the SK model with spin-S whose energy function described by

$$\mathcal{E}_{\mathrm{SK}}(\boldsymbol{S}) = -\sum_{i<j} w_{ij} S_i S_j. \tag{33}$$

The random variable S_i takes any value belonging to the set $\{-1, -1+1/S, \ldots, 1\}$. Each weight w_{ij} is generated from the Gaussian distribution defined by

$$P(w_{ij}) = \left(\frac{N}{2\pi w^2}\right)^{\frac{1}{2}} \exp\left\{-\frac{N}{2w^2}\left(w_{ij} - \frac{w_0}{N}\right)^2\right\}, \tag{34}$$

independently. When we take the limit $S \to \infty$, the model can be reduced to our model with $a = -1$, $b = 1$ and $w_{ii} = 0$ for all i. Katayama and Horiguchi analyzed the model in the case of $N \to \infty$ and formulated the Helmholtz free energy in the model [8].

We calculate the Helmholtz free energy numerically by using the naive mean-field approximation and the TAP equation for the model, respectively, and then, we compare the results given by both approximations with the analytic solution given by Katayama and Horiguchi [8]. We employ their RS solution as the analytic solution in this experiment. Note that Helmholtz free energies of both approximations are obtained by using the Legendre transform of Gibbs free energies in Eqs. (20) and (23), respectively. Therefore, the Helmholtz free energies of the naive mean-field equation and of the TAP equation are obtained by

$$F_{\mathrm{MF}} = G_{\mathrm{MF}} - \sum_{i=1}^{N} \theta_i m_i \tag{35}$$

and

$$F_{\mathrm{TAP}} = G_{\mathrm{TAP}} - \sum_{i=1}^{N} \theta_i m_i, \tag{36}$$

respectively. Equations (21) and (24) express extremal conditions of the approximate Helmholtz free energies F_{MF} and F_{TAP} with respect to $\{m_i\}$, respectively. The moments $\{m_i\}$ in Eqs. (35) and (36) are calculated by Eqs. (21) and (24), respectively.

Figure 1 shows a comparison of the Helmholtz free energy (per node) of analytic solution with those of the naive mean-field equation and of the TAP equation. In these numerical experiments, we set $N = 1500$, $a = -1$, $b = 1$ and $w_{ii} = 0$ for all i, and the parameters w_{ij} are generated from the Gaussian distribution (34) independently. To obtain values of F_{MF} and F_{TAP}, we solve Eqs. (22) and (24), respectively. We set $\{m_i\}$ in Eqs. (22) and (24) randomly within the interval $[-1, 1]$ as initial values, and we solve Eqs. (22) and (24) numerically using a simple iterative method. Each plot represents an average of 300 samples. We set $\beta = 1$ and $w_0 = 0$, and then we experiment with several ws. This numerical experiment is carried out within the paramagnetic phase of the SK model with spin-S at $S \to \infty$. Since the

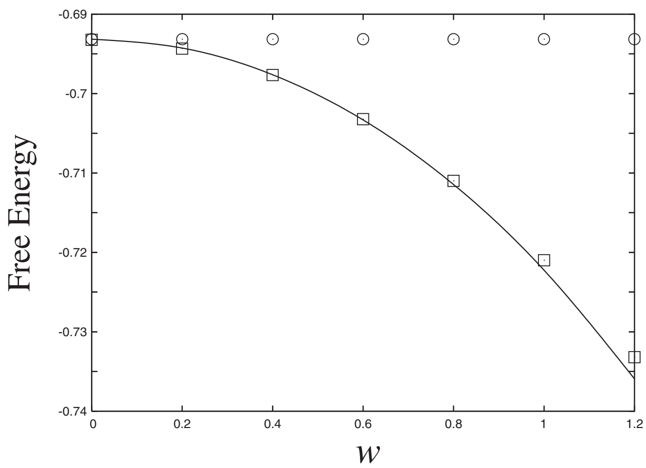

Fig. 1. The Helmholtz free energy per node of analytic solution versus those of the naive mean-field equation and of the TAP equation.

AT condition is satisfied [8], the analytic solution used in this numerical experiment is considered to express the true Helmholtz free energy at $N \to \infty$. The solid line, open circle and open square express the analytic solution, F_{MF}/N and F_{TAP}/N, respectively. The values of F_{TAP} are significantly closer to the analytic solution than those of F_{MF}. Thus, we find that the TAP equation gives us better accuracy than the naive mean-field approximation in the present case.

4. Concluding Remarks

In this paper, we have proposed the Boltzmann machine with bounded continuous random variables and have given the approximate algorithm to calculate some statistical quantities for it. We have shown our formulation of the TAP equation for the proposed model includes Downs' TAP equation for the NNBM as a special case. From our numerical experiments, we have shown that the TAP equation provides better accuracy than the naive mean-field equation for the proposed model.

However, it does not bear out that the proposed model and its TAP equation are available for practical learning problems. We need to verify the availability of the proposed Boltzmann machine and its approximate algorithms for learning tasks involving practical data. It is also required that we check performances of the learning of the proposed Boltzmann machine and compare it with the learning of the NNBM.

We are also interested in how far the present TAP equation can describe the spin glass phase in the SK model with spin-S at $S \to \infty$. Since the spin glass phase has great complexity and rich structures, it is expected to provide us with some new perspectives from which to view the performance of the machine learning for complex data by studying the behavior of the proposed algorithm in the spin glass phase. This is a task that needs to be addressed in the future.

Acknowledgements

The present work was partly supported by the Grants-In-Aid (No. 14084101, No. 14084203, No. 17500134 and No. 18079002) for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

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