Multiple-valued energy function in neural networks with asymmetric connections

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We apply the graphic transformation method [K. Mogi, J. Theor. Biol. **162**, 337 (1993)] to obtain the steady-state distribution of asymmetric Boltzmann machines as an extension of the symmetric equilibrium case. We give the magnitude of deviation from the equilibrium explicitly as a function of asymmetry in the connections between the neurons. We show that the steady state of asymmetric Boltzmann machines is characterized by multiple energy values, rather than by a single energy value as in the equilibrium state of symmetric Boltzmann machines. The equilibrium scalar energy function is generalized to a multiple-valued energy function in the case of asymmetric Boltzmann machines.

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I. INTRODUCTION

In an effort to understand the mechanism of brain function, the artificial neural networks have been studied as a model of the function of a population of neurons. Since the time Hopfield [1,2] formulated the problem of artificial neural networks within a physical framework, the study of neural networks has increasingly attracted the interest of the physicists.

In an artificial neural network, the neurons are assumed to interact with each other through reciprocal connections, which correspond to the synapses in biological neural networks. In biological neural networks, the connections between the neurons are, in general, asymmetric. It is therefore interesting to study the properties of artificial neural networks with asymmetric connections [3–10].

The graphic method has been applied to various aspects of biology [11–13]. In particular, the graphic representation of the solution of a linear system of equations introduced by King and Altman [14–16] has found many applications in the kinetic analysis of enzyme catalyzed reactions in biological systems. Recently, a new graphic technique, the graphic transformation method, has been developed by the author [17,18]. The graphic transformation method is based on an interesting property of the "spanning in-trees," a class of graphs that is used in the King and Altman method. With the graphic transformation method, we can express the steady state as an extension of the equilibrium. The deviation from the equilibrium is given explicitly as a geometrical property of the graphic representation of the system.

In the scheme of the artificial neural networks, the equilibrium state corresponds to the case where the connections between the neurons are symmetric. In the case of general neural networks with asymmetric connections, an equilibrium state does not exist, and only a steady state can exist as a solution. Due to the lack of appropriate mathematical techniques, it has been difficult to analyze the steady state of the neural networks with asymmetric connections.

In this paper, we apply the graphic transformation method to the study of asymmetric neural networks. The subject of our present study is the Boltzmann machine [19–22], a general formalism of artificial neural networks with stochastic dynamics. We obtain the steady-state distribution of asymmetric Boltzmann machines as an extension of the equilibrium distribution. We give the magnitude of deviation from the equilibrium explicitly as a function of asymmetry in the connections between the neurons. We show that the steady state is characterized by multiple energy values, rather than by a single energy value as in the equilibrium.

II. THE KINETIC TREATMENT OF THE BOLTZMANN MACHINE

In order to apply the graphic method to the study of the Boltzmann machines, we first need to derive a kinetic version of the transition rule of the Boltzmann machine.

The Boltzmann machine can be considered as a stochastic version of the Hopfield network [1,2]. The Boltzmann machine consists of N neurons. At a given instant, each neuron takes a value of either 0 (nonfiring state) or 1 (firing state). The states of the N neurons are therefore expressed as the vertices of the N-dimensional hypercube:

$$S=(s_1,\ldots,s_N)\in\{0,1\}^N .$$

The neurons are coupled via a real $N\times N$ matrix $W=\|w_{ij}\|$. We assume that

$$w_{ii}=0 .$$

In biological neural networks, there are, in general, more than one synapsis connecting a pair of neurons, but we represent the collective effect of these synapses with one weight.

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In the following discussion, we indicate a particular state in $\{0,1\}^N$ as S^k, where $k=1,2,\ldots,2^N$. Let us assume that the neurons are randomly chosen and called to update [23] with rates of activation $F(i)$, where i denotes the index of the neuron that is called to update. The rate of transition from the state S^q to the state S^p can be written as

$$K(S^p,S^q)=F(i_c)\frac{1}{1+e^{-\beta(1-2s_{i_c}^q)U_{i_c}(S^q)}}\ , \tag{1}$$

where i_c denotes the index of the neuron that is called to update and changes its state in the transition from the state S^q to the state S^p. $U_i(S)$ is the input signal on the ith neuron given as

$$U_i(S)=\sum_{j=1}^{N} w_{ij}s_j-\theta_i\ , \tag{2}$$

where θ_i represents the threshold.

If we assume that the connections between the neurons are symmetric, the system has an equilibrium solution characterized by the equilibrium energy values

$$E(S)=-\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} w_{ij}s_is_j+\sum_{i=1}^{N} s_i\theta_i\ . \tag{3}$$

We assume that only one neuron changes its state at a particular time of transition (the serial update method). Namely, we have the relations

$$\begin{aligned} s_{i_c}^q&=1-s_{i_c}^p\ ,\\ s_i^p&=s_i^q\quad (i\neq i_c)\ . \end{aligned} \tag{4}$$

The evolution of the system is described by the master equation

$$\frac{\partial\rho(S^p,t)}{\partial t}=\sum_{S^q}[K(S^p,S^q)\rho(S^q)-K(S^q,S^p)\rho(S^p)]\ , \tag{5}$$

where $\rho(S)$ is the probability distribution for the state S.

From Eq. (1), we can derive the relations between the rate constants

$$\begin{aligned} \frac{K(S^p,S^q)}{K(S^q,S^p)}&=\frac{1+e^{-\beta(1-2s_{i_c}^p)U_{i_c}(S^p)}}{1+e^{-\beta(1-2s_{i_c}^q)U_{i_c}(S^q)}}\\ &=e^{-\beta(1-2s_{i_c}^p)U_{i_c}(S^p)}\\ &=e^{-\beta[s_{i_c}^qU_{i_c}(S^q)-s_{i_c}^pU_{i_c}(S^p)]}\\ &=\exp\left\{-\beta\left[\left[-\sum_j w_{i_cj}s_{i_c}^ps_j^p+\sum_j w_{i_cj}s_{i_c}^qs_j^q\right]+(s_{i_c}^p-s_{i_c}^q)\theta_{i_c}\right]\right\}\ , \end{aligned} \tag{6a}$$

where we have used the equality

$$U_{i_c}(S^p)=U_{i_c}(S^q)\ .$$

Equation (6a) can be further transformed by using the relations

$$\begin{aligned} (s_{i_c}^p-s_{i_c}^q)\theta_{i_c}&=\sum_i s_i^p\theta_i-\sum_i s_i^q\theta_i\ ,\\ \sum_j w_{i_cj}s_{i_c}s_j&=\frac{1}{2}\left[\sum_i\sum_j w_{ij}s_is_j-\sum_{i\neq i_c}\sum_{j\neq j_c} w_{ij}s_is_j\right.\\ &\qquad\left.+\sum_j(w_{i_cj}-w_{ji_c})s_{i_c}s_j\right] \end{aligned}$$

as

$$\frac{K(S^p,S^q)}{K(S^q,S^p)}=e^{-\beta[E(S^p)-E(S^q)+d(S^p,S^q)]}\ , \tag{6b}$$

where $E(S^p)$ and $E(S^q)$ are the equilibrium energy values given by Eq. (2), and the "asymmetric energy term"

$$d(S^p,S^q)=-\frac{1}{4}\sum_i\sum_j(w_{ij}-w_{ji})(s_i^p-s_i^q)(s_j^p+s_j^q) \tag{7}$$

is a measure of the deviation from the equilibrium.

We note that

$$d(S^q,S^p)=-d(S^p,S^q)\ . \tag{8}$$

It is clear that $d(S^p,S^q)=0$ when the connection between the neurons are symmetric. Note that the asymmetric energy term can be alternatively written as

$$\begin{aligned} d(S^p,S^q)&=-\frac{1}{4}\sum_j(w_{i_cj}-w_{ji_c})(s_{i_c}^p-s_{i_c}^q)(s_j^p+s_j^q)\\ &=-\tfrac{1}{2}\sum_{\langle j\rangle}(w_{i_c\langle j\rangle}-w_{\langle j\rangle i_c})(s_{i_c}^p-s_{i_c}^q)\ , \end{aligned} \tag{9}$$

where $\langle j\rangle$ denotes the subset of the values of the index j for which $s_j^p=s_j^q=1$.

Now we are ready to study the steady-state properties of asymmetric Boltzmann machines. In a steady state, the state distribution $\rho(S)$ is given by the balance equation

$$\sum_{S^q} [K(S^p,S^q)\rho(S^q)-K(S^q,S^p)\rho(S^p)]=0 \ . \tag{10}$$

The normalization condition is

$$\sum_{S} \rho(S)=1 \ . \tag{11}$$

The steady-state distribution of the Boltzmann machine can be obtained as the solution for Eqs. (6b), (10), and (11).

III. THE GRAPHIC ANALYSIS

A. The graphic representation of the state distribution

The steady-state distribution satisfying Eqs. (6b), (10), and (11) can be represented by the graphic method. As the graphic method has not been previously applied to the study of artificial neural networks, we briefly review some terms that are used in the following discussion.

A connected graph G is a graph such that there is at least one path between any given pair of vertices belonging to it. A subgraph of a graph G is a graph the vertices and edges of which is a subset of the vertices and edges of graph G. A tree is a connected graph which contains no cycles. Let us assume that G is a connected directed graph (digraph). A spanning in-tree in G is defined as a subgraph of G which satisfies the following conditions: (i) It contains every vertex of G; (ii) it is a tree; (iii) its directed edges all point toward a certain vertex (the *sink*). An underlying graph of a directed graph G is the graph obtained by removing the direction from every edge of G.

In 1956, King and Altman introduced the graphic method to the analysis of enzyme kinetics [14]. In the graphic method, we first consider the set of all possible spanning in-trees with the states of the neurons represented as the vertices (Fig. 1).

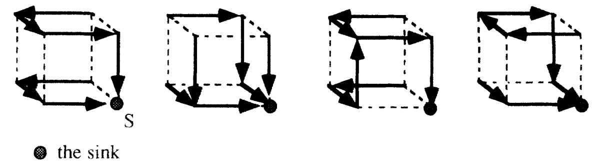

FIG. 1. Some examples of spanning in-trees in $\{0,1\}^3$. Some examples of spanning in-trees $G_S(m)$ which have the state S (indicated by the filled circle) as the sink are shown. In this figure, the number of neurons is taken to be 3. The vertices represent the neural states $\{0,1\}^3$. In the case of N neurons, a hypercube in N dimensions should be used.

We express the spanning in-tree which have a particular state S as the sink as $G_S(m)$ $(m=1,2,3,\ldots,n_g)$, where n_g is the number of spanning in-trees [24] of the hypercube $\{0,1\}^N$ and is the same for all S. From the matrix tree theorem [25], n_g can be calculated as [26]

$$n_g=2^{(2^N-N-1)}\prod_{i=1}^{N} i^{\binom{N}{i}} \ . \tag{12}$$

It is known that the solution for Eq. (10) is given formally by Cramer's rule as

$$\rho(S)=\frac{W(S)}{\sum_S W(S)} \ ,$$

where

$$W(S)=\begin{array}{cc} & \begin{array}{cccccc} & & & \text{column for } S & & \\ & & & \downarrow & & \end{array} \\ & \begin{vmatrix} \sum_S K(S^1,S) & -K(S^2,S^1) & \cdots & 0 & \cdots & -K(S^{2^N},S^1) \\ -K(S^1,S^2) & \sum_S K(S^2,S) & \cdots & 0 & \cdots & -K(S^{2^N},S^2) \\ \vdots & \vdots & & \vdots & & \vdots \\ 1 & 1 & \cdots & 1 & \cdots & 1 \\ \vdots & \vdots & & \vdots & & \vdots \\ -K(S^1,S^{2^N}) & -K(S^2,S^{2^N}) & \cdots & 0 & \cdots & \sum_S K(S^{2^N},S) \end{vmatrix} \begin{array}{l} \\ \\ \\ \leftarrow \text{row for } S. \\ \\ \\ \end{array} \end{array}$$

King and Altman showed that the weight $W(S)$ for the state S in the above formula can be alternatively written in a graphic form as

$$W(S)=\sum_m \prod_{(S^p,S^q)\in G_S(m)} K(S^p,S^q) \ , \tag{13}$$

where

$$\prod_{(S^p,S^q)\in G_S(m)} K(S^p,S^q) \tag{14}$$

represents the product of the rate constants corresponding to the directed edges of the spanning in-tree $G_S(m)$. The term (S^p,S^q) represents the ordered pair of states corresponding to the directed edges of the spanning in-tree $G_S(m)$. We define the indexing of the spanning in-trees in such a way that the spanning in-trees with the same index share the same underlying graph.

Since the introduction by King and Altman, the graphic method has been used in the analysis of kinetic pathways in biological and other systems. A review of the graphic method can be found in Ref. [16].

B. The graphic transformation method

We now introduce the graphic transformation method. The graphic transformation method is a graphic procedure introduced by the author with which we can obtain the steady-state distribution as a generalization of the equilibrium Boltzmann distribution. With the graphic transformation, we can express the deviation from the equilibrium distribution explicitly as a function of the asymmetry in the system. The graphic transformation method has been initially applied to the question of enzyme coupled reactions [18], and is applied to the problem of neural networks for the first time here [17].

In the procedure of the graphic transformation, we first normalize the graphic expression (13) by the spanning in-trees contributing to the graphic expressions of a state S^0, where S^0 is the standard state for normalization taken as arbitrary. Namely, we transform the spanning in-trees $G_S(m)$ $(m=1,2,3,\ldots,n_g)$ into the spanning in-trees $G_{S^0}(m)$ $(m=1,2,3,\ldots,n_g)$. This can be accomplished by the following procedure. Let us consider $P_{SS^0}(m)$, which is defined as the subgraph of $G_S(m)$ connecting the states S and S^0 (by the definition of a tree, there is only one subgraph of $G_S(m)$ that satisfies this condition). We then reverse the directed edges of $P_{SS^0}(m)$. As a result, we obtain $P_{S^0S}(m)$, which is the corresponding subgraph of $G_{S^0}(m)$ (Fig. 2). Note that the above procedure is always possible, as $P_{SS^0}(m)$ and $P_{S^0S}(m)$ share the same underlying graph.

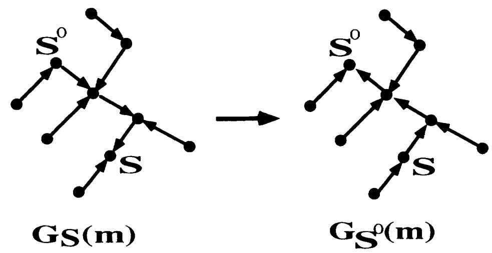

FIG. 2. The graphic transformation method. In order to derive the steady-state distribution of the asymmetric Boltzmann machine as a generalization of the symmetric equilibrium case, we perform the graphic transformation method. In this figure, the spanning in-tree $G_S(m)$ is transformed into the spanning in-tree $G_{SS^0}(m)$. In order to do so, it is necessary and sufficient to reverse the direction of the directed edges belonging to the path $P_{SS^0}(m)$. The corresponding rate constants are accordingly transformed.

As the result of the graphic transformation, the graphic representation of the weight $W(S)$ is transformed as

$$\begin{aligned}
W(S)&=\sum_m \prod_{(S^p,S^q)\in G_S(m)} K(S^p,S^q)\\
&=\sum_m \prod_{(S^p,S^q)\in G_S(m)-P_{SS^0}(m)} K(S^p,S^q) \prod_{(S^p,S^q)\in P_{SS^0}(m)} K(S^p,S^q)\\
&=\sum_m \prod_{(S^p,S^q)\in G_S(m)-P_{SS^0}(m)} K(S^p,S^q) \prod_{(S^p,S^q)\in P_{SS^0}(m)} K(S^q,S^p)e^{-\beta[E(S^p)-E(S^q)+d(S^p,S^q)]}\\
&=e^{-\beta[E(S)-E(S^0)]}\sum_m \prod_{(S^p,S^q)\in G_S(m)-P_{SS^0}(m)} K(S^p,S^q) \prod_{(S^p,S^q)\in P_{SS^0}(m)} K(S^q,S^p)e^{-\beta d\{S^p,S^q)}\\
&=e^{-\beta[E(S)-E(S^0)]}\sum_m \prod_{(S^p,S^q)\in G_{S^0}(m)-P_{S^0S}(m)} K(S^p,S^q) \prod_{(S^p,S^q)\in P_{S^0S}(m)} K(S^p,S^q) \prod_{(S^p,S^q)\in P_{SS^0}(m)} e^{-\beta d\{S^p,S^q)}\\
&=e^{-\beta[E(S)-E(S^0)]}\sum_m \exp\left[-\beta\left[\sum_{(S^p,S^q)\in P_{SS^0}(m)} d(S^p,S^q)\right]\right] \prod_{(S^p,S^q)\in G_{S^0}(m)} K(S^p,S^q)\ .
\end{aligned}\tag{15}$$

Note that the exponential terms involving the equilibrium energy cancel except for the states on both ends of the reversed path, S and S^0. This is the most important property of the graphic transformation method. Also note that we have replaced $G_S(m)-P_{SS^0}(m)$ with $G_{S^0}(m)-P_{S^0S}(m)$, as they are equivalent. By use of the graphic transformation method, we have successfully separated the contributions of the equilibrium energy term and the asymmetric energy terms in the weight $W(S)$.

In Eq. (15), the term due to $E(S^0)$ is a common normalization factor. The weight $W(S)$ normalized by the state S^0 can therefore be written as

$$W(S)=e^{-\beta E(S)}\sum_m \exp\left[-\beta\left[\sum_{(S^p,S^q)\in P_{SS^0}(m)} d(S^p,S^q)\right]\right] \prod_{(S^p,S^q)\in G_{S^0}(m)} K(S^p,S^q)\ .\tag{16}$$

Equation (16) expresses the steady-state distribution of the states of the neurons as an extension of the equilibrium distribution. From Eq. (16), we define the vectors

$$\mathbf{K}=\left[\prod_{(S^p,S^q)\in G_{S^0}(1)} K(S^p,S^q),\ldots,\prod_{(S^p,S^q)\in G_{S^0}(n_g)} K(S^p,S^q)\right], \tag{17}$$

$$\mathbf{D}(S)=\left\{\exp\left[-\beta\left[\sum_{(S^p,S^q)\in P_{SS^0}(1)} d(S^p,S^q)\right]\right],\ldots,\exp\left[-\beta\left[\sum_{(S^p,S^q)\in P_{SS^0}(n_g)} d(S^p,S^q)\right]\right]\right\}, \tag{18}$$

where $\mathbf{K}$ is the "spanning in-tree product" vector which is common for all the states, and $\mathbf{D}(S)$ is the "distortion" vector which gives the magnitude of deviation from the equilibrium for each state. Note that these vectors are defined with the state S^0 as the standard state for normalization. Note also that the dimension of the vectors n_g is not a measure of asymmetry of the neural network or the deviation from the equilibrium, as n_g is a quantity that is determined solely by the number of neutrons.

We can then normalize the distribution (16) by dividing by a common denominator as

$$\frac{W(S)}{\sum_m \prod_{(S^p,S^q)\in G_{S^0}(m)} K(S^p,S^q)}=e^{-\beta E(S)}\frac{\sum_m \exp\left[-\beta\left[\sum_{(S^p,S^q)\in P_{SS^0}(m)} d(S^p,S^q)\right]\right]\prod_{(S^p,S^q)\in G_{S^0}(m)} K(S^p,S^q)}{\sum_m \prod_{(S^p,S^q)\in G_{S^0}(m)} K(S^p,S^q)}$$

$$=e^{-\beta E(S)}\frac{\mathbf{K}\cdot\mathbf{D}(S)}{\mathbf{K}\cdot\mathbf{U}}. \tag{19a}$$

The ratio

$$\frac{\mathbf{K}\cdot\mathbf{D}(S)}{\mathbf{K}\cdot\mathbf{U}}, \quad \text{where } \mathbf{U}=(1,\ldots,1) \tag{19b}$$

gives the magnitude of deviation from equilibrium distribution.

It is easily seen that the distribution (16) reduces to the equilibrium distribution when the connections between the neurons are made symmetric ($w_{ij}=w_{ji}$). The distortion vector $\mathbf{D}(S)$ is then equal to the vector $\mathbf{U}$, and the ratio (19b) reduces to 1.

Finally, we define the "weight vector" $\mathbf{W}(S)$ as

$$\mathbf{W}(S)=e^{-\beta E(S)}\mathbf{D}(S)$$

$$=\left\{\exp\left[-\beta\left[E(S)+\sum_{(S^p,S^q)\in P_{SS^0}(1)} d(S^p,S^q)\right]\right],\ldots,\exp\left[-\beta\left[E(S)+\sum_{(S^p,S^q)\in P_{SS^0}(n_g)} d(S^p,S^q)\right]\right]\right\}. \tag{20}$$

Using the weight vector, the state distribution $\rho(S)$ can be written as

$$\rho(S)=\frac{\mathbf{K}\cdot\mathbf{W}(S)}{\mathbf{K}\cdot\sum_R \mathbf{W}(R)}. \tag{21}$$

Equation (21) is the "weight vector" representation of the steady-state distribution of the asymmetric Boltzmann machines.

IV. MULTIPLE ENERGY VALUES CHARACTERIZING THE STEADY STATE

It is interesting to consider the significance of the "weight vector" representation we obtained above. From representation (21), we see that in order to describe the steady state of asymmetric Boltzmann machines, we need n_g energy values

$$\mathbf{E}(S)=\left[E(S)+\sum_{(S^p,S^q)\in P_{SS^0}(1)} d(S^p,S^q),\ldots,E(S)+\sum_{(S^p,S^q)\in P_{SS^0}(n_g)} d(S^p,S^q)\right]$$
$$=\left[E(S)-\frac{1}{4}\sum_{(S^p,S^q)\in P_{SS^0}(1)}\sum_i\sum_j (w_{ij}-w_{ji})(s_i^p-s_i^q)(s_j^p+s_j^q),\ldots,E(S)\right.$$
$$\left.-\frac{1}{4}\sum_{(S^p,S^q)\in P_{SS^0}(n_g)}\sum_i\sum_j (w_{ij}-w_{ji})(s_i^p-s_i^q)(s_j^p+s_j^q)\right] . \tag{22}$$

Namely, we see that the steady state of asymmetric Boltzmann machines is characterized by the multiple-valued energy function $\mathbf{E}(S)$. The energy values are expressed as the sum of the equilibrium energy term and an extra term due to the asymmetric energy term. The asymmetric energy term is summed over the transition pathways connecting the state S and the standard state S^0. Note that when the connections between the neurons are symmetric, the n_g energy values reduce to a single value, $E(S)$. Therefore, the multiple-valued energy function $\mathbf{E}(S)$ defined above can be considered as a generalization of the single-valued scalar energy function for a symmetric Boltzmann machine.

From the representation (21), we also see that the relative importance of the multiple energy values in determining the state density $\rho(S)$ is given by the components of the "spanning in-tree product vector" $\mathbf{K}$. Specifically, the relative importance of the energy value corresponding to the mth spanning in-tree.

$$E(S)+\sum_{(S^p,S^q)\in P_{SS^0}(m)} d(S^p,S^q)$$

is given by

$$\prod_{(S^p,S^q)\in G_{S^0}(m)} K(S^p,S^q) .$$

We can now define a generalized entropy for a steady state. It is known that the equilibrium Boltzmann distribution is given by maximizing the "entropy"

$$-\sum_S \rho(S)\ln\rho(S) \tag{23}$$

under the conditions

$$\sum_S \rho(S)=1 , \tag{24a}$$

$$\sum_S E(S)\rho(S)=E \quad (\text{const}) . \tag{24b}$$

We see that the distribution (21) for asymmetric Boltzmann machines is obtained by maximizing the generalized entropy

$$-\sum_S \rho(S)\ln\rho'(S) , \tag{25a}$$

where

$$\rho'(S)=\frac{\rho(S)}{\mathbf{K}\cdot\mathbf{D}(S)/\mathbf{K}\cdot\mathbf{U}} \tag{25b}$$

under the conditions of (24a) and (24b).

We can therefore conclude that, formally, the steady state can be characterized as the state for which the generalized entropy (25a) is maximum under the conditions of (24a) and (24b). Note that the generalized entropy (25a) reduces to the equilibrium entropy (23) when the connections between the neurons are symmetric, as the denominator in Eq. (25b) reduces to 1.

We note that the generalized entropy (25a) for the steady state can be alternatively expressed as the sum of the equilibrium entropy term and an extra term as

$$-\sum_S \rho(S)\ln\rho'(S)=-\sum_S \rho(S)\ln\frac{\rho(S)}{\mathbf{K}\cdot\mathbf{D}(S)/\mathbf{K}\cdot\mathbf{U}}$$
$$=-\sum_S \rho(S)\ln\rho(S)-\sum_S \rho(S)\ln\frac{\mathbf{K}\cdot\mathbf{U}}{\mathbf{K}\cdot\mathbf{D}(S)} , \tag{26a}$$

where

$$-\sum_S \rho(S)\ln\frac{\mathbf{K}\cdot\mathbf{U}}{\mathbf{K}\cdot\mathbf{D}(S)}=-\sum_S \rho(S)\ln\frac{\sum_m \prod_{(S^p,S^q)\in G_{S^0}(m)} K(S^p,S^q)}{\sum_m \exp\left[-\beta\left[\sum_{(S^p,S^q)\in P_{SS^0}(m)} d(S^p,S^q)\right]\right]\prod_{(S^p,S^q)\in G_{S^0}(m)} K(S^p,S^q)} \tag{26b}$$

is the extra entropy term characterizing the deviation of the steady state from the equilibrium.

V. STEADY FLOW IN THE SYSTEM AND THE ASYMMETRY IN NEURAL CONNECTIONS

A. Expression of the steady flow

In previous sections, we have applied the graphic transformation method to the analysis of asymmetric Boltzmann machines. The weight vector representation (21) is novel and interesting from a mathematical point of view. However, the question naturally arises as to whether the mathematical method we introduced here is useful as well. In order to establish the validity of the graphic transformation method, we investigate the relation between the steady flow and the asymmetric energy term (7), using the weight vector representation (21).

The steady flow from the state S^y to state S^x, $F(S^x,S^y)$, is defined as

$$F(S^x,S^y)=K(S^x,S^y)\rho(S^y)-K(S^y,S^x)\rho(S^x)\ . \tag{27}$$

We note that

$$F(S^y,S^x)=-F(S^x,S^y)\ . \tag{28}$$

In the equilibrium state, the steady flow is zero. In the case of the steady state, the steady flow is, in general, not zero. The steady flow is therefore an important property characterizing the steady state. The steady flow can be transformed using the weight vector representation as

$$\begin{aligned}F(S^x,S^y)&=K(S^x,S^y)\rho(S^y)-K(S^y,S^x)\rho(S^x)\\&=K(S^x,S^y)\frac{\mathbf{K}\cdot\mathbf{W}(S^y)}{\mathbf{K}\cdot\sum_R\mathbf{W}(R)}-K(S^y,S^x)\frac{\mathbf{K}\cdot\mathbf{W}(S^x)}{\mathbf{K}\cdot\sum_R\mathbf{W}(R)}\\&=\frac{\mathbf{K}[K(S^x,S^y)\mathbf{W}(S^y)-K(S^y,S^x)\mathbf{W}(S^x)]}{\mathbf{K}\cdot\sum_R\mathbf{W}(R)}\\&=\frac{K(S^x,S^y)\mathbf{K}\cdot[\mathbf{W}(S^y)-e^{\beta[E(S^x)-E(S^y)+d(S^x,S^y)]}\mathbf{W}(S^x)]}{\mathbf{K}\cdot\sum_R\mathbf{W}(R)}\\&=\frac{\mathbf{K}\cdot\mathbf{F}(S^x,S^y)}{\mathbf{K}\cdot\sum_R\mathbf{W}(R)}\ ,\end{aligned} \tag{29}$$

where

$$\mathbf{F}(S^{\lambda}\ S^y)=K(S^x,S^y)[\mathbf{W}(S^y)-e^{\beta[E(S^x)-E(S^y)+d(S^x,S^y)]}\mathbf{W}(S^x)] \tag{30}$$

is the "steady-flow vector" which represents the net flow from the state S^y to the state S^x.

We now note that

$$\begin{aligned}&e^{\beta[E(S^x)-E(S^y)+d(S^x,S^y)]}\mathbf{W}(S^x)\\&\quad=e^{\beta[E(S^x)-E(S^y)+d(S^x,S^y)]}\left\{\exp\left[-\beta\left[E(S^x)+\sum_{(S^p,S^q)\in P_{S^xS^0}(1)}d(S^p,S^q)\right]\right],\ldots,\right.\\&\qquad\qquad\left.\exp\left[-\beta\left[E(S^x)+\sum_{(S^p,S^q)\in P_{S^xS^0}(n_g)}d(S^p,S^q)\right]\right]\right\}\\&\quad=\left\{\exp\left[-\beta\left[E(S^y)+\sum_{(S^p,S^q)\in P_{S^xS^0}(n_g)}d(S^p,S^q)+d(S^y,S^x)\right]\right],\ldots,\right.\\&\qquad\left.\exp\left[-\beta\left[E(S^y)+\sum_{(S^p,S^q)\in P_{S^xS^0}(n_g)}d(S^p,S^q)+d(S^y,S^x)\right]\right]\right\}\ .\end{aligned}$$

The mth element of the steady-flow vector can therefore be expressed as

$$K(S^x,S^y)\left\{\exp\left[-\beta\left[E(S^y)+\sum_{(S^p,S^q)\in P_{S^yS^0}(m)} d(S^p,S^q)\right]\right]-\exp\left[-\beta\left[E(S^y)+\sum_{(S^p,S^q)\in P_{S^xS^0}(m)} d(S^p,S^q)+d(S^y,S^x)\right]\right]\right\}$$

$$=K(S^x,S^y)e^{-\beta E(S^y)}\left\{1-\exp\left[-\beta\left[\sum_{(S^p,S^q)\in P_{S^xS^0}(m)} d(S^p,S^q)+d(S^y,S^x)-\sum_{(S^p,S^q)\in P_{S^yS^0}(m)} d(S^p,S^q)\right]\right]\right\}\exp\left[-\beta\sum_{(S^p,S^q)\in P_{S^yS^0}(m)} d(S^p,S^q)\right].$$

At this point, $\mathcal{L}_{\text{loop}}(S^x,S^y,m)$ is defined as the loop obtained by adding the directed edge (S^y,S^x) to the path $P_{S^xS^y}(m)$ in the spanning in-tree $G_S(m)$ [Fig. 3(a)].

We then note that

$$\sum_{(S^p,S^q)\in P_{S^xS^0}(m)} d(S^p,S^q)+d(S^y,S^x)-\sum_{(S^p,S^q)\in P_{S^yS^0}(m)} d(S^p,S^q)$$
$$=\sum_{(S^p,S^q)\in P_{S^xS^0}(m)} d(S^p,S^q)+\sum_{(S^p,S^q)\in P_{S^0S^y}(m)} d(S^p,S^q)+d(S^y,S^x)$$
$$=\sum_{(S^p,S^q)\in P_{S^xS^y}(m)} d(S^p,S^q)+d(S^y,S^x)$$
$$=\sum_{(S^p,S^q)\in \mathcal{L}_{\text{loop}}(S^xS^y,m)} d(S^p,S^q)\,. \tag{31}$$

The steady-flow vector is finally expressed as

$$\mathbf{F}(S^x,S^y)=K(S^x,S^y)e^{-\beta E(S^y)}\left(\left\{1-\exp\left[-\beta\left[\sum_{(S^p,S^q)\in\mathcal{L}_{\text{loop}}(S^x,S^y,1)} d(S^p,S^q)\right]\right]\right\}\exp\left[-\beta\sum_{(S^p,S^q)\in P_{S^yS^0}(1)} d(S^p,S^q)\right],\dots,\right.$$
$$\left\{1-\exp\left[-\beta\left[\sum_{(S^p,S^q)\in\mathcal{L}_{\text{loop}}(S^x,S^y,n_g)} d(S^p,S^q)\right]\right]\right\}$$
$$\left.\times\exp\left[-\beta\sum_{(S^p,S^q)\in P_{S^yS^0}(n_g)} d(S^p,S^q)\right]\right). \tag{32}$$

In Eq. (32), we have expressed the largeness of the steady flow from the state S^y to the state S^x as a function of the asymmetry in the connections between the neurons. Specifically, the largeness of the steady flow is related to the sum of the asymmetric energy terms over the loops containing the two states in question. Generally speaking, the steady state is distinguished from the equilibrium state in that the detailed balancing [27] does not hold. The largeness of the steady flow is a measure of the violation of the detailed balancing. We therefore see that Eq. (32) relates the measure of the violation of the detailed balancing to a geometrical property (the sum of the asymmetric energy terms over the loops) of the network.

B. Contribution of tangled pairs of flip-flop transitions to the steady flow

We now show that in considering the sum of the asymmetric energy terms in Eq. (32), it is important to distinguish two classes of transition sequences of neural states. The sequence of transitions in $\mathcal{L}_{\text{loop}}(S^x,S^y,m)$ is made of flip-flop transitions. Let us assume that the $\mathcal{L}_{\text{loop}}(S^x,S^y,m)$ consists of $2K(m)$ transitions, where

$$1\le K(m)\le\left[\frac{N}{2}\right].$$

$[x]$ is defined as the largest integer not exceeding x.

We write the neural state after the kth transition as $S(p)$ $[p=0,1,2,\dots,2K(m)]$. We have $S(0)=S^y$, $S(2K(m)-1)=S^x$, and $S(2K(m))=S^y$. These transitions are composed of $K(m)$ flip-flop transitions. Let us write the index of the neuron involved in the kth flip-flop transition as $i(k)$ $[k=1,2,\dots,K(m)]$. Note that it is possible that a neuron is involved in more than one flip-flop transitions, so that in some cases

$$i(k)=i(k') \text{ even though } k\neq k' .$$

We write the indices of pair of transitions that constitute the kth flip-flop transition as k_1 and k_2. We define the ordering of the flip-flop transitions by the first (i.e., "flip") transition. Namely,

$$k<k' \text{ when } k_1<k_1' .$$

We write the index of neuron that changes its state in the kth flip-flop transition as $i(k)$. The loop term (31) can now be written as the sum over flip-flop transitions as

$$\begin{aligned}
&\sum_{(S^p,S^q)\in\mathcal{L}_{\text{loop}}(S^x,S^y,m)} d(S^p,S^q)\\
&=-\frac{1}{4}\sum_{(S^p,S^q)\in\mathcal{L}_{\text{loop}}(S^x,S^y,m)}\sum_i\sum_j (w_{ij}-w_{ji})(S_i^p-S_i^q)(S_j^p+S_j^q)\\
&=-\frac{1}{4}\sum_{k=1}^{K(m)}\sum_j (w_{i(k)j}-w_{ji(k)})\{[s(k_1)_{i(k)}-s(k_1-1)_{i(k)}][s(k_1)_j+s(k_1-1)_j]\\
&\qquad\qquad +[s(k_2)_{i(k)}-s(k_2-1)_{i(k)}][s(k_2)_j+s(k_2-1)_j]\}\\
&=-\frac{1}{2}\sum_{k=1}^{K(m)}\sum_j (w_{i(k)j}-w_{ji(k)})[s(k_1)_{i(k)}-s(k_2)_{i(k)}][s(k_1)_j-s(k_2)_j] ,
\end{aligned} \tag{33}$$

where we have used the relations

$$s(k_2)_{i(k)}-s(k_2-1)_{i(k)}=-[s(k_1)_{i(k)}-s(k_1-1)_{i(k)}] ,$$
$$s(k_1-1)_{i(k)}=s(k_2)_{i(k)} ,$$
$$s(k_2-1)_{i(k)}=s(k_1)_{i(k)} ,$$
$$s(k_1)_j=s(k_1-1)_j \quad [j\neq i(k)] ,$$
$$s(k_2)_j=s(k_2-1)_j \quad [j\neq i(k)] .$$

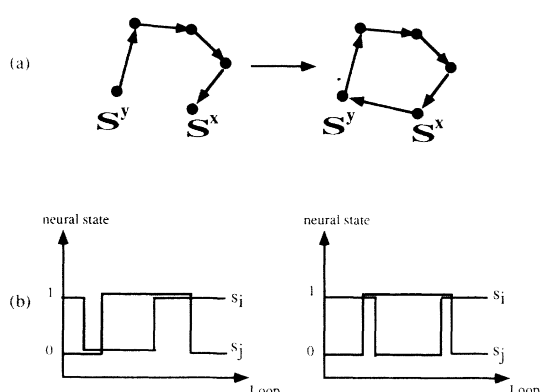

FIG. 3. (a) The formation of the $\mathcal{L}_{\text{loop}}(S^x,S^y,m)$ from the path $P_{S^xS^y}(m)$. In the calculation of the steady-flow vector, we obtain a loop by adding the directed edge (S^y,S^x) to the path $P_{S^xS^y}(m)$ in the spanning in-tree $G_S(m)$. The steady-flow vector is then expressed as a function of the sum of the asymmetric energy terms over these loops. (b) "Tangled" and "untangled" pair of flip-flop transitions in the sum of the asymmetric energy terms over the loops. In the calculation of the sum of the asymmetric energy terms over a loop, the nonvanishing terms arise from the "tangled" pairs of flip-flop transitions. The terms from the "untangled" pairs of flip-flop transitions cancel out.

Let us now consider a pair of flip-flop transitions involving the neurons with indices $i(k)$ and $i(k')$, where $k<k'$ and $i(k)\neq i(k')$. A "tangled" pair of flip-flop transitions is defined as a pair of flip-flop transitions that satisfies

$$k_1<k_1'<k_2<k_2' .$$

When a pair of flip-flop transitions satisfies

$$k_1<k_2<k_1'<k_2'$$

or

$$k_1<k_1'<k_2'<k_2 ,$$

we call it an "untangled" pair of flip-flop transitions [Fig. 3(b)].

Let us now consider two "tangled" flip-flop transitions that involve the kth flip-flop transition, (k,k') and (k,k''), where $k<k'$ and $k<k''$. It is easy to see that $i(k'')\neq i(k')$ when $k''\neq k'$.

From Eq. (33), we can then show that the only nonzero contributions come from a "tangled" pair of flip-flop transitions. Let us indicate a "tangled" pair of flip-flop transitions in $\mathcal{L}_{\text{loop}}(S^x,S^y,m)$ by their indices as (k,k'), where we assume that $k<k'$. Let us write the set of such a "tangled" pair of flip-flop transitions as $X(S^x,S^y,m)$. We can then transform Eq. (33) further as

$$\sum_{(S^p,S^q)\in\mathcal{L}_{\text{loop}}(S^x,S^y,m)} d(S^p,S^q)$$
$$=-\frac{1}{2}\sum_{k=1}^{K(m)}\sum_j (w_{i(k)j}-w_{ji(k)})[s(k_1)_{i(k)}-s(k_2)_{i(k)}][S(k_1)_j-s(k_2)_j]$$
$$=-\frac{1}{2}\sum_{(k,k')\in X(S^x,S^y,m)}\{(w_{i(k)i(k')}-w_{i(k')i(k)})[s(k_1)_{i(k)}-s(k_2)_{i(k)}]$$
$$\times[s(k_2')_{i(k')}-s(k_1')_{i(k')}]+(w_{i(k')i(k)}-w_{i(k)i(k')})[s(k_1')_{i(k')}-s(k_2')_{i(k')}]$$
$$\times[s(k_1)_{i(k)}-s(k_2)_{i(k)}]\}$$
$$=\sum_{(k,k')\in X(S^x,S^y,m)}(w_{i(k)i(k')}-w_{i(k')i(k)})[s(k_1)_{i(k)}-s(k_2)_{i(k)}][s(k_1')_{i(k')}-s(k_2')_{i(k')}]\ , \tag{34}$$

where we have used the relations

$$s(k_1)_{i(k')}=s(k_2')_{i(k')}\ ,$$
$$s(k_2)_{i(k')}=s(k_1')_{i(k')}\ .$$

In conclusion, the sum of asymmetric energy terms over $\mathcal{L}_{\text{loop}}(S^x,S^y,m)$ that appear in expression (32) can be expressed as the sum of contributions from the "tangled" flip-flop transition in $\mathcal{L}_{\text{loop}}(S^x,S^y,m)$.

In this section, we have expressed the largeness of the steady flow explicitly as a function of the asymmetric energy terms. We have shown that the steady flow can be related to the sum of the asymmetric energy terms over a loop, which can be considered as a measure of the "distortion" in the space $\{0,1\}^N$ due to the existence of multiple energy values (22). We expect such a geometrical property of the network [28] to play an essential role in the future studies of the nature of the steady state of asymmetric Boltzmann machines.

VI. CONCLUSION

In this paper, we have applied the graphic method to study of artificial neural networks. Specifically, we have applied the graphic transformation method to the study of asymmetric Boltzmann machines, and successfully expressed the state distribution of asymmetric Boltzmann machines as an extension of the equilibrium distribution.

We have shown that the steady state of asymmetric Boltzmann machines is characterized by multiple energy values, rather than by a single scalar energy function as in the case of symmetric equilibrium case. The single-valued scalar energy function for the equilibrium state of symmetric Boltzmann machines is generalized to a multiple-valued energy function in the case of the steady state of asymmetric Boltzmann machines.

We have defined a generalized entropy for the steady state of asymmetric Boltzmann machines. The generalized entropy is obtained by dividing each state density appearing in logarithm by a state-dependent denominator, which represents the largeness of deviation from the equilibrium state. The generalized entropy can alternatively be expressed as the sum of the equilibrium entropy and an extra entropy term, where the latter term is a measure of the largeness of deviation from the equilibrium.

We have expressed the steady flow between two neural states as a function of the asymmetry between the neurons. The existence of a nonzero steady flow can be considered as a result of the difference between the multiple energy values characterizing the steady state. We have shown that the steady flow is related to the sum of asymmetric energy terms over a loop including the two adjacent neural states in question. In the context of the study on artificial neural networks, our present study can be regarded as an attempt to understand the properties of an asymmetric neural network as geometrical features of the network. The graphic approach we introduced in this paper is expected to be valuable in such a line of research.

It is expected that the graphic transformation method has a wide applicability in questions relating to the nature of a steady state as compared to the equilibrium state. The graphic transformation method can be applied, for example, to an Ising spin system [29] with asymmetric exchange interactions, or to the question of coupling in biological systems [18]. However, it should be pointed out that at present there is a difficulty when we try to apply the graphic method to practical purposes, since the number of spanning in-trees given in formula (12) increases rapidly as the number of neurons increases. We should therefore devise some technique to overcome this problem, e.g., by calculating the exact number of independent energy values in the multiple-valued energy function given in (22). We note that this is one of the most important open problems in the graphic approach to artificial networks that we proposed in this paper.

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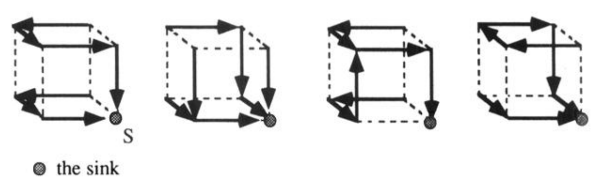

FIG. 1. Some examples of spanning in-trees in $\{0,1\}^3$. Some examples of spanning in-trees $G_S(m)$ which have the state S (indicated by the filled circle) as the sink are shown. In this figure, the number of neurons is taken to be 3. The vertices represent the neural states $\{0,1\}^3$. In the case of N neurons, a hypercube in N dimensions should be used.