Convergence Rates to Optimal Distribution of the Boltzmann Machine on Simulated Annealing

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In this paper, explicit estimations of the convergence rates of the Boltzmann machine on simulated annealing are given. As its applications, quantitative bounds of the temperature and the transition times of the Boltzmann machine to optimal distribution are given.

KEYWORDS: Boltzmann machine, Markov chain, Gibbs matrix, total variation distance, convergence rates

1. Introduction

Since the nineteen eighties, many studies of simulated annealing, so called the Boltzmann machine searching the minimum of a given function have been done. But, effective estimation of the convergence rates might be so far still unknown. However, the convergence rates of Markov chains have widely been studied (cf. [2], [3], [4], [5], [7], [10], [11], [12], [13], [14], [15], [16], [18]). In this paper, applying the result of Diaconis and Stroock [3] on the estimate of the convergence rates of Markov chains, we give an explicit estimation of the convergence rates to the optimal distribution of the Boltzmann machine (cf. Theorem 1.2). Moreover, we give concrete estimations of the temperature and transition time of the Gibbs-Boltzmann distributions of simulated annealing to optimal distribution in the simplest cases in which the number of states are four or eight (cf. Theorem 1.3 and Proposition 4.1). Even though the simplest case, our situation is completely general, and our estimation explains very well the character of the Boltzmann machine (See Remark 1.4).

Let us explain our situation, more precisely. We consider a function F on a finite set S having a minimum $F_{\min}$ on a subset S_0 of S . Let us consider an optimal distribution q_0 given by

$$q_0(x) := \begin{cases} \frac{1}{|S_0|}, & x \in S_0, \\ 0, & x \in S \setminus S_0. \end{cases}$$

It is well known (cf. see [1], for example) that

- (1) the Gibbs distribution q_T with temperature $T > 0$ converges to q_0 when T tends to 0, and
- (2) the distribution $r G_T^m$ converges to the Gibbs distribution q_T when m tends to infinity for every initial distribution r .

But, so far, it has been unknown how much T and m one should take rigorously in order to approximate q_T and $r G_T^m$ enough to q_0 . In this paper, we want to answer to this question.

Let us recall several notations which are necessary for later use. For every distribution r on S , $r G_T^m$ on S is given by

$$(r G_T^m)(x) := \sum_{y \in S} r(y) G_T^m(y, x),$$

where G_T^m is the m -th power of the Gibbs matrix G_T with temperature T , that is,

$$G_T^m(x, y) := \sum_{z_1, \dots, z_m \in S} G_T(x, z_1) \cdots G_T(z_m, y).$$

The Gibbs matrix $G_T = (G_T(x, y))_{x, y \in S}$ is given by definition as

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$$G_T(x, y) = \begin{cases} P(x, y)A_T(x, y) & \text{if } x \neq y, \\ 1 - \sum_{z \neq x} P(x, z)A_T(x, z) & \text{if } x = y, \end{cases} \quad (1.1)$$

$P = (P(x, y))_{x, y \in S}$ is the *generating probability matrix* and $A_T = (A_T(x, y))_{x, y \in S}$ is the *accepting matrix*, which is given by

$$A_T(x, y) = g\left(\frac{q_T(y)}{q_T(x)}\right), \quad (1.2)$$

where $g(u)$ is the *accepting function* on the open interval $(0, \infty)$ into the interval $(0, 1]$ satisfying that

$$g(u) = u g\left(\frac{1}{u}\right), \quad 0 < u < \infty.$$

Furthermore, let us recall the definition of *Gibbs distribution* q_T :

$$q_T(x) = \frac{e^{-\frac{1}{T}F(x)}}{Z}, \quad x \in S, \quad (1.3)$$

where Z is the *Boltzman constant* which is by definition

$$Z = \sum_{y \in S} e^{-\frac{1}{T}F(y)}. \quad (1.4)$$

Then, G_T is *reversible* with respect to q_T , that is,

$$q_T(x) G_T(x, y) = q_T(y) G_T(y, x), \quad \forall x, y \in S, \quad (1.5)$$

and q_T is the *equilibrium distribution*, that is,

$$\sum_{x \in S} q_T(x) G_T(x, y) = q_T(y), \quad \forall y \in S. \quad (1.6)$$

It is well known that G_T is *irreducible*, that is, for all x and y in S , there exists a positive integer k such that $G_T^k(x, y) > 0$. Furthermore, G_T is *aperiodic*, that is, $\gcd\{k; G_T^k(x, y) > 0\} = 1$. Due to *ergodic theorem*, it holds (cf. [1]) that

Theorem 1.1. *For all initial distribution r ,*

$$\lim_{m \rightarrow \infty} r G_T^m = q_T. \quad (1.7)$$

Now, let us recall the notion of the *total variation distance* between two probability distributions μ and μ' on S :

$$\begin{aligned} \|\mu - \mu'\|_{TV} &:= \sup\{|\mu(A) - \mu'(A)| : A \in \mathcal{B}\} \\ &= \frac{1}{2} \sum_{x \in S} |\mu(x) - \mu'(x)|, \end{aligned} \quad (1.8)$$

where $\mathcal{B}$ is the σ -algebra of all Borel sets in S . Diaconis and Stroock [3] estimated the total variation distance between any reversible Markov chain G (with respect to π) and the stationary distribution π in terms of the eigenvalues of G (See the next section). Applying their result to the Boltzmann machine, we have:

Theorem 1.2. *For every $T > 0$ and $m = 1, 2, \dots$,*

$$\|r G_T^m - q_0\|_{TV} \leq \frac{\sqrt{|S|}}{2} \beta_*^m \left(|S_0| + \sum_{y \in S \setminus S_0} e^{\frac{1}{2T}(F(y) - F_{\min})} \right) + \frac{\sum_{x \in S \setminus S_0} e^{-\frac{1}{T}(F(x) - F_{\min})}}{|S_0| + \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}(F(x) - F_{\min})}}, \quad (1.9)$$

where $0 \leq \beta_* := \max\{\beta_1, |\beta_{a-1}|\} < 1$. Here, we write the eigenvalues of the Gibbs matrix G_T as

$$1 = \beta_0 > \beta_1 \geq \dots \geq \beta_{a-1} \geq -1, \quad (\text{where } a := |S|).$$

Applying this estimation (1.9) to the simplest set S of states with $|S| = 4$, we can concretely estimate T and m such that

$$\|r G_T^m - q_0\|_{TV} < \epsilon = 0.1. \quad (1.10)$$

For the case $|S| = 8$, see Section Four. In the case $|S| = 4$, more precisely, let us consider the function F on $S = \{a, b, c, d\}$ with four values, say

$$0 > -v_1 > -v_2 > -w_{12} - v_1 - v_2 \quad (1.11)$$

without loss of generality. We choose the accepting function g as

$$g(u) = \frac{u}{1+u} = \frac{1}{1+u^{-1}} =: \tau(u). \quad (1.12)$$

How much $0 < T < \infty$ and m can one take to search the point of $S = \{a, b, c, d\}$ at which F attains the minimum value $-w_{12} - v_1 - v_2$ by simulated annealing? Our answer is this:

Theorem 1.3. If $0 < T \leq \frac{w_{12}+v_1}{2.70806}$ and

$$m \geq 31.2415 \times \frac{w_{12} + v_1 + v_2}{T} + 169.207 \quad (1.13)$$

in the case $w_{12} > 0$, or

$$m \geq 1.06382 \times \frac{w_{12} + v_1 + v_2}{T} + 5.76176 \quad (1.14)$$

in the case $w_{12} < 0$, then

$$\|r G_T^m - q_0\|_{TV} < \frac{1}{10} = 0.1. \quad (1.15)$$

Remark 1.4. By Theorem 1.3, if we take T and m as in this theorem, the Boltzmann machine can search the point of S at which F attains the minimum with probability 90%. This estimation explains the character of the Boltzmann machine very well. Indeed, in order to estimate the convergence rates of the simulated annealing lower than 0.1, one should set the temperature T lower than $\frac{w_{12}+v_1}{2.70806}$. But, if one sets for the temperature T to be too low, a large transition time m is necessary.

Remark 1.5. The right hand side of (1.9) in Theorem 1.2 does not depend on the initial state r on S . The first term of the right hand side converges to zero if m tends to infinity since $0 \leq \beta_* < 1$. The second term converges to zero if T tends to zero. Be careful that the factor of the first term, $\sum_{y \in S \setminus S_0} e^{\frac{1}{2T}(F(y) - F_{\min})}$ goes to infinity if T tends to zero.

2. Proof of Theorem 1.2

We first prove

Theorem 2.1.

$$\|q_T - q_0\|_{TV} = \frac{|S_0|}{Z} e^{-\frac{1}{T}F_{\min}} - 1 = \frac{1}{Z} \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}F(x)} \quad (2.1)$$

$$= \frac{\sum_{x \in S \setminus S_0} e^{-\frac{1}{T}(F(x) - F_{\min})}}{|S_0| + \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}(F(x) - F_{\min})}}. \quad (2.2)$$

Proof. By (1.8), we have

$$\|q_T - q_0\|_{TV} = \frac{1}{2} \sum_{x \in S} \left| \frac{1}{Z} e^{-\frac{1}{T}F(x)} - \frac{1}{|S_0|} \chi_{S_0}(x) \right|, \quad (2.3)$$

where χ_{S_0} is the characteristic function of S_0 in S . The right hand side of (2.3) coincides with

$$\frac{1}{2} \sum_{x \in S_0} \left| \frac{1}{Z} e^{-\frac{1}{T}F(x)} - \frac{1}{|S_0|} \chi_{S_0}(x) \right| + \frac{1}{2} \sum_{x \in S \setminus S_0} \left| \frac{1}{Z} e^{-\frac{1}{T}F(x)} - \frac{1}{|S_0|} \chi_{S_0}(x) \right|,$$

which is equal to

$$\frac{|S_0|}{2Z} \left| e^{-\frac{1}{T}F_{\min}} - \frac{Z}{|S_0|} \right| + \frac{1}{2Z} \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}F(x)}. \quad (2.4)$$

But, we have

$$\begin{aligned} Z &= \sum_{x \in S} e^{-\frac{1}{T}F(x)} = \sum_{x \in S_0} e^{-\frac{1}{T}F(x)} + \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}F(x)} \\ &= |S_0| e^{-\frac{1}{T}F_{\min}} + \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}F(x)}, \end{aligned} \quad (2.5)$$

which implies that

$$-e^{-\frac{1}{T}F_{\min}} + \frac{Z}{|S_0|} = \frac{1}{|S_0|} \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}F(x)} \geq 0, \quad (2.6)$$

so that we have (2.1). By (2.5),

$$\frac{1}{Z} \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}F(x)} = \frac{\sum_{x \in S \setminus S_0} e^{-\frac{1}{T}F(x)}}{|S_0|e^{-\frac{1}{T}F_{\min}} + \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}F(x)}} = \frac{\sum_{x \in S \setminus S_0} e^{-\frac{1}{T}(F(x)-F_{\min})}}{|S_0| + \sum_{x \in S \setminus S_0} e^{-\frac{1}{T}(F(x)-F_{\min})}}, \quad (2.7)$$

which implies (2.2). $\square$

Next, we have

Theorem 2.2.

$$\|r G_T^m - q_T\|_{TV} \leq \beta_*^m \cdot \frac{1}{2} \sum_{y \in S} r(y) \left(\frac{1 - q_T(y)}{q_T(y)} \right)^{\frac{1}{2}}. \quad (2.8)$$

Before going into the proof of Theorem 2.2, let us recall the results due to Diaconis and Stroock (cf. [3]) of the transition probability $G(x, y)$ for an irreducible Markov chain reversible relative to the stationary distribution π , that is

$$\pi(x) G(x, y) = \pi(y) G(y, x), \quad \forall x, y \in S.$$

We denote all the eigenvalues of the matrix $G = (G(x, y))_{x, y \in S}$ by

$$1 = \beta_0 > \beta_1 \geq \beta_2 \geq \cdots \geq \beta_{a-1} \geq -1,$$

where $a = |S|$. Then, it holds (cf. [3]) that

$$2\|G^m(x, \cdot) - \pi(\cdot)\|_{TV} \leq \left(\frac{1 - \pi(x)}{\pi(x)} \right)^{1/2} \beta_*^m, \quad (2.9)$$

where $\beta_* := \max\{\beta_1, |\beta_{a-1}|\}$.

By applying (2.9) to G_T , we have

$$2\|G_T^m(x, \cdot) - q_T(\cdot)\|_{TV} \leq \left(\frac{1 - q_T(x)}{q_T(x)} \right)^{1/2} \beta_*^m. \quad (2.10)$$

(Proof of Theorem 2.2). We have by definition and (1.8)

$$\begin{aligned} \|r G_T^m - q_T\|_{TV} &= \left\| \sum_{y \in S} r(y) G_T^m(y, \cdot) - q_T(\cdot) \right\|_{TV} \\ &= \frac{1}{2} \sum_{x \in S} \left| \sum_{y \in S} r(y) G_T^m(y, x) - q_T(x) \right| \\ &= \frac{1}{2} \sum_{x \in S} \left| \sum_{y \in S} r(y) (G_T^m(y, x) - q_T(x)) \right| \\ &\leq \frac{1}{2} \sum_{x \in S} \sum_{y \in S} r(y) |G_T^m(y, x) - q_T(x)| \\ &= \sum_{y \in S} r(y) \frac{1}{2} \sum_{x \in S} |G_T^m(y, x) - q_T(x)| \\ &= \sum_{y \in S} r(y) \|G_T^m(y, \cdot) - q_T(\cdot)\|_{TV} \\ &\leq \sum_{y \in S} r(y) \frac{1}{2} \left(\frac{1 - q_T(y)}{q_T(y)} \right)^{1/2} \beta_*^m, \end{aligned} \quad (2.11)$$

which follows from (2.10). (2.11) is the desired one. $\square$

To estimate the right hand side of (2.8), we have

Proposition 2.3. (1) For the upper bound,

$$\sum_{y \in S} r(y) \left(\frac{1 - q_T(y)}{q_T(y)} \right)^{1/2} \leq |S|^{1/2} \left(|S_0| + \sum_{y \in S \setminus S_0} e^{\frac{1}{2T}(F(y)-F_{\min})} \right). \quad (2.12)$$

(2) For the lower bound,

$$\sum_{y \in S} r(y) \left(\frac{1 - q_T(y)}{q_T(y)} \right)^{1/2} \geq |S_0|^{1/2} \sum_{y \in S \setminus S_0} r(y) e^{\frac{1}{2T}(F(y) - F_{\min})}. \quad (2.13)$$

Proof. (1) Since $0 \leq r(y) \leq 1$ and $q_T(y) \leq 1$, we have

$$\sum_{y \in S} r(y) \left(\frac{1 - q_T(y)}{q_T(y)} \right)^{1/2} \leq \sum_{y \in S} q_T(y)^{-1/2} = Z^{1/2} \cdot \sum_{y \in S} e^{\frac{1}{2T}F(y)}. \quad (2.14)$$

Here, by definition of Z , we have

$$e^{\frac{1}{2T}F_{\min}} Z = |S_0| + \sum_{z \in S \setminus S_0} e^{-\frac{1}{2T}(F(z) - F_{\min})} \leq |S_0| + |S \setminus S_0| = |S|. \quad (2.15)$$

Then, by (2.15), we have

$$\begin{aligned} Z^{1/2} \cdot \sum_{y \in S} e^{\frac{1}{2T}F(y)} &\leq |S|^{1/2} e^{-\frac{1}{2T}F_{\min}} \sum_{y \in S} e^{\frac{1}{2T}F(y)} \\ &= |S|^{1/2} \sum_{y \in S} e^{\frac{1}{2T}(F(y) - F_{\min})} \\ &= |S|^{1/2} \left(|S_0| + \sum_{y \in S \setminus S_0} e^{\frac{1}{2T}(F(y) - F_{\min})} \right), \end{aligned}$$

which is (2.12).

For (2), by definition of q_T , we have, for every $y_0 \in S \setminus S_0$,

$$\frac{1 - q_T(y_0)}{q_T(y_0)} = \frac{1 - e^{-\frac{1}{T}F(y_0)}/Z}{e^{-\frac{1}{T}F(y_0)}/Z} = e^{\frac{1}{T}F(y_0)} Z - 1. \quad (2.16)$$

Here, we have

$$\begin{aligned} e^{\frac{1}{T}F(y_0)} Z &= e^{\frac{1}{T}F(y_0)} \left(|S_0| e^{-\frac{1}{T}F_{\min}} + \sum_{y \in S \setminus S_0} e^{-\frac{1}{T}F(y)} \right) \\ &= |S_0| e^{\frac{1}{T}(F(y_0) - F_{\min})} + \sum_{y \in S \setminus S_0} e^{\frac{1}{T}(F(y_0) - F(y))} \\ &= |S_0| e^{\frac{1}{T}(F(y_0) - F_{\min})} + 1 + \sum_{y_0 \neq y \in S \setminus S_0} e^{\frac{1}{T}(F(y_0) - F(y))} \\ &\geq |S_0| e^{\frac{1}{T}(F(y_0) - F_{\min})} + 1. \end{aligned} \quad (2.17)$$

Thus, we have, for every $y_0 \in S \setminus S_0$,

$$\frac{1 - q_T(y_0)}{q_T(y_0)} \geq |S_0| e^{\frac{1}{T}(F(y_0) - F_{\min})}, \quad (2.18)$$

which yields (2.13). □

By Theorems 2.1, 2.2 and Proposition 2.3, we have Theorem 1.2. □

3. The Boltzmann Machine of Neural Networks

Now we apply our estimate to the Boltzmann machine coming from neural networks. The set S of states is given by $S = \{(x_1, x_2, \dots, x_n); x_i = 0 \text{ or } 1 (i = 1, \dots, n)\}$ ($|S| = 2^n$), and our function F on S is given by

$$F(x) = -\frac{1}{2} \sum_{i,j=1}^n w_{ij} x_i x_j - \sum_{i=1}^n v_i x_i, \quad (3.1)$$

where $w_{ii} = 0$ and $w_{ij} = w_{ji}$ ($i, j = 1, \dots, n$). For two states x and y in S , the transition probability from x to y is given by

$$P(x, y) = \begin{cases} \frac{1}{n} & \text{if } x \sim y \\ 0 & \text{otherwise,} \end{cases} \quad (3.2)$$

where $x \sim y$ stands that the Hamming distance on S between x and y is 1. The accepting matrix A_T is given by

$$A_T(x, y) = \tau\left(-\frac{F(y) - F(x)}{T}\right), \quad (3.3)$$

where the accepting function τ is given by (1.12). For $x = (x_1, x_2, \dots, x_n)$ and $y = x(k) = (x_1, x_2, \dots, x_{k-1}, 1 - x_k, x_{k+1}, \dots, x_n)$, we have

$$A_T(x, x(k)) = \tau\left(-\frac{(2x_k - 1)U_k(x)}{T}\right), \quad (3.4)$$

where

$$u_k = U_k(x) = \sum_{j=1}^n w_{kj}x_j + v_k \quad (k = 1, \dots, n) \quad (3.5)$$

which is called the *interior voltage* of k -th neuron. All the elements belonging to the set S are ordered as small as the function $N(x) = \sum_{k=1}^n k x_k$ ($x = (x_1, \dots, x_n) \in S$).

In the sequel of this section, we treat with the case $|S| = 4$ ($n = 2$), and will treat with the case $|S| = 8$ ($n = 3$) in the next section. In the case $|S| = 4$ ($n = 2$), we can calculate P , A_T and G_T as follows.

$$P = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix},$$

and

$$G_T = \begin{pmatrix} 1 - \frac{1}{2}A - \frac{1}{2}B & \frac{1}{2}A & \frac{1}{2}B & 0 \\ \frac{1}{2} - \frac{1}{2}A & \frac{1}{2} + \frac{1}{2}A - \frac{1}{2}D & 0 & \frac{1}{2}D \\ \frac{1}{2} - \frac{1}{2}B & 0 & \frac{1}{2} + \frac{1}{2}B - \frac{1}{2}C & \frac{1}{2}C \\ 0 & \frac{1}{2} - \frac{1}{2}D & \frac{1}{2} - \frac{1}{2}C & \frac{1}{2}C + \frac{1}{2}D \end{pmatrix},$$

where

$$A = \tau\left(\frac{v_1}{T}\right), \quad B = \tau\left(\frac{v_2}{T}\right), \quad C = \tau\left(\frac{w_{12} + v_1}{T}\right), \quad D = \tau\left(\frac{w_{12} + v_2}{T}\right).$$

By using “Mathematica”, one can compute the eigenvalues of G_T as follows:

$$\left\{ 1 > \frac{1}{2} \left(1 + \sqrt{(A - C)(B - D)} \right) > \frac{1}{2} \left(1 - \sqrt{(A - C)(B - D)} \right) > 0 \right\}.$$

Thus, we obtain

$$\beta_* = \frac{1}{2} \left(1 + \sqrt{(A - C)(B - D)} \right). \quad (3.6)$$

Now, we take $\epsilon = \frac{1}{10}$, $|S| = 4$, $|S_0| = 1$ and $|S \setminus S_0| = 3$. By Theorems 1.2 or 2.1, if $0 < T \leq T_0$,

$$\|q_T - q_0\|_{TV} \leq \frac{1}{20}, \quad (3.7)$$

where

$$\begin{aligned} T_0 &= \frac{F_1 - F_{\min}}{-\log \epsilon + \log 2 - \log |S| + \log |S \setminus S_0|} \\ &= \frac{w_{12} + v_1}{2.70806}. \end{aligned} \quad (3.8)$$

Here, we put

$$F_{\max} = 0 > F_2 = -v_1 > F_1 = -v_2 > F_{\min} = -w_{12} - v_1 - v_2 \quad (3.9)$$

satisfying that

$$0 < v_1 < v_2, \quad \text{and} \quad 0 < w_{12} + v_1. \quad (3.10)$$

On the other hand, for the above $T > 0$, by Theorems 1.1 or 2.2, and Proposition 2.3, to satisfy $\|r G_T^m - q_T\|_{TV} < \frac{\epsilon}{2}$, it suffices to take for any m satisfying that

$$\beta_*^m \frac{|S|^{3/2}}{2} e^{\frac{1}{2T}(F_{\max} - F_{\min})} < \frac{\epsilon}{2} \quad (3.11)$$

which is equivalent to the following:

$$\begin{aligned} m &> \frac{1}{-\log \beta_*} \left\{ -\log \epsilon + \frac{3}{2} \log |S| + \frac{1}{2T} (F_{\max} - F_{\min}) \right\} \\ &= \frac{1}{-\log \beta_*} \left\{ \log 10 + 3 \log 2 + \frac{1}{2T} (w_{12} + v_1 + v_2) \right\} \\ &= \frac{1}{-\log \beta_*} \left\{ 4.38203 + \frac{1}{2T} (w_{12} + v_1 + v_2) \right\}, \end{aligned} \quad (3.12)$$

since $\epsilon = \frac{1}{10}$, $|S| = 4$, $F_{\max} = 0$, and $F_{\min} = -w_{12} - v_1 - v_2$.

Here, $\beta_* = \frac{1}{2}(1+x)$ with $0 < x < 1$ which is given by

$$\begin{aligned} x &= \sqrt{\left(\tau\left(\frac{v_1}{T_0}\right) - \tau\left(\frac{w_{12}+v_1}{T_0}\right) \right) \left(\tau\left(\frac{v_2}{T_0}\right) - \tau\left(\frac{w_{12}+v_2}{T_0}\right) \right)} \\ &= \left\{ \frac{e^{-\frac{v_1}{T_0}}}{1+e^{-\frac{v_1}{T_0}}} \right\}^{1/2} \left\{ \frac{e^{-\frac{v_2}{T_0}}}{1+e^{-\frac{v_2}{T_0}}} \right\}^{1/2} \\ &\quad \times \left\{ \frac{1}{1+e^{-\frac{w_{12}+v_1}{T_0}}} \right\}^{1/2} \left\{ \frac{1}{1+e^{-\frac{w_{12}+v_2}{T_0}}} \right\}^{1/2} |e^{-\frac{w_{12}}{T_0}} - 1| \end{aligned} \quad (3.13)$$

$$\begin{aligned} &= \left\{ \frac{e^{\frac{v_1}{T_0}}}{1+e^{\frac{v_1}{T_0}}} \right\}^{1/2} \left\{ \frac{e^{\frac{v_2}{T_0}}}{1+e^{\frac{v_2}{T_0}}} \right\}^{1/2} \\ &\quad \times \left\{ \frac{1}{1+e^{\frac{w_{12}+v_1}{T_0}}} \right\}^{1/2} \left\{ \frac{1}{1+e^{\frac{w_{12}+v_2}{T_0}}} \right\}^{1/2} |e^{\frac{w_{12}}{T_0}} - 1|. \end{aligned} \quad (3.14)$$

If $w_{12} \geq 0$, by (3.13), we have

$$\frac{1}{-\log \beta_*} \leq 62.9842. \quad (3.15)$$

And if $w_{12} < 0$, by (3.14), we have

$$\frac{1}{-\log \beta_*} \leq 2.12764. \quad (3.16)$$

We obtain the desired lower bound of m . □

4. The Boltzmann Machine for the Case $|S| = 8$

In this section, we retain the general setting for the Boltzmann machine for neural networks and set $|S| = 8$ ($n = 3$). For simplicity, we assume that

$$v_1 = v_2 = v_3 = v > 0, \quad w_{12} = w_{13} = w_{23} = w > 0. \quad (4.1)$$

Then, the matrices P , A_T , and G_T can be calculated as follows.

$$P = \begin{pmatrix} 0 & \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} \\ \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} \\ 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} \\ 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 \end{pmatrix},$$

Fig. 1. Neural Network for $n = 3$.

and G_T is equal to

$$\begin{pmatrix} 1-3a & a & a & 0 & a & 0 & 0 & 0 \\ \frac{1}{3}-a & \frac{2}{3}+a-2b & 0 & b & 0 & b & 0 & 0 \\ \frac{1}{3}-a & 0 & \frac{2}{3}+a-2b & b & 0 & 0 & b & 0 \\ 0 & \frac{1}{3}-b & \frac{1}{3}-b & \frac{1}{3}+2b-c & 0 & 0 & 0 & c \\ \frac{1}{3}-a & 0 & 0 & 0 & \frac{2}{3}+a-2b & b & b & 0 \\ 0 & \frac{1}{3}-b & 0 & 0 & \frac{1}{3}-b & \frac{1}{3}+2b-c & 0 & c \\ 0 & 0 & \frac{1}{3}-b & 0 & \frac{1}{3}-b & 0 & \frac{1}{3}+2b-c & c \\ 0 & 0 & 0 & \frac{1}{3}-c & 0 & \frac{1}{3}-c & \frac{1}{3}-c & 3c \end{pmatrix},$$

where $a = \frac{1}{3}\tau(\frac{v}{T})$, $b = \frac{1}{3}\tau(\frac{w+v}{T})$, and $c = \frac{1}{3}\tau(\frac{2w+v}{T})$.

By using “Mathematica”, the eigenvalues of G_T are given as follows:

$$\left\{ 1, 0, \frac{1}{2}(1+a-c \pm \alpha) \text{ (with multiplicities 2)}, \frac{1}{2}(1-a+2c \pm \beta) \right\},$$

where

$$\alpha = \frac{1}{3}\sqrt{1+6a+9a^2-12b-72ab+108b^2+6c+18ac-72bc+9c^2}$$

$$\beta = \frac{1}{3}\sqrt{1-12a+36a^2+24b-72ab-12c+72ac-72bc+36c^2}.$$

Then, we obtain that the β^* in Theorem 1.2 is given by

$$\beta^* = \max \left\{ \frac{1}{2}(1+a-c+\alpha), \frac{1}{2}(1-a+2c+\beta) \right\}. \quad (4.2)$$

Note that $0 < \beta^* < 1$.

The set of values of the function F is given as

$$F_{\max} = 0 > F_2 = -v > F_1 = -w - 2v > F_{\min} = -3w - 3v, \quad (4.3)$$

and $S_0 = \{x \in S; F(x) = F_{\min}\} = \{(1, 1, 1)\}$, so we have $|S_0| = 1$, and $|S \setminus S_0| = 7$.

Then, the right hand side of (1.9) of Theorem 1.2 can be calculated as follows: The first term of the right hand side of (1.9) coincides with

$$\sqrt{2} \beta^{*m} (1 + e^{\frac{1}{2T}(3w+3v)} + 3e^{\frac{1}{2T}(3w+2v)} + 3e^{\frac{1}{2T}(2w+v)}) \leq 8\sqrt{2} \beta^{*m} e^{\frac{1}{2T}(3w+3v)}, \quad (4.4)$$

and the second term of the right hand side of (1.9) coincides with

$$\frac{e^{-\frac{1}{T}(3w+3v)} + 3e^{-\frac{1}{T}(3w+2v)} + 3e^{-\frac{1}{T}(2w+v)}}{1 + e^{-\frac{1}{T}(3w+3v)} + 3e^{-\frac{1}{T}(3w+2v)} + 3e^{-\frac{1}{T}(2w+v)}} \leq 7e^{-\frac{1}{T}(2w+v)}. \quad (4.5)$$

Therefore, the right hand side of (1.9) is smaller than or equal to

$$8\sqrt{2} \beta^{*m} e^{\frac{1}{2T}(3w+2v)} + 7e^{-\frac{1}{T}(2w+v)}. \quad (4.6)$$

Thus, we obtain

Proposition 4.1. *For every $T > 0$ and $m = 1, 2, \dots$,*

$$\|r G_T^m - q_0\|_{TV} \leq 8\sqrt{2} \beta^{*m} e^{\frac{1}{2T}(3w+2v)} + 7e^{-\frac{1}{T}(2w+v)}. \quad (4.7)$$

Here, β^* is given by (4.2).

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