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Memory effects of the multi-charge network model

Kazuo Nokura

Shonan Institute of Technology, Fujisawa 251-8511, Japan

E-mail: nokura@la.shonan-it.ac.jp

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Abstract

We propose a spin glass model which has interactions characterized by P kinds of charges carried by N kinds of particles. When the densities of the particles are assumed to be Ising spin variables, this model becomes a spin glass model which has an opposite interactional sign to the Hopfield model with P memorized patterns. The number of local minimum states and remanent magnetization are studied to clarify the memory effects of the model. We find that, as P/N decreases, both quantities tend to the maximum possible values of the thermodynamic limit.

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1. Introduction

In recent years, in the studies of spin glass models, it has been shown that inhomogeneous interactions among simple degrees of freedom induce interesting collective behaviours among them. This idea provides fruitful points of view to look at the biological systems which are expected to be described by the concept of networks.

Among the many properties of biological systems, learning and memory are attractive subjects which can be studied naturally in terms of spin glass models. Due to the effect of inhomogeneous interactions, spin glass models have many local minimum states of the energy function. Since they are fixed points of the dynamics, we expect that any initial configuration will evolve into one of the local minimum states close to the initial configuration, implying a memory effect. The properties of these fixed points are controlled by changing interactions and this corresponds to a kind of learning if it is done according to the effects of external information.

As a typical infinite-range spin glass model, the Sherrington–Kirkpatrick (SK) model has been studied intensively by the methods of statistical mechanics [1, 2]. In this model, interactions between spin variables are random and uncorrelated with each other. Among the various studies, the study of the number of local minimum states directly shows the complexity of the energy landscape. For the model with Ising variables, it was shown that the number

of local minimum states is given by 2^{Nc} with $c \sim 0.3$, where N is the system size, i.e. the number of Ising variables [3]. This number is compared with the number of all configurations of the system 2^N . On the other hand, the memory effect is directly measured by remanent magnetization, which has been studied intensively to clarify the dynamical properties [4, 5]. From these studies, we know that the SK model has a complex energy landscape and really works as a memory.

To model biological systems by spin glass models, the statistics of interactions should be prescribed according to the biological aspects of the problems. In neural network models, spin variables correspond to states of the neuron and synaptic interactions are usually assumed to obey the well-known Hebb rule or something similar [6]. By the Hebb rule, interactions become correlated and we have spin-glass-like models of neural networks which show interesting properties, including an associative memory [7, 8].

Another interesting suggestion from neural networks is unlearning [9, 10]. It was found that spin models are modified nontrivially by unlearning the paramagnetic configurations [11]. When this idea is applied to the SK model, interactions become correlated, resulting in a nontrivial spin glass model, which is practically similar to the Hopfield model but with an opposite interactional sign, which may be called the anti-Hopfield model [12].

In the previous paper, we have studied the anti-Hopfield model by the replica method. In spite of the simplicity, this model has properties quite different from the SK model. In particular, the spin glass phase transition becomes dynamical for small numbers of ‘memorized’ patterns P . To identify this dynamical phase transition, we need to find a replica solution which satisfies the marginality condition [13, 14]. In addition, the structure of the energy function implies a strong degeneracy of energy for small P . These observations suggest that the anti-Hopfield model will have attractive properties as a model of memory. However, the interactions are not familiar in statistical and biological physics. It is desirable to give some direct physical reasoning for this type of interaction, apart from unlearning.

We have two purposes in this paper. In section 2, we describe a physical meaning for the anti-Hopfield model. By the arguments in this section, we realize that the parameter P in the anti-Hopfield model corresponds to the number of kinds of charges if the spin variables are regarded as the densities of the charged particles. In sections 3 and 4, we evaluate the memory effects of the model by studying the number of local minimum states and remanent magnetization. Section 5 is devoted to some discussion.

2. The multi-charge network model

The anti-Hopfield model is defined by reversing the sign of the Hopfield interactions. This model was motivated by the observation on unlearning in the SK model. In this section, we suggest another reason for this type of interaction and discuss the features of the energy function.

Let us imagine that there are many kinds of particles which are characterized by P kinds of charges. These charges are expressed by $\xi_i^\mu = \pm 1$, $\mu = 1, 2, \dots, P$ for particles of kind i . There can be 2^P kinds of different particles characterized by these charges. Then, assuming that different charges do not interact, the interaction energy between the kind i and kind j particles will be a function of the particle coordinates multiplied by $\sum_\mu \xi_i^\mu \xi_j^\mu$. Although the statistical mechanics will be studied by specifying the numbers of each kinds of particles, the neutralization of the system is nontrivial in some situations.

Now let us introduce the simple problem for the system of these particles. We first assume that only N kinds of particles out of 2^P can appear in the system. These kinds of particles are specified in advance. Then we have quenched charges ξ_i^μ with $i = 1, 2, \dots, N$. With

this condition, we consider the problem to find the densities of particles which make the energy minimum. The relevant cost function will be obtained by averaging the energy over the coordinates of particles. By the mean-field-like approximation, we will obtain the energy as a quadratic function of densities of the particles. In this way, denoting their densities by S_i , the energy function of the system will be expressed by

$$H = -\frac{1}{2} \sum_{ij} J_{ij} S_i S_j \quad (1)$$

where

$$J_{ij} = -\frac{1}{N} \sum_{\mu} \xi_i^{\mu} \xi_j^{\mu}. \quad (2)$$

This energy function is equal to that of the anti-Hopfield model if the $i = j$ terms are irrelevant. The above argument naturally suggests calling this model the multi-charge network (MCN) model.

To define the model completely, we should specify ξ_i^{μ} and S_i . We simply assume that ξ_i^{μ} are generated randomly, although some specific assignments may give quite different models. We can further simplify the problem by assuming S_i to be binary variables which express the presence or absence of each kind of particles. In this paper, we restrict ourselves to the Ising variables $S_i = \pm 1$ to simplify the following arguments.

We give some remarks on the technical aspects of the model. In the mean field theory, P should be assumed to be proportional to N . On the other hand, in the framework of charged particles, P and N are weakly related. We note that different kinds of particles should be characterized by different sets of charges ξ_i^{μ} . Thus, when ξ_i^{μ} are generated randomly, N , the number of kinds of particles in the network, should be much smaller than 2^P . This leads to the inequality $P \gg \ln N / \ln 2$, or $\alpha = P/N \gg \ln N / (N \ln 2)$, which gives the lower bound of α to define the particle network model with randomly generated ξ_i^{μ} . This lower bound becomes zero as $N \rightarrow \infty$. Thus, the MCN model with $\alpha \sim 0$ is relevant for the description of the particle networks if N is chosen properly. Note that the antiferromagnet, i.e. $P = 1$, which creates only two kinds of particles, does not satisfy the condition for $N > 2$.

In the earlier paper [12], we have studied the statistical mechanics of the MCN model with Ising S_i by the replica method. What we found for the MCN model is summarized as follows. There are two regions of $\alpha \equiv P/N$ which show different properties. For large α , the model is similar to the SK model. This is a direct consequence of the fact that the correlation among interactions disappears as $\alpha \rightarrow \infty$. On the other hand, below $\alpha = \alpha_c \sim 1.4$, the property of the spin glass phase transition changes to a dynamical one, which requires a marginality condition on the one-step replica symmetry breaking ansatz to be identified. This aspect is very similar to other spin glass models such as the random orthogonal model [13, 14]. For $\alpha < \alpha_c$, we expect that there are a large number of large local minimum states with moderate energies and annealing configurations are easily trapped by one of them, implying a dynamical phase transition

The strong dependence on α of this model is qualitatively understood if we see that the structures of the energy function are quite different between $\alpha > 1$ and $\alpha < 1$. It also gives some idea on the local minimum states. The energy function can be viewed as a problem-searching N -component vector $\mathbf{S} = \{S_i\}$ which is orthogonal to all $\xi^{\mu} = \{\xi_i^{\mu}\}$. This is seen by writing the energy function in the form

$$H = \frac{1}{2N} \sum_{\mu} \left(\sum_i \xi_i^{\mu} S_i \right)^2 - \frac{1}{2} P \quad (3)$$

which is minimized by the configurations perpendicular to all ξ^μ . Physically, the requirement $\sum_i \xi_i^\mu S_i = 0$ for all μ corresponds to the neutralization of all kinds of charges. The solutions are given by $(N - P)$ -dimensional space for $N > P$, whereas there is no solution space for $N < P$. For discontinuous spin variables, the finite-dimensional solution space for $N > P$ will imply a strong degeneracy of energies of local minimum states, especially for $\alpha \sim 0$.

In the following sections, we report studies on the local minimum states and remanent properties of the MCN model in order to discuss the memory effect of the model. A parameter α controls the proximity to the SK model. We are especially interested in the model with small α , which is located far from the SK model.

3. Number of local minimum states of the MCN model

To study the memory effect of the Ising spin model, we begin with the study of the number of local minimum states, which are spin configurations stable to a flip of any spin. We follow the standard method of the saddle point approximation presented first for the SK model [3].

The local minimum states are defined by the conditions

$$S_i \sum_j J_{ij} S_j > 0 \quad (4)$$

for all i . The number of local minimum states is given by

$$G = \sum_{\{S\}} \prod_i \int_0^\infty \delta\left(S_i \sum_j J_{ij} S_j - h_i\right) dh_i. \quad (5)$$

The details of the following calculations are presented in the appendix, which also gives definitions of the saddle point variables A, \bar{A} and B, \bar{B} . After averaging ξ_i^μ , which is denoted by $\langle \cdot \cdot \cdot \rangle$, we reach the problem to find the extremum:

$$\langle G \rangle = \text{Extr} \{ \exp Ng \} \quad (6)$$

with

$$g = \ln 2 - \frac{1}{2} \alpha \ln \{ (1 + B)^2 - A \} + \alpha B - \bar{A} A - \bar{B} B + \ln \Phi \left(\frac{\bar{B}}{\sqrt{2\bar{A}}} \right) \quad (7)$$

where

$$\Phi(x) = \int_{-\infty}^x \exp\left(-\frac{1}{2}t^2\right) \frac{dt}{\sqrt{2\pi}}. \quad (8)$$

The SK limit is achieved by replacing J_{ij} by $J_{ij}/\sqrt{\alpha}$ in (5) and putting $\alpha \rightarrow \infty$, resulting in terms up to the second order of B in (7). The saddle point value of g is denoted by g_m .

The α dependence of $g_m/\ln 2$ is presented in figure 1. As expected, g_m is larger than the SK value 0.198 in the studied region. We found that g_m tends to the SK value quite gradually as α increases, while, as α decreases, g_m increases monotonically. In particular, with α smaller than 0.2, g_m increases drastically and tends to the possible maximum value $\ln 2 = 0.693$ as $\alpha \rightarrow 0$. In the appendix we discuss this limit analytically and find

$$g_m \sim \ln 2 - \frac{1}{2} \alpha \ln \left(4 + \frac{2}{\alpha} \ln \frac{1}{\alpha} \right) + \frac{1}{2} \alpha \quad (9)$$

which is also plotted in figure 1. We should note that this result does not mean that all configurations become local minimum states for $\alpha \rightarrow 0$, which is logically impossible. In g_m , there will be some corrections which disappear in the thermodynamic limit.

The result is rather interesting and should be confirmed by some other approaches. In the next section, we will study the population of local minimum states from different points of view.

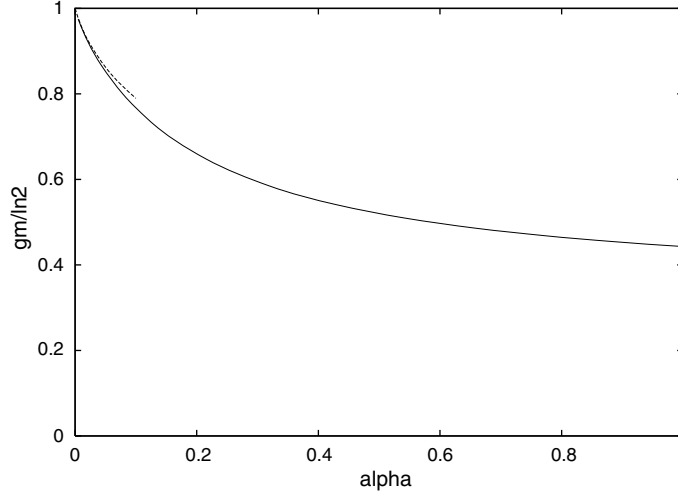


Figure 1. The α dependence of the number of local minimum states obtained by the saddle point method. The full curve represents $g_m/\ln 2$ obtained by numerical studies of the saddle point equations. The broken curve on the left is drawn by using the analytic result in the text, which is obtained by the approximation for $\alpha \rightarrow 0$.

4. Remanent magnetization

The result for the number of local minimum states is very interesting and it is highly desirable to confirm it by some numerical methods. However, it is not easy to study directly the number of local minimum states numerically due to the enormous number of them. In the context of the memory effect, the large number of local minimum states implies a large remanent effect if local minimum states are not correlated in configuration space. We have no idea about the correlation among local minimum states, but it is plausible that the remanent effect increases if the number of local minimum states increases. In addition, the remanent effect is easier to address numerically than the number of local minimum states. For the SK model, there have been many studies on remanent magnetization by numerical simulations and the dynamical mean field method [5]. In this section, we study the remanent magnetization of the MCN model by the standard simulation method.

Remanent magnetization is defined by the overlap between initial configuration and final configuration which is obtained by spin dynamics from an initial configuration. To be thorough, we review the numerical procedure to obtain this quantity.

We first generate a random spin configuration $S_i(0)$. This configuration is relaxed to a local minimum state by asynchronous spin dynamics defined by

$$S_i(t+1) = \text{sgn}\left(\sum_j J_{ij} S_j(t)\right). \quad (10)$$

A local minimum is achieved when $S_i(t_0+1) = S_i(t_0)$. Then, the remanent magnetization m is obtained by

$$m = \frac{1}{N} \sum_i S_i(0) S_i(t_0). \quad (11)$$

We perform averages of m over N_I initial configurations and N_S realizations of ξ_i^μ for each α .

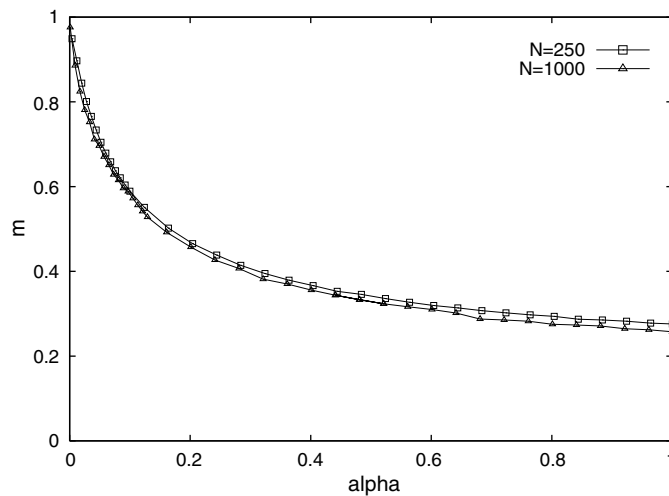


Figure 2. The α dependence of remanent magnetization m obtained numerically for $N = 250$ with $N_I = 100$, $N_S = 100$ and $N = 1000$ with $N_I = 10$, $N_S = 10$. The curves are to guide the eye.

For the SK model, m was found to be about 0.1 [4]. It is known that m shows strong system-size dependence. The system sizes we have studied are $N = 250, 1000$, which may not be large enough to achieve the thermodynamic limit. Here, we restrict ourselves to the α dependence of m . We have chosen an odd P to avoid $J_{ij} = 0$ for small α .

In figure 2, averages of m are presented as a function of α for $N = 250, 1000$. The α studied are slightly different for different N since we used odd P . The numerical results show a monotonic increase of m as α decreases: in particular, m tends to 1 as $\alpha \rightarrow 0$. The drastic change below 0.2 is quite consistent with that of g_m . We notice that m with $N = 1000$ are systematically smaller than the ones with $N = 250$, implying the system size dependence of m . Although some systematic studies are needed on this point, our numerical results suggest that the remanent magnetizations tend to 1 as $\alpha \rightarrow 0$, in accordance with the behaviour of g_m .

5. Discussion

In this paper, we first discussed a physical reason for the anti-Hopfield model, which suggests calling this model the MCN model, and then we studied the memory effects of the model.

The physical reasoning of the MCN model is summarized as follows. We introduce the system which consists of N kinds of particles. Each kind of particles is characterized by P kinds of charges $\xi_i^\mu = \pm 1$, where $i = 1, 2, \dots, N$. They are assumed to interact with each other by these charges. To find the simple nontrivial problem, we restrict ourselves to the problem of finding the densities of the particles which make the energy minimum. This leads to the energy function of the MCN model which is a quadratic function of densities of particles S_i . The energy function becomes a minimum by neutralization of all kinds of charges.

To evaluate the memory effects of the Ising MCN model, we have studied the number of local minimum states and remanent magnetization. These quantities show consistent α dependence in the parameter region studied. In particular, as α decreases, these two quantities tend to the possible maximum values of the thermodynamic limit. This implies that α is a relevant parameter for controlling the complexity of the energy landscape.

Let us comment on an interesting problem in the MCN model. In this model, the system is specified by N kinds of particles. These particles are implicitly assumed to be produced by the system. Then we may ask what happens if a new kind of particle, which has a set of charges different from all ξ_i , gets into the system. The energy function for this situation is easily obtained by introducing ξ_0^μ and fixed S_0 , which represent the charges and the density of the new particle. The structure of the energy function implies that the charges of new particles should be neutralized by the system. It will be interesting to study the minimum of the energy function from this point of view.

The introduction of several charges may look unphysical, but this is a natural way of introducing randomness characterized by sites instead of bonds. In addition, the introduction of many charges naturally provides a simple description of the diversity of species in the system. This leads to the application of the model to systems which consist of many kinds of complex particles, such as protein molecules in the immune system. It is known that many types of shape-complementary-shape interactions control the interactions between protein molecules. Although there will be several points to be clarified, we expect that the system of particles with many kinds of charges may capture this aspect of biological systems.

Apart from our modelling, the similarity between the nervous system and immune system has been pointed out, concerning their functions to external stimuli [15, 16]. Both biological systems respond adequately to external information which is foreign to themselves. They need to memorize and learn information coming from outside to stabilize themselves. To do this, it will be convenient to have an enormous number of dynamical fixed points in the configuration space. Studies of the MCN model will hopefully provide some insight into the functions of these biological networks.

Appendix

In this appendix, we first review the derivation of saddle point equations for the number of local minimum states and then discuss the solution in the $\alpha \rightarrow 0$ limit.

Introducing integral representations for the delta functions, (5) is expressed as

$$G = \sum_{\{S\}} \prod_i \int_0^\infty \int_{-i\infty}^{i\infty} \exp \left[\phi_i \left(S_i \sum_j J_{ij} S_j - h_i \right) \right] \frac{d\phi_i dh_i}{2\pi i}. \quad (\text{A.1})$$

In the exponential, summation over i and j gives

$$\sum_i \phi_i \left(S_i \sum_j J_{ij} S_j \right) = - \sum_\mu a_\mu b_\mu + \alpha \sum_i \phi_i \quad (\text{A.2})$$

where $a_\mu = \sum_i \xi_i^\mu S_i / \sqrt{N}$ and $b_\mu = \sum_i \xi_i^\mu \phi_i S_i / \sqrt{N}$. For each μ , we introduce Gaussian variables x_μ and y_μ and write

$$\exp(-ab) = \iint \exp \left\{ -\frac{1}{2}(x^2 + y^2) + x \frac{a-b}{\sqrt{2}} + iy \frac{a+b}{\sqrt{2}} \right\} \frac{dx dy}{2\pi} \quad (\text{A.3})$$

where the index μ are dropped for simplicity. Introducing $z = (x + iy)/\sqrt{2}$ and $\bar{z} = (x - iy)/\sqrt{2}$, and after ξ_i^μ averages, we obtain

$$\langle \exp(-ab) \rangle = \int \exp \left\{ -z\bar{z} + \frac{1}{2}(Az^2 - 2Bz\bar{z} + \bar{z}^2) \right\} \frac{dx dy}{2\pi} \quad (\text{A.4})$$

where $A = \sum_i \phi_i^2 / N$ and $B = \sum_i \phi_i / N$. After integrating over x_μ and y_μ , we obtain

$$\langle G \rangle = 2^N \int_0^\infty \int_{-i\infty}^{i\infty} \exp \left(-\frac{1}{2} P \ln \{ (1+B)^2 - A \} + PB - \sum_i \phi_i h_i \right) \prod_i \frac{d\phi_i dh_i}{2\pi i}.$$

Then, by expressing 1 by the delta functions

$$\int \delta\left(\sum_i \phi_i^2 - NA\right) N dA = \iint \exp\left[\bar{A}\left(\sum_i \phi_i^2 - NA\right)\right] \frac{N dA d\bar{A}}{2\pi i}$$

$$\int \delta\left(\sum_i \phi_i - NB\right) N dB = \iint \exp\left[\bar{B}\left(\sum_i \phi_i - NB\right)\right] \frac{N dB d\bar{B}}{2\pi i}$$

and replacing ϕ_i by $i\phi_i$, we obtain

$$g = \ln 2 - \frac{1}{2}\alpha \ln\{(1+B)^2 - A\} + \alpha B - \bar{A}A - \bar{B}B + \ln \Phi\left(\frac{\bar{B}}{\sqrt{2\bar{A}}}\right) \quad (\text{A.5})$$

where irrelevant constants are omitted.

Let us briefly discuss the solution of the saddle point equations in the $\alpha \rightarrow 0$ limit. The saddle point equations are given by

$$\bar{A} = \frac{1}{2} \frac{\alpha}{(1+B)^2 - A}$$

$$\bar{B} = \alpha - \alpha \frac{1+B}{(1+B)^2 - A}$$

$$A = -\frac{1}{2} \frac{\Phi'}{\Phi} \frac{\bar{B}}{\bar{A}\sqrt{2\bar{A}}}$$

$$B = \frac{1}{\sqrt{2\bar{A}}} \frac{\Phi'}{\Phi}.$$

By numerical inspection, we found that $-A$ is positive and become larger than $1/\alpha$, while B remains finite as $\alpha \rightarrow 0$. Thus we assume $-A$ becomes infinite as $\alpha \rightarrow 0$. Then, by the first and second equations, $\bar{A} \sim \alpha/(-2A)$ and $\bar{B} \sim \alpha$, which give $\bar{B}/\sqrt{2\bar{A}} \sim \sqrt{-\alpha A}$, which also becomes large. Putting these relations in the third and fourth equations, we have $B \sim 1$, which implies

$$|A| \sim 2\pi\alpha \exp(\alpha|A|) \quad (\text{A.6})$$

where we used $\Phi'/\Phi \sim \exp(-\alpha|A|/2)/\sqrt{2\pi}$. By this equation, we find $|A| \sim 2(1/\alpha) \ln(1/\alpha)$ asymptotically. Putting these results in g , we find (9) as $\alpha \rightarrow 0$.

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