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Proposal of a checking parameter in the simulated annealing method applied to the spin glass model

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ABSTRACT

We propose a checking parameter utilizing the breaking of the Jarzynski equality in the simulated annealing method using the Monte Carlo method. This parameter is based on the Jarzynski equality. By using this parameter, to detect that the system is in global minima of the free energy under gradual temperature reduction is possible. Thus, by using this parameter, one is able to investigate the efficiency of annealing schedules. We apply this parameter to the $\pm J$ Ising spin glass model. The application to the Gaussian Ising spin glass model is also mentioned. We discuss that the breaking of the Jarzynski equality is induced by the system being trapped in local minima of the free energy. By performing Monte Carlo simulations of the $\pm J$ Ising spin glass model and a glassy spin model proposed by Newman and Moore, we show the efficiency of the use of this parameter.

1. Introduction

The studies of spin glass models have been widely done [1,2]. The spin glass models have the randomness and the frustration. The combination of the randomness and the frustration causes various interesting dynamics as well as the static properties. For the spin glass model, there is a problem that it is difficult for the system to reach global minima of the free energy by using the Monte Carlo method, although the Monte Carlo method is known as a powerful method for investigating spin models. When the system has reached the global minima of the free energy by the Monte Carlo method, the system is in equilibrium or the ground state. On the other hand, when the system has not reached the global minima of the free energy by the Monte Carlo method, the system is in non-equilibrium.

We propose a checking parameter in the simulated annealing method using the Monte Carlo method. The simulated annealing method originally uses the Metropolis method [3,4] and is originally made for the ground-state search [4]. The simulated annealing method [4,5] performs gradual temperature reduction (annealing). It is known that, if $T(k) \geq \frac{c}{\log(1+k)}$ is applied as the time schedule (annealing schedule), the system always goes in the ground state for any model, where T is the temperature, c is a constant, and k is the number of site replacements [5]. However, this time schedule is not practical for simulation time. In addition, because the difficulty for finding the ground state depends on each model, each proper annealing schedule can also depend on each model. In the cases of the complex systems such as the spin glass model, if annealing schedules are not appropriate, the systems go in local minima of the free energy, and one cannot obtain the physical quantities in equilibrium or the ground state. If appropriate annealing schedules are chosen, the systems go in global minima of the free energy, and one can obtain the physical quantities in equilibrium or the ground state. Therefore, when performing the simulated annealing method, one has to choose appropriate annealing schedules.

The understandings for solving optimization problems by using annealing processes are recently becoming significant in relation to the D-Wave chip [6]. This chip is designed to perform a quantum annealing for solving optimization problems. The present study is related to a thermal annealing, but the relationship with a quantum annealing [7] is straightforward. The application to the quantum annealing is mentioned in Section 5.

There are two interests for investigating the spin glass model by using the Monte Carlo method at least. One is to clear the nature of the material, and another is to find a powerful Monte Carlo method. The spin glass model also works as a test bed for optimization methods [4]. This study has a relationship with both of the two interests, because the study for gradual temperature reduction is proposed as an optimization method called the simulated annealing method [4,5] and the study for gradual temperature reduction is also done for investigating dynamical features of the spin glass model [8].

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We apply the Jarzynski equality to the spin glass model. The Jarzynski equality is an equality that connects the work in non-equilibrium and the ratio of the partition functions [9,10]. The work is performed in switching an external parameter of the system. The Jarzynski equality for temperature-change process is also proposed [11,12]. We use the Jarzynski equality for temperature-change process. The Jarzynski equality is also derived in the Markov process with discrete time in Ref. [13], and it is pointed out in Ref. [13] that the Metropolis method [3] based on the Markov process with discrete time is a suited example for applying the Jarzynski equality.

We propose a checking parameter in this article. By using this checking parameter, to detect that the system is in global minima of the free energy is possible. The checking parameter means that, by using this parameter, one can check whether annealing schedules are appropriate or not. The meaning of the value of the present checking parameter is different from that of the study of the energy decrease as the temperature decreases, although this parameter uses the values of the energies. In the case of the study of the energy decrease, one can see that the energy does not decrease for long Monte Carlo time, however, one cannot determine whether the system is in global minima of the free energy or not. On the other hand, because the value of a quantity estimated by the Monte Carlo method and the exact analytical value of the quantity are compared, by using the present checking parameter, one can determine whether the system is in global minima of the free energy or not.

In this article, in order to show the features of the present checking parameter, we apply the Glauber dynamics [8,14], although other Monte Carlo methods, which include the Metropolis method [3], based on the Markov process with discrete time are also applicable. The Glauber dynamics is suited to the study of the dynamical features of physical systems [8,14]. If one uses the present checking parameter as a powerful optimization method, applying more powerful Monte Carlo methods [15,16], instead of the Glauber dynamics or the Metropolis method, would be necessary.

We apply the present parameter to the $\pm J$ Ising spin glass model [1]. The present technique is also applicable to the Gaussian Ising spin glass model [2]. The application to the Gaussian model is also mentioned in this article.

There are previous studies for investigating the relationship between the spin glass model and the Jarzynski equality in Refs. [12,17–19]. We describe the difference between this study and the previous studies. We propose a checking parameter. By using this parameter, one is able to investigate the efficiency of annealing schedules. In the previous studies, this parameter is not mentioned, the breaking of the Jarzynski equality is not mentioned, and the treatment under a uniform external magnetic field is also not mentioned. In this article, these are described.

In addition, in order to confirm the behavior of the present checking parameter, a glassy spin model [20] by Newman and Moore is also investigated.

This article is organized as follows. The present checking parameter is explained in Section 2, and the breaking of the Jarzynski equality is discussed in Section 3. The results of Monte Carlo simulations are given in Section 4. The concluding remarks of this article are described in Section 5.

2. A checking parameter

We investigate the $\pm J$ Ising spin glass model. The Hamiltonian $\mathcal{H}$ for Ising spin glass models is given by [1,2]

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{i,j} S_i S_j - h\sum_i S_i, \tag{1}$$

where $\langle i,j\rangle$ denotes nearest-neighbor pairs, S_i is a state of the spin at site i, $S_i = \pm 1$, and h is an external magnetic field. The value of $J_{i,j}$ is given with a distribution $P(J_{i,j})$. The distribution $P^{(\pm J)}(J_{i,j})$ of $J_{i,j}$ for the $\pm J$ model is given by [1]

$$P^{(\pm J)}(J_{i,j}) = \frac{1}{2}\,\delta_{J_{i,j},J} + \frac{1}{2}\,\delta_{J_{i,j},-J}, \tag{2}$$

where δ is the Kronecker delta, $J > 0$, and J is the strength of the exchange interaction between spins.

We explain the Jarzynski equality [9,10,13]. We consider a non-equilibrium process of λ_t from λ_0 to λ_τ. λ_t is an externally controlled parameter, and $t = 0, 1, 2, \ldots, \tau$. The initial and final states in equilibrium are assumed, and the states in the process from λ_0 to λ_τ are in non-equilibrium. The Jarzynski equality is equivalently given by [9,10,13]

$$\overline{e^{-\beta W}} = \frac{Z(\beta,\lambda_\tau)}{Z(\beta,\lambda_0)}, \tag{3}$$

where W is the work performed in the process from λ_0 to λ_τ, β is the inverse temperature of the reservoir, $\beta = 1/k_B T$, T is the temperature, and k_B is the Boltzmann constant. The overbar indicates an ensemble average over all possible paths through phase space. Z is the partition function given by $Z = \sum \exp(-\beta\mathcal{H})$. The left-hand side of Eq. (3) is the non-equilibrium measurements, and the right-hand side of Eq. (3) is the equilibrium information. By using Eq. (3), to extract the equilibrium information from the ensemble of non-equilibrium is possible. The work W is given by [13]

$$W = \sum_{t=0}^{\tau-1}[E(i_t,\lambda_{t+1}) - E(i_t,\lambda_t)], \tag{4}$$

where $E(i_t,\lambda_t)$ is the energy at state i_t under the externally controlled parameter λ_t. The Jarzynski equality for temperature-change process is proposed in Refs. [11,12]. In Ref. [13], the Jarzynski equality is derived in the Markov process with discrete time. Then, the inverse temperature β and the energy $E(i_t,\lambda_t)$ always appear as a couple. Therefore, the Jarzynski equality also holds for process of $\beta_t E(i_t)$ instead of $\beta E(i_t,\lambda_t)$, where β_t is the inverse temperature with discrete time t, and $E(i_t)$ is the energy at state i_t with discrete time t. Then, the Jarzynski equality for the process of the inverse temperature β_t from β_0 to β_τ is given by

$$\overline{e^{-\Upsilon}} = \frac{Z(\beta_\tau)}{Z(\beta_0)}, \tag{5}$$

where Υ is a pseudo work given by

$$\Upsilon = \sum_{t=0}^{\tau-1}(\beta_{t+1}-\beta_t)E(i_t). \tag{6}$$

Only the values of the energies just before the temperature changes contribute to the value of Υ.

We consider a quantity $[\overline{e^{-\Upsilon}}]_R$, where $[\,]_R$ is the random configuration average for exchange interactions. $[\overline{e^{-\Upsilon}}]_R$ is a quantity for Υ, and $[\overline{e^{-\Upsilon}}]_R$ is also a quantity for the ratio of the partition functions. Note that, strictly speaking, the quantity $[\overline{e^{-\Upsilon}}]_R$ is not the free energy difference, because the free energy difference is given by $-\frac{1}{\beta_\tau}[\ln Z(\beta_\tau)]_R + \frac{1}{\beta_0}[\ln Z(\beta_0)]_R$ and is not a function for $[\overline{e^{-\Upsilon}}]_R$, but the quantity $[\overline{e^{-\Upsilon}}]_R$ is useful as described in this article. When $\beta_0 = 0$ and $\beta_\tau = \beta$, by applying Eq. (5) to the $\pm J$ Ising spin glass model, we obtain

$$\begin{aligned}[\overline{e^{-\Upsilon}}]_R^{(\pm J)} &= \frac{1}{2^{N_B}}\sum_{\{J_{i,j}\}}\frac{\sum_{\{S_i\}} e^{\beta\sum_{\langle i,j\rangle}J_{i,j}S_iS_j+\beta h\sum_i S_i}}{2^N}\\ &= \exp\{N_B\ln[\cosh(\beta J)] + N\ln[\cosh(\beta h)]\},\end{aligned} \tag{7}$$