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Deterministic replica-exchange method without pseudo random numbers for simulations of complex systems

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ABSTRACT

We propose a replica-exchange method (REM) which does not use pseudo random numbers. For this purpose, we first give a conditional probability for Gibbs sampling replica-exchange method (GSREM) based on the heat bath method. In GSREM, replica exchange is performed by conditional probability based on the weight of states using pseudo random numbers. From the conditional probability, we propose a new method called deterministic replica-exchange method (DETREM) that produces thermal equilibrium distribution based on a differential equation instead of using pseudo random numbers. This method satisfies the detailed balance condition using a conditional probability of Gibbs heat bath method and thus results can reproduce the Boltzmann distribution within the condition of the probability. We confirmed that the equivalent results were obtained by REM and DETREM with two-dimensional Ising model. DETREM can avoid problems of choice of seeds in pseudo random numbers for parallel computing of REM and gives analytic method for REM using a differential equation.

1. Introduction

The enhancement of sampling during Monte Carlo (MC) and molecular dynamics (MD) simulations is very important for complex systems. Replica-exchange method (REM) (or parallel tempering) is one of the most popular ways to improve sampling efficiency [1–4] including biomolecular system in explicit solvent [5,6] or biomembrane [7,8] (for reviews, see, e.g., Refs. [9,10]). To realize a thermal equilibrium distribution, REM uses Metropolis criterion with pseudo random numbers. However, random numbers sometimes give inaccurate results of simulations [11]. Moreover, generation of high quality random numbers is often difficult and does not assure good simulation results [12]. REM and its extension is suited for parallel computing [13–16]. Most of pseudo random number generators decrease the scalability in parallelization [17]. Hence, the complementary method producing the same results without pseudo random numbers is meaningful.

In addition, the analytic approach for temperature selections in REM has been performed [18,19]. For performance and the condition of REM, several works were also performed. For example, Nymeyer [20] showed how efficient REM is than conventional simulations using the number of independent configurations. Abraham and Gready introduced some measurement and compared the results [21]. Rosta and Hummer [22] evaluated the practical efficiency of REM simulation for protein folding with a two-state model. However, the examination of the condition for convergence of REM is difficult partly because the mixing of temperature in REM is determined by pseudo random numbers with Metropolis criteria. As a result, most of analyses estimated the REM performance by simulation results.

Recently, Suzuki et al. proposed a method to produce a thermal equilibrium state without using random numbers for spin models by a differential equation based on the conditional probability of Gibbs sampling heat bath method, which is referred to as chaotic Boltzmann machines [23,24]. The differential equation controls spin states at each site and the staying time of each spin state is proportional to the weights of the thermal equilibrium distribution. They reproduced the results of a conventional MC method in some spin systems.

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Moreover, Boltzmann machine [25] has its mathematical framework [26]. The method was analyzed by mean field approximation [27], algebraic geometry and informative geometry. For example, a linear convergence of parameters in Boltzmann machine was suggested by a learning algorithm of Fisher information matrices [28], and a upper boundary for performance was obtained by algebraic geometry [29]. By introducing the differential equation for replica-exchange method, the previous results in the fields can be applied for the REM analysis. This means that analytic approach for Boltzmann machine will be applied for REM by this extension. Moreover, this new implementation of REM will be related to hierarchical structure of Boltzmann machine, which is similar to deep Boltzmann machine [30,31]. Developments in Boltzmann machine to accelerate convergence of sampling such as Contrastive Divergence method [32] have been proposed.

We here generalize this Chaotic Boltzmann machine to REM. We first have to extend the conditional probability for replica exchange not based on Metropolis criterion but on a Gibbs sampling heat bath method. The heat bath formalism has already been given in Ref. [33], we refer to this method as Gibbs sampling replica-exchange method (GSREM). (A similar approach based on global balance condition [34] was also developed [35].) We then introduce a differential equation for replica exchange to modify GSREM. This method is referred to as the deterministic replica-exchange method (DETREM). We then tested the effectiveness of DETREM by comparing the results of simulation of 2-dimensional Ising model with those by the conventional REM.

The organization of this paper is as follows. In Section 2, the theory for the new method and conventional REM is presented. In Section 3, we give the results of DETREM together with REM. The final section is devoted to conclusions.

2. Methods

We first briefly review the conventional REM. We prepare M non-interacting replicas at M different temperatures. Let the label $i\,(=1,\ldots,M)$ stand for the replica index and label $m\,(=1,\ldots,M)$ for the temperature index. Here, i and m are related by the permutation functions by

$$\begin{cases} i = i(m) \equiv f(m), \\ m = m(i) \equiv f^{-1}(i), \end{cases} \tag{1}$$

where $f(m)$ is a permutation function of m and $f^{-1}(i)$ is the inverse. We represent the state of the entire system of M replicas by $X = \left\{x^{[1]}_{m(1)}, \ldots, x^{[M]}_{m(M)}\right\}$, where $x^{[i]}_m = \left\{q^{[i]}, p^{[i]}\right\}_m$ are the set of coordinates $q^{[i]}$ and momenta $p^{[i]}$ of particles in replica i (at temperature T_m). The probability weight factor for state X is given by a product of Boltzmann factors:

$$W_{\mathrm{REM}}(X) = \prod_{i=1}^{M} \exp[-\beta_{m(i)} H(q^{[i]}, p^{[i]})], \tag{2}$$

where $\beta_m (=1/k_{\mathrm{B}}T_m)$ is the inverse temperature and $H(q, p)$ is the Hamiltonian of the system. We consider exchanging a pair of replicas i and j corresponding to temperatures T_m and T_n, respectively:

$$X = \left\{\ldots, x^{[i]}_m, \ldots, x^{[j]}_n, \ldots\right\} \to X' = \left\{\cdots, x^{[j]'}_m, \ldots, x^{[i]'}_n, \ldots\right\}, \tag{3}$$

where $x^{[i]'}_n \equiv \left\{q^{[i]}, p^{[i]'}\right\}_n$, $x^{[j]'}_m \equiv \left\{q^{[j]}, p^{[j]'}\right\}_m$, and $p^{[j]'} = \sqrt{\frac{T_m}{T_n}}\, p^{[j]}$, $p^{[i]'} = \sqrt{\frac{T_n}{T_m}}\, p^{[i]}$ [4]. The exchange of replicas introduces a new permutation function f':

$$\begin{cases} i = f(m) \to j = f'(m), \\ j = f(n) \to i = f'(n). \end{cases} \tag{4}$$

We remark that this process is equivalent to exchanging a pair of temperatures T_m and T_n for the corresponding replicas i and j.

Here, the transition probability $\omega(X \to X')$ of Metropolis criterion is given by

$$\omega(X \to X') = \min\left(1, \frac{W_{\mathrm{REM}}(X')}{W_{\mathrm{REM}}(X)}\right) = \min(1, \exp(-\Delta)), \tag{5}$$

where

$$\Delta = \Delta_{m,n} = (\beta_n - \beta_m)(E(q^{[i]}) - E(q^{[j]})). \tag{6}$$

REM is performed by repeating the following two steps:

1. We perform a conventional MD or MC simulation of replica $i\,(=1,\ldots,M)$ at temperature T_m $(m = 1,\ldots,M)$ simultaneously and independently for short steps.
2. Selected pairs of replicas are exchanged based on the above Metropolis criterion in Eqs. (5) and (6). A pseudo random number is used to judge the criterion.

Without loss of generality we can assume $T_1 < T_2 < \cdots < T_M$. Note that in Step 2 we usually exchange only pairs of replicas corresponding to neighboring temperatures, because the acceptance probability for replica exchange decreases exponentially with the difference of the two inverse temperatures and potential energy terms because of Eq. (6). This replica exchange can be written as

$$X = \left\{\cdots, x^{[i]}_m, \ldots, x^{[j]}_{m+1}, \cdots\right\} \to X' = \left\{\cdots, x^{[j]'}_m, \ldots, x^{[i]'}_{m+1}, \cdots\right\}, \tag{7}$$

where in Eq. (5) Δ is now given by

$$\Delta_m = (\beta_{m+1} - \beta_m)(E(q^{[i]}) - E(q^{[j]})). \tag{8}$$

The REM method makes a random walk in temperature space during the simulation. The canonical ensemble is reconstructed by the multiple-histogram reweighting technique, or weighted histogram analysis method (WHAM) [36,37].

We next present GSREM [33]. As in the conventional REM, we usually consider the neighboring temperature exchange in Eq. (7). The conditional probability $\omega(x^{[j']}_m, x^{[i']}_{m+1} \mid x^{[k\neq i(m),j(m+1)]}_{m(k)})$, in which the new state selects the temperature exchanged state of replicas i and j with T_{m+1} and T_m from the no-exchange state of replicas i and j with temperatures T_m and T_{m+1}, is given by

$$\omega(x^{[j']}_m, x^{[i']}_{m+1} \mid x^{[k\neq i(m),j(m+1)]}_{m(k)}) = \frac{W(x^{[j']}_m, x^{[i']}_{m+1} \mid x^{[k\neq i(m),j(m+1)]}_{m(k)})}{W(x^{[i]}_m, x^{[j]}_{m+1} \mid x^{[k\neq i(m),j(m+1)]}_{m(k)}) + W(x^{[j']}_m, x^{[i']}_{m+1} \mid x^{[k\neq i(m),j(m+1)]}_{m(k)})} \tag{9}$$

$$= \frac{1}{1 + \frac{W(x^{[i]}_m, x^{[j]}_{m+1} \mid x^{[k\neq i(m),j(m+1)]}_{m(k)})}{W(x^{[j']}_m, x^{[i']}_{m+1} \mid x^{[k\neq i(m),j(m+1)]}_{m(k)})}}. \tag{10}$$

In GSREM, the above procedure for the conventional REM is performed, where Step 2 for the GSREM is performed based on Eq. (A.1). Here, in Step 2, the conditional probability of a temperature set based on Eq. (A.1) is calculated, and this assigns weights between 0 and 1 for exchanged states and a no-exchange state. Finally, after a pseudo random number is generated, the state corresponding to the random number with the assigned region is selected. For the Boltzmann distribution, this equation in Eq. (9) can be rewritten as

$$\omega(x^{[j']}_m, x^{[i']}_{m+1} \mid x^{[k\neq i(m),j(m+1)]}_{m(k)}) = \frac{1}{1 + \exp(\Delta_m)}, \tag{11}$$

where Δ_m is given by Eq. (8). This is the Gibbs sampling replica-exchange method when an equilibrium state is produced by this