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Simulating thermal boundary conditions of spin–lattice models with weighted averages

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ABSTRACT

Thermal boundary conditions have played an increasingly important role in revealing the nature of short-range spin glasses and is likely to be relevant also for other disordered systems. Diffusion method initializing each replica with a random boundary condition at the infinite temperature using population annealing has been used in recent large-scale simulations. However, the efficiency of this method can be greatly suppressed because of temperature chaos. For example, most samples have some boundary conditions that are completely eliminated from the population in the process of annealing at low temperatures. In this work, I study a weighted average method to solve this problem by simulating each boundary conditions separately and collect data using weighted averages. The efficiency of the two methods is studied using both population annealing and parallel tempering, showing that the weighted average method is more efficient and accurate.

1. Introduction

Thermal boundary conditions (TBC) include the set of all combinations of periodic/antiperiodic boundary conditions in each spatial dimension [1–3]. For example in three dimensions ($d = 3$), there are $2^d = 8$ possible choices. Each boundary condition i occurs in the thermal ensemble with weight p_i depends on its free energy F_i as $p_i = \exp[-\beta(F_i - F)]$, where F is the total free energy of the system in TBC and β is the inverse temperature. TBC was initially motivated to reduce domain-wall effects in spin glasses [1] and was later shown to be useful in studying temperature chaos and bond chaos via boundary condition crossings, i.e, the weights $\{p_i\}$ change chaotically as a function of temperature or couplings [2,3]. Previously, thermal boundary conditions were used with exact algorithms for finding ground states of two-dimensional spin glasses [4,5] (referred to as "extended" boundary conditions). A restricted version of thermal boundary conditions using periodic and anti-periodic boundary conditions in a single direction (a subset of TBC) was also used in Refs. [6–9].

Simulating the full TBC ensemble in Refs. [1–3] was done using population annealing (PA) [10–13]. See Ref. [14] for a recent discussion of the algorithm. Population annealing works with a population of replicas and aims to maintain thermal equilibrium while lowering the temperature. When temperature is decreased, the population is resampled according to the Boltzmann weights of the replicas, followed by regular Monte Carlo sweeps to all replicas in the population. In this work, the Metropolis algorithm is used. Simulating TBC using the diffusion method with PA is very simple. One can initialize each replica with a random boundary condition at $\beta = 0$ and then boundary conditions are resampled along with the replicas. The word "diffusion" would become apparent when one implements the method in parallel tempering, as discussed in Section 2.3.

It was noticed in Refs. [1,2] that the efficiency of the diffusion method can be greatly suppressed by temperature chaos. Some boundary conditions can be totally removed from the population. This is not satisfactory as there is no mechanism to recover these lost boundary conditions once they are eliminated from the population. Furthermore, temperature chaos predicts that these boundary conditions could become important again at lower temperatures. Therefore, it is worth studying a new method that does not have this problem. The most natural way is to simulate each boundary condition separately and combine the observables using weighted averages with free energy. How to weight different kinds of observables is discussed in Section 2.4. Since it is also interesting to study the performance of parallel tempering (PT) in simulating the full set of thermal boundary conditions, the two methods are therefore studied in both PA and PT.

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The paper is organized as follows: Section 2 introduces the Edwards–Anderson model, measured quantities, the diffusion method and the weighted average method. Numerical results are shown in Section 3, followed by concluding remarks and future challenges in Section 4.

2. Models, observables and methods

2.1. The Edwards–Anderson model

The Edwards–Anderson (EA) Hamiltonian is defined as

$$H = -\sum_{\langle ij\rangle} J_{ij} S_i S_j, \tag{1}$$

where $\{S_i = \pm 1\}$ are the spin degrees of freedom defined on a three-dimensional cubic lattice. The sum over $\langle ij\rangle$ means sum over all nearest neighbors. J_{ij} is the coupling between spins S_i and S_j and all couplings are independently chosen from the standard Gaussian distribution with mean 0 and variance 1. Thermal boundary conditions are applied to all instances.

2.2. Observables

There are three classes of observables that need to be treated differently using weighted averages. The first class is observables that are functions of a single replica like the energy E or the magnetization m. The second class is the thermodynamic observables of the free energy F and the entropy S. There is a third class of observables in spin glasses due to the nature of the symmetry breaking which is functions of two replicas like the spin overlap q defined as

$$q_{ab} = \frac{1}{N}\sum_i S_i^a S_i^b, \tag{2}$$

where micro-states a, b are chosen independently from the Boltzmann distribution. Note that a, b can be chosen from the same boundary conditions or different boundary conditions. Another quantity in this class is the link overlap which needs some care in the definition due to the change of boundary conditions, the link overlap q_ℓ is defined as

$$q_{\ell ab} = \frac{1}{dN}\sum_{\langle ij\rangle} S_i^a \mathrm{sign}(J_{ij}^a) S_j^a S_i^b \mathrm{sign}(J_{ij}^b) S_j^b, \tag{3}$$

where the sign function is ± 1 depends on whether the argument is positive or negative respectively. The definition has nothing to do with the weighted average method, but this is a more useful definition in the TBC setting for studying the nature of spin glasses. In this way, the difference of the link overlap of two different boundary conditions arises only from the domain walls, not from a mixture of domain walls and boundary condition differences. In the following, I will focus on the spin overlap function and will refer to it as the overlap function where no confusion arises. Note also that there is a 8×8 overlap function matrix in the TBC ensemble. An important statistic I, which quantifies the weight of an overlap distribution near $q = 0$, is defined as

$$I = \int_{-0.2}^{0.2} P(q)dq, \tag{4}$$

where $P(q)$ is an overlap distribution function.

2.3. The diffusion method

We have already discussed the diffusion method in population annealing, which initializes each replica with a random boundary condition at $\beta = 0$. For completeness, I also introduce and study the diffusion method in parallel tempering because parallel tempering is widely used in spin-glass simulations. Following the same strategy, one can simulate the TBC using parallel tempering by generating random states with random boundary conditions at $\beta = 0$. Then the boundary conditions diffuse along with the replicas under the swap moves of parallel tempering, hence the name the diffusion method. The convenience of working with $\beta = 0$ is because proposing a boundary condition change at finite temperatures can be costly as many bonds are affected when boundary condition changes. Furthermore, this is also essential to measure the absolute free energy.

The implementation of this method is simple and detailed balance is satisfied. However, the efficiency of the method still needs to be studied. Since in this method, PA and PT work in a similar way, one may expect that PT should suffer from temperature chaos too. This turns out to be the case as discussed in Sections 3.1 and 3.2. The effect of boundary condition eliminations in PA is replaced by one or more diffusion bottlenecks in PT. In the next, I discuss the weighted average method, which does not have this problem.

2.4. The weighted average method

It was shown that the absolute free energy can be measured very accurately using the free energy perturbation method in both population annealing and parallel tempering [11,15]. It can be shown from statistical mechanics that the average energy, entropy, free energy and the spin overlap distribution should be averaged as

$$E = \sum_i E_i p_i, \tag{5}$$

$$S = \sum_i S_i p_i - \sum_i p_i \log p_i, \tag{6}$$

$$F = \sum_i F_i p_i + T\sum_i p_i \log p_i, \tag{7}$$

$$P(q) = \sum_{ij} P_{ij}(q) p_i p_j, \tag{8}$$

where $p_i = \frac{e^{-\beta F_i}}{\sum_j e^{-\beta F_j}}$, E_i, S_i and F_i are the energy, entropy and free energy of boundary condition i and $P_{ij}(q)$ is the overlap distribution between the boundary conditions i and j.

It is worth noting that the weighted average method generates a lot more information than the diffusion method. For example, the overlap matrix is briefly discussed in Section 4. For now, we discuss briefly of the implementation of the weighted average method in PA and PT. In the weighted average method, each boundary condition is simulated independently. It is only when computing the spin overlaps that one needs communications between replicas with different boundary conditions. Therefore, in this way, PT can be simulated using parallel computing too. Since it is usually a practice to simulate two independent sets of replicas of each boundary condition, one can use 8 or 16 threads in the simulation. This is not doable in the diffusion method of PT. On the other hand, PA is intrinsically parallel and is also much more flexible with the number of threads. In my simulations, I have used OpenMP parallel computing for both PA and PT. For the equilibration measure of PA, one can either use the weighted average or the minimum of the entropy of families [14] of all boundary conditions.

3. Results

In this section, I investigate the performance of the diffusion method and the weighted average method. I first compare PA and PT for the diffusion method in Section 3.1. The conclusion is that