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An efficient Monte Carlo algorithm for overcoming broken ergodicity in the simulation of spin systems

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Abstract

A new Monte Carlo algorithm which provides enhanced sampling in the calculation of equilibrium thermodynamic properties of spin systems is presented. The algorithm proposed performs trial moves based on the generalized statistical distributions derived from a modification of the Gibbs–Shannon entropy by Tsallis. Results for a two-dimensional Ising model demonstrate that the algorithm leads to a greatly enhanced rate of barrier crossing and convergence in the calculation of equilibrium thermodynamic averages. Comparison is made with standard Metropolis Monte Carlo.

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1. Introduction

“Broken ergodicity” is a common challenge in computer explorations of phase space for systems for which the simulation time is shorter than an important relaxation time. Such a problem appears in complex disordered systems such as the spin glasses where the potential energy surface is rugged and regions of configurational space may be separated by free energy barriers which are much greater than the thermal energy. Enhanced sampling algorithms which accelerate the search of phase space are essential if reliable equilibrium averages are to be computed.

In this paper we propose an enhanced sampling algorithm based on the generalized statistical mechanics introduced by Tsallis [1]. We present the equilibrium distributions

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and define a Monte Carlo algorithm for the sampling of these distributions. The algorithm generates a Monte Carlo trajectory through a well-defined generalized statistical distribution. However, an appropriately weighted average allows us to calculate equilibrium thermodynamic averages for the Gibbs–Boltzmann canonical ensemble. Because of the delocalized character of the generalized distribution, the sampling is enhanced.

2. Tsallis statistics

In the generalized statistical mechanics proposed by Tsallis, the “generalized entropy” for a system with N degrees of freedom is *postulated* to be [1,2]

$$S_q = \frac{k}{q-1} \int p_q(\mathbf{r}^N) (1 - [p_q(\mathbf{r}^N)]^{q-1}) d\mathbf{r}^N, \quad (1)$$

where q is a real number. The definition is reminiscent of the “replica trick” in the theory of disordered systems, where $\langle \ln Z \rangle = \lim_{n \rightarrow 0} (\langle Z^n \rangle - 1)/n$, where Z^n is the partition function of a collection of n replicas of the system. When $q \rightarrow 1$ it can be shown that S_q tends to the Gibbs–Shannon entropy, $S = -k \int p(\mathbf{r}^N) \ln p(\mathbf{r}^N) d\mathbf{r}^N$.

In the way the Gibbs–Boltzmann distribution is derived in the canonical ensemble by the method of Lagrange multipliers, the generalized entropy may be extremized subject to the constraints $\int p_q(\mathbf{r}^N) d\mathbf{r}^N = 1$ and $\int [p_q(\mathbf{r}^N)]^q E(\mathbf{r}^N) d\mathbf{r}^N = E_q$, where $E(\mathbf{r}^N)$ is the energy. The probability density is found to be

$$p_q(\mathbf{r}^N) = \frac{1}{Z_q} [1 - (1-q)\beta E(\mathbf{r}^N)]^{1/(1-q)}, \quad (2)$$

where $Z_q = \int [1 - (1-q)\beta E(\mathbf{r}^N)]^{1/(1-q)} d\mathbf{r}^N$ is the generalized partition function. Having this generalized partition function, the rest of the statistical mechanics à la Gibbs can be derived, in a generalized fashion. For example, one can define the Tsallis free energy as $F_q = E_q - TS_q$, and generalize the standard formalism of the canonical ensemble. The equilibrium average over configuration space for a given observable $O(\mathbf{r}^N)$ is defined to be the “ q -expectation value”

$$\langle O \rangle_q = \int d\mathbf{r}^N O(\mathbf{r}^N) p_q^q(\mathbf{r}^N). \quad (3)$$

The Tsallis formalism was shown to preserve the Legendre transformations between thermodynamic state functions [2]. Also, for any q , there exist generalized versions of the von Neumann equation [3], the Ehrenfest theorem [4], the Boltzmann H-theorem [5], the Langevin and Fokker–Planck equations [6] and the fluctuation-dissipation theorem [7].

It is known that the normal diffusion of random walks can be obtained by extremizing the Gibbs–Shannon entropy subject to two constraints: normalization of the probability density and finiteness of the second moment. By extremizing the *Tsallis entropy* with the norm constraint plus the constraint that the q -expectation value of the second moment is finite, super-diffusive walks are naturally derived [8,9]. In general, the Tsallis

statistical distributions will be broader, for values of $q > 1$, than the Gibbs distribution, so the higher probabilities to be in regions of high potential compared to the Gibbs factor at the same temperature will enhance the sampling of a phase space partitioned by tall energy barriers.

3. Tsallis statistical Monte Carlo

3.1. Acceptance criterion and detailed balance

Previously, we have proposed a generalized Monte Carlo algorithm based on the acceptance probability

$$p = \min \left[1, \left(\frac{p_q(\mathbf{r}_{\text{new}}^N)}{p_q(\mathbf{r}_{\text{old}}^N)} \right)^q \right]. \tag{4}$$

This algorithm was used to sample according to the equilibrium distribution $[p_q(\mathbf{r}^N)]^q$ in the conformational optimization (energy minimization) of a tetrapeptide [10]. It was found that due to the delocalized nature of the distribution function when $q > 1$, the search of conformational space was greatly enhanced over standard Metropolis Monte Carlo methods. The standard Metropolis Monte Carlo acceptance probability corresponds to the $q = 1$ limit of Eq. (4).

In this paper, we propose to explore a modification of the Tsallis statistical MC. It is based on the Glauber acceptance probability sometimes known as Barker sampling. In the computation of equilibrium thermodynamic averages for spin systems it was shown [11] that for two-state problems such as the Ising model the Glauber (Barker) acceptance is favorable. The so-called asymmetric acceptance in Eq. (4) is just one of the solutions that guarantees convergence towards the distribution probability in Eq. (2). It is known from the theory of Monte Carlo simulation that a symmetrical solution of the type

$$W(x \rightarrow x') = T(x \rightarrow x') \frac{\rho_{x'}}{\rho_x + \rho_{x'}}, \tag{5}$$

where $T(x \rightarrow x')$ is the a priori symmetric transition matrix and ρ_x the probability distribution function for the x state, also satisfies detailed balance. Thus, by constructing the acceptance probability

$$p = \frac{1}{2} [1 - \tanh(\beta \Delta \bar{E} / 2)], \tag{6}$$

where $\bar{E} = [q/\beta(q-1)] \ln[1 - (1-q)\beta E]$, we retrieve a form reminiscent of the Glauber function [12], widely used in simulations of spin systems. A simulation using this acceptance probability will also tend towards the generalized probability distribution of Tsallis, just as Eq. (4) did. It will obey detailed balance,

$$[p_q(x)]^q W(x \rightarrow x') = [p_q(x')]^q W(x' \rightarrow x), \tag{7}$$

where $W(x \rightarrow x')$ is an element of the transition matrix and, by making $q \rightarrow 1$ as the temperature decreases, it will behave like a steepest descent.

3.2. Implementation using single flip algorithm

We performed simulations on a two-dimensional Ising spin system, with a 16-site cell with periodic boundary conditions (wrapped around a torus). Because of the form of the Tsallis probability, the energy cannot be negative for $q > 1$. For this reason we have chosen the following expression of the Ising Hamiltonian, with 0 and 1 for the possible values of the spin:

$$E = J \sum (1 - \delta_{s_i, s_j}), \quad (8)$$

where the sum extends over nearest-neighbor spin pairs. The energy of a spin pair is 0 if the spins are parallel and 1 if anti-parallel. We have implemented the generalized Monte Carlo algorithm using a single spin-flip procedure composed of the following steps:

- (i) A spin is picked at random and flipped.
- (ii) The change of energy is calculated. Because of the short-range interactions of the Ising systems, only nearest neighbors count.
- (iii) The spin configuration is accepted or rejected according to the criterion Eq. (6).
- (iv) Return to 1.

Since this acceptance will exactly satisfy detailed balance, the walk will converge towards sampling the equilibrium distribution $[p_q(x)]^q$.

3.3. Exact calculation of equilibrium averages

We used the enhanced sampling algorithm to calculate standard, Gibbs–Boltzmann equilibrium thermodynamic averages over a trajectory which samples the generalized statistical distribution.

Using the definition of the “ q -expectation value” in Eq. (3), the equilibrium thermodynamic average of O in the $q = 1$ canonical ensemble may be written

$$\langle O \rangle_1 = \left\langle \frac{O e^{-\beta E(\mathbf{r}^N)}}{[1 - (1 - q)\beta E(\mathbf{r}^N)]^{q/(1-q)}} \right\rangle_q \left\langle \frac{e^{-\beta E(\mathbf{r}^N)}}{[1 - (1 - q)\beta E(\mathbf{r}^N)]^{q/(1-q)}} \right\rangle_q^{-1}. \quad (9)$$

Using this expression, the standard $q = 1$ equilibrium average properties may be calculated over a trajectory which samples the Tsallis statistical distribution for $q \neq 1$. We show in Fig. 1 the results of such a simulation, shown with a continuous line, compared with results of Metropolis Monte Carlo, shown with a dotted line. The simulation was performed at the reduced temperature of 2. As can be seen, the two methods converge to the same average, with a much broader walk for the Tsallis acceptance method. This feature may be desirable in overcoming critical slowing down encountered in

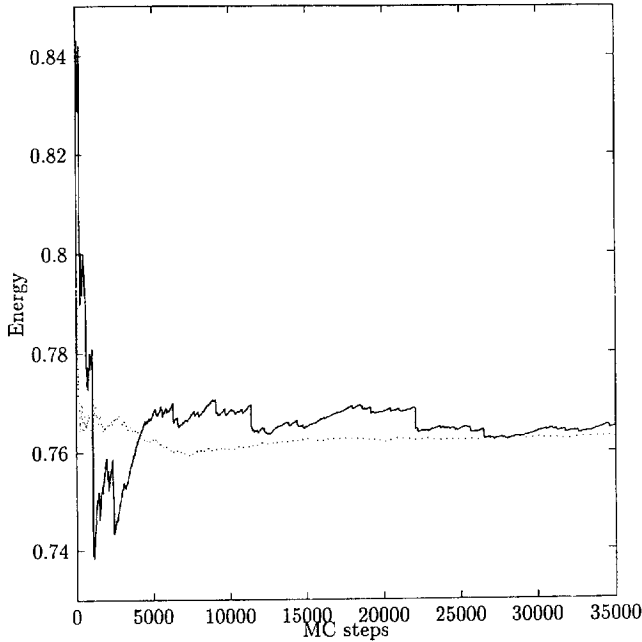


Fig. 1. For explanation see text.

spin systems near a phase transition. Further work will be performed at lower temperatures and we expect to see the broader characteristic of the $q > 1$ distribution function taking effect. Also, the algorithm we have presented can be used in connection with global (cluster) moves [13] to speed up even more the exploration of the phase space.

4. Discussion

We conclude with a specialized discussion of case of a first-order phase transition below the critical temperature. To go from one region to the other there is a bottle neck with a corresponding high free energy barrier. The height of the free energy barrier will be proportional to the area of the surface separating the two phases L^{d-1} , where L is the size of the system and d the dimension of the space. Due to the Boltzmann weight, a Metropolis Monte Carlo walk would be exponentially slowed down, and the simulation time would scale as $L^{2d} e^{L^{d-1}}$.

Now suppose each point in the configuration space is visited with a constant probability. This is the case of “multicanonical Monte Carlo”. Then it can be argued [14] that the Monte Carlo trajectory is a one-dimensional random walk in potential energy. The simulation time will scale as U^2 or, equivalently, as L^{2d} .

Now suppose the simulation is performed in the Tsallis ensemble. The slowing down reduces from an exponential to a power law. For example, if $q = 2$, the time scales as

$L^{2(2d-1)}$. The power-law scaling is similar to the multicanonical method [14], a powerful method used for simulation of phase transitions and frustrated systems. For Tsallis statistical MC the probability density function is known and need not be binned in advance. In the multicanonical method, a “production” run must be performed to estimate the weight of each phase point that would give the “multicanonical” distribution.

References

- [1] C. Tsallis, *J. Stat. Phys.* 52 (1988) 479.
- [2] E.M.F. Curado, C. Tsallis, *J. Phys. A: Math. Gen.* 24 (1991) L69.
- [3] A.R. Plastino, A. Plastino, *Physica A* 202 (1994) 438.
- [4] A.R. Plastino, A. Plastino, *Phys. Lett. A* 177 (1993) 177.
- [5] A.M. Mariz, *Phys. Lett. A* 165 (1992) 409.
- [6] D.A. Stariolo, *Phys. Lett. A* 185 (1994) 262.
- [7] A. Chame, E.V.L. de Mello, *J. Phys. Math A: Math. Gen.* 27 (1994) 3663.
- [8] P.A. Alemany, D.H. Zanette, *Phys. Rev. E* 49 (1994) R956.
- [9] C. Tsallis, S.V.F. Levy, A.M.C. de Souza, R. Maynard, *Phys. Rev. Lett.* 13 (1995) 3589.
- [10] I. Andricioaei, J.E. Straub, *Phys. Rev. E* 53 (1996) R3055.
- [11] G.W. Cunningham, P.H.E. Meijer, *J. Comput. Phys.* 20 (1976) 50.
- [12] R.J. Glauber, *J. Math. Phys.* 4 (1963) 294.
- [13] R.H. Swendsen, J.S. Wang, *Phys. Rev. Lett.* 58 (1987) 86.
- [14] B.A. Berg, T. Neuhaus, *Phys. Lett. B* 267 (1991) 249.