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Performance of Wang–Landau algorithm in continuous spin models and a case study: Modified XY-model

Suman Sinha, Soumen Kumar Roy *

Department of Physics, Jadavpur University, Kolkata 700032, India

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ABSTRACT

Performance of Wang–Landau (WL) algorithm in two continuous spin models is tested by determining the fluctuations in energy histogram. Finite size scaling is performed on a modified XY-model using different WL sampling schemes. Difficulties faced in simulating relatively large continuous systems using WL algorithm are discussed.

The Wang–Landau (WL) algorithm for Monte Carlo (MC) simulation, introduced in 2001 [1] has since been applied to a wide range of problems in statistical physics [2–6]. In most of these investigations the authors have applied the WL algorithm to systems with discrete energy levels which include the Ising and the Potts model. Relatively fewer papers have so far appeared on continuous models [7–9] and in such systems one uses a discretization scheme to divide the energy range of interest into a number of bins which label the macrostates of the system.

In the WL algorithm, one directly determines the density of states $\Omega(E_i)$ (in practice, its logarithm $g(E_i)$) of the system with $i = 1, 2, \ldots, n$ being the bin index. These macrostates are sampled with a probability which is inversely proportional to the current value of the density of states. If a trial move passes the probability test, $g(E_j)$ for the new energy E_j is modified as $g(E_j) \to g(E_j) + \ln f$, where the modification factor f is $\geqslant 1$ in the beginning of the simulation. In case a trial move fails, the density of states corresponding to the old value E_i of the energy is modified. A histogram record $H(E_i)$ of all states visited is maintained throughout the simulation. When the $g(E_i)$ corresponding to a certain macrostate is modified by adding $\ln f$ to it, the corresponding $H(E_i)$ is modified as $H(E_i) \to H(E_i) + 1$. In the beginning of the simulation the $g(E_i)$'s for all macrostates are initialized to zero. In the original version of WL algorithm, an iteration is considered to be complete when the histogram satisfies a "flatness" criterion. This means that $H(E_i)$ for all values of i, has attained 90% (or some other preset value) of the average of all $H(E_i)$. In the following iteration f is reduced, the $H(E_i)$'s are reset to zero, and the process is continued till $\ln f$ is as small as 10^{-8} or 10^{-9}. Since the history of the entire sampling process determines the density of states, the WL algorithm is non-Markovian besides being multicanonical in nature.

In course of the random walk in a WL simulation, the fluctuation of the energy histogram, for a given modification factor f, initially grows with the number of Monte Carlo sweeps and then saturates to a certain value. Because of the nature of the WL algorithm, which has been described above, the value of the histogram fluctuation determines the error which is generated in the resulting density of states. Zhou and Bhatt [10] carried out a mathematical analysis of the WL algorithm. They proved the convergence of the iterative procedure and have shown that the error in the density of states, for a given f, is of the order of $\sqrt{\ln f}$. This finding has been tested by Lee et al. [11] who performed extensive numerical test in two discrete models. In Monte Carlo simulation on two two-dimensional Ising models, namely, the ferromagnetic Ising model (FMIM) and the fully frustrated Ising model (FFIM), Lee et al. have shown that the fluctuation in the histogram increases during an initial accumulation stage and then saturates to

* Corresponding author. Tel.: +91 9331910161; fax: +91 33 24146584.
E-mail addresses: ssinha@research.jdvu.ac.in (S. Sinha), skroy@phys.jdvu.ac.in (S.K. Roy).

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a value which is inversely proportional to $\sqrt{\ln f}$ and they were of the view that this feature is generic to the WL algorithm. As is shown in Refs. [10] and [11] and also in the later part of this Letter, the resulting error in the density of states is then of the order of $\sqrt{\ln f}$, which is in agreement with the prediction of Zhou and Bhatt.

Methods which are alternatives to the requirement of the histogram flatness, for deciding where to stop an iteration for a given modification factor, have been proposed in the work described in Refs. [10] and [11]. Zhou and Bhatt [10] were of the opinion that an iteration may be stopped when the minimum number of visits to each macrostate is $1/\sqrt{\ln f}$. On the other hand, Lee et al. [11] proposed that an iteration can be stopped when the number of Monte Carlo sweeps, for a given value of f, is such that the saturation of the histogram fluctuation has been reached, since continuing the simulation for this particular modification factor is unlikely to reduce the error in the density of states any further. Subsequently, there have been a number of proposed improvements and studies of the efficiency and convergence of this algorithm [12–14].

In this Letter we first present the results of our investigation on the growth of histogram fluctuations in two continuous models. One of our aims is to check if the conjecture of Lee et al., that the nature of the dependence of the maximum of the histogram fluctuation on the modification factor f is model independent, can be extended to lattice spin models with continuous energy spectrum. For this purpose, we have chosen a two-dimensional spin system, where the spins, confined to a square lattice and free to rotate in a plane, say the xy-plane (having no z-component) interact with the nearest neighbours via a potential,

$$V(\theta) = 2\left[1 - \left(\cos^2\frac{\theta}{2}\right)^{p^2}\right], \tag{1}$$

where θ is the angle between the interacting spins and p^2 is a parameter to be chosen. This model, now known as the modified XY-model, was first introduced by Domany et al. in 1984 [15]. For $p^2 = 1$, the model is simply the conventional two-dimensional XY-model, which is known to exhibit a quasi-long-range-order–disorder phase transition mediated by the unbinding of topological defects [16]. For large values of p^2, the potential of Eq. (1) has a sharp well structure for small values of θ and the model exhibits a rather strong first order phase transition. Thus, the model with interaction determined by Eq. (1), for values of $p^2 = 1$ and 50, effectively behaves like two different models, having characteristically different phase transitions, although the symmetry of the Hamiltonian and the lattice and the spin dimensionalities remain the same. A similar change in the nature of the phase transition has been observed in the two-dimensional Lebwohl–Lasher (LL) model and a modified version of it [17]. In this model, with spin dimensionality $n = 3$ and lattice dimensionality $d = 2$, the nearest neighbour spins interact via a potential $-P_2(\cos\theta_{ij})$ and in the modified (LL) model this is $-P_4(\cos\theta_{ij})$ where, P_2 and P_4 are the second and the fourth Legendre polynomials respectively. Both models have the $O(3)$ as well as the local Z_2 symmetry. But as the nature of the interacting potential is modified, the transition changes from continuous to a sharply first order one. It has also been observed that for the $n = 3$ and $d = 3$ LL model, if one adds a P_4 interaction to the usual P_2 term, the nature of the phase transition changes from a weakly first order one to one where the discontinuities, which characterize the first order transition, grow sharply [18–23].

The $p^2 = 50$ model has very large fluctuations in energy, which is manifested in a huge peak in the specific heat. This is accompanied by very long relaxation times that make it difficult to obtain good statistics in the simulation using the conventional canonical sampling as is done in the Metropolis method [24]. In their original work, Domany et al. [15] had to carry out the simulation of this model in the roughening representation [25] and employ long runs.

Using different approaches mentioned below, we have also tested the performance of the WL algorithm in simulating the $p^2 = 50$ model. In the first method, which we call 'a', a preassigned number of MC sweeps, determined from the saturation of the histogram fluctuation, is used to stop an iteration with a given modification factor. In the other two methods, 'b' and 'c', a minimum number of visits to each macrostate (bins) namely $1/\sqrt{\ln f}$ and $1/(\ln f)$ respectively, have been used. So, in our work three different criteria, instead of testing the flatness of the histogram, have been used for stopping a particular iteration. Besides the methods 'a' and 'b' suggested in Refs. [11] and [10] respectively, we have chosen method 'c' because the proposition of $1/\sqrt{\ln f}$ visits to each macrostate does not directly follow from the fact that the error in the density of states is of the order of $\sqrt{\ln f}$. We have exercised this option, although it leads to a huge increase in the amount of computation, to see in particular if it leads to any improvement in the results of simulation. This is necessary particularly in view of the fact that, we have worked in a continuous model and the number of microstates which correspond to each bin is enormously large.

Before presenting our results we explain in detail the notations and symbols relevant to the problem. We represent by β_k, the saturation value of the energy histogram fluctuation in the kth iteration. Let f_k be the modification factor for the kth iteration. One usually starts with a modification factor $f = f_1 \geqslant 1$ and uses a sequence of decreasing f_k's ($k = 1, 2, 3, \ldots$) defined in some manner. One MC sweep is taken to be completed when the number of attempted single particle moves equals the number of particles in the system. The error in the density of states after the nth iteration has been performed, is directly related to β_i for $i > n$, the saturation values of the fluctuations.

In the WL algorithm the logarithm of the density of states after n iterations is given by

$$g_n(E_i) = \sum_{k=1}^{n} H_k(E_i)\ln(f_k), \tag{2}$$

where $H_k(E_i)$ is the accumulated histogram count for the ith energy bin during the kth iteration. In order to get an idea of the fluctuations in the histogram and its growth with the number of MC sweeps we subtract the minimum of the histogram count h_k^j which occurs in the histogram after the jth MC sweeps has been completed during the kth iteration, i.e. we consider the quantity

$$\tilde{H}_k^j(E_i) = H_k^j(E_i) - h_k^j. \tag{3}$$

(It may be noted that h_k^j does not refer to any particular bin and may occur randomly in any of the bins.)

The quantity $\tilde{H}_k^j(E_i)$ is now summed over all bins to give ΔH_k^j:

$$\Delta H_k^j = \sum_i \tilde{H}_k^j(E_i). \tag{4}$$

ΔH_k^j is thus a measure of the fluctuations which occurs in the jth MC sweeps during kth iteration and is a sort of average over all macrostates or bins. ΔH_k^j fluctuates with j because of statistical errors and its mean value taken over j is nothing but β_k. The error in the logarithm of the density of states, summed over all energy levels or bins, after the completion of n iterations is therefore given by

$$\eta_n = \sum_{k=n+1}^{\infty} \beta_k \ln(f_k). \tag{5}$$