

Reweighting for nonequilibrium Markov processes using sequential importance sampling methods

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We present a generic reweighting method for nonequilibrium Markov processes. With nonequilibrium Monte Carlo simulations at a single temperature, one calculates the time evolution of physical quantities at different temperatures, which greatly saves computational time. Using the dynamical finite-size scaling analysis for the nonequilibrium relaxation, one can study the dynamical properties of phase transitions together with the equilibrium ones. We demonstrate the procedure for the Ising model with the Metropolis algorithm, but the present formalism is general and can be applied to a variety of systems as well as with different Monte Carlo update schemes.

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The Monte Carlo simulation has served as a standard method to treat many-body problems in statistical physics [1]. Metropolis *et al.* [2] used the importance sampling, which generates the states with a probability proportional to the Boltzmann factor. The importance sampling method can be considered as a reweighting technique in a sense that one samples a trial distribution and takes an average for the true distribution with reweighting. A more direct way of reweighting is found in the histogram reweighting method due to Ferrenberg and Swendsen [3], where equilibrium thermal averages for a range of temperatures can be calculated from a single simulation. This method greatly improves the efficiencies of Monte Carlo simulations; however, the histogram reweighting technique must be used only to calculate equilibrium properties.

Recently, the nonequilibrium relaxation method has been successfully applied to the study of critical phenomena [4–7]. In the nonequilibrium relaxation method, simulations were performed for several temperatures; the critical temperature, the dynamical exponent, and other quantities are estimated using the scaling behavior of the nonequilibrium process. If we combine the strength of nonequilibrium relaxation method with a reweighting technique, we can expect an effective method of simulation.

In this paper, we will present a generic reweighting method that is applicable to both equilibrium and nonequilibrium systems. With reweighting at nonequilibrium, only a simulation at a single temperature is required. Our method of reweighting may also be applicable in a multitude of other nonequilibrium processes, such as the contact process [8] and the driven diffusive systems [9].

Reweighting at nonequilibrium can be easily understood as follows. Consider every simulation up to the t th Monte Carlo step as a sequence of states (or path),

$$\vec{x}_t = (\sigma_1, \sigma_2, \dots, \sigma_t), \quad (1)$$

where σ_t is the system configuration at time t . Hereafter, we refer to the Monte Carlo step simply as the time of simulation. Such a path \vec{x}_t can be generated using any Monte Carlo method at a temperature T . The objective is to calculate the

relative probability of generating the same path \vec{x}_t at another temperature T' .

Suppose many simulations were performed at an inverse temperature $\beta = 1/k_B T$ to obtain a set of paths \vec{x}_t^j , $j = 1, \dots, n$. (From now on, β will be sometimes referred to as temperature.) The dynamical thermal average of some quantity $Q(t)$ can be obtained by $\langle Q(t) \rangle_\beta = (1/n) \sum_{j=1}^n Q(\vec{x}_t^j)$. To calculate the dynamical thermal average at another temperature β' , the measured quantity $Q(\vec{x}_t^j)$ has to be reweighted with a set of weights w_t^j . For the same set of paths \vec{x}_t^j , the thermal average at β' is obtained as

$$\langle Q(t) \rangle_{\beta'} = \frac{\sum_{j=1}^n w_t^j Q(\vec{x}_t^j)}{\sum_{j=1}^n w_t^j}. \quad (2)$$

Although not labeled explicitly in Eq. (2), the set of weights w_t^j depend on the simulation temperature β and the new temperature β' . To calculate the weights, the following algorithm is implemented for each path \vec{x}_t^j , $j = 1, \dots, n$.

(1) Assume that the Monte Carlo simulation is carried out at a temperature β , and a path $\vec{x}_t^j = (\sigma_1^j, \dots, \sigma_t^j)$ for some arbitrary time t is obtained.

(2) To go from time t , let σ'^j be a trial configuration and $T(\sigma'^j | \sigma_t^j)$ be the probability to select this configuration. If the trial move is accepted with the acceptance probability $A_\beta(\sigma'^j | \sigma_t^j)$, then the new configuration at $t+1$ becomes $\sigma_{t+1}^j = \sigma'^j$. If the move is not accepted, $\sigma_{t+1}^j = \sigma_t^j$.

(3) In terms of the transition probability $P_\beta(\sigma_{t+1}^j | \sigma_t^j)$, we may write it as $P_\beta(\sigma_{t+1}^j | \sigma_t^j) = T(\sigma'^j | \sigma_t^j) A_\beta(\sigma'^j | \sigma_t^j)$ if the move is accepted and as $P_\beta(\sigma_{t+1}^j | \sigma_t^j) = T(\sigma'^j | \sigma_t^j) [1 - A_\beta(\sigma'^j | \sigma_t^j)]$ otherwise.

(4) Then the appropriate weights w_{t+1}^j can be obtained by

$$w_{t+1}^j = \frac{P_{\beta'}(\sigma_{t+1}^j | \sigma_t^j)}{P_\beta(\sigma_{t+1}^j | \sigma_t^j)} w_t^j \quad \text{with } w_1^j = 1. \quad (3)$$

(5) Repeat steps 2 to 4 until t reaches some predetermined maximum simulation time.

For each path \vec{x}_t^j , $j = 1, \dots, n$, these steps are repeated. Step 2 is simply the standard Monte Carlo procedure of accep-

tance and rejection. Step 3 calculates the transition probability after the decision on acceptance is made. Step 4 updates the appropriate weight. In this method, essentially, the usual Monte Carlo update is carried out, and at the same time the weights are updated.

The proof of Eq. (3) involves two ingredients, the sequential importance sampling (SIS) [10–12] method and a generic Monte Carlo method. A brief description of the SIS method will be discussed here. The SIS method assumes that the distribution for a multidimensional state $\vec{x}_t = (\sigma_1, \sigma_2, \dots, \sigma_t)$ is known and let it be denoted by $\pi_t(\vec{x}_t)$. Implementation of the SIS algorithm is as follows:

(1) Draw σ_{t+1}^j from a trial distribution $g_{t+1}(\sigma_{t+1}^j | \vec{x}_t)$ to form $\vec{x}_{t+1}^j = (\vec{x}_t^j, \sigma_{t+1}^j)$.

(2) The importance weight at $t+1$ is given by

$$w_{t+1}^j = \frac{\pi_{t+1}(\vec{x}_{t+1}^j)}{\pi_t(\vec{x}_t^j) g_{t+1}(\sigma_{t+1}^j | \vec{x}_t^j)} w_t^j. \quad (4)$$

The key to understanding the reweighting method is to realize that in a Monte Carlo simulation, the time sequence \vec{x}_t^j is sampled from the true probability distribution of the path at some temperature β . The Monte Carlo method is Markovian and the probability of obtaining the path is given by

$$P_\beta(\vec{x}_t^j) = P_\beta(\sigma_1^j | \sigma_{t-1}^j) \cdots P_\beta(\sigma_t^j | \sigma_{t-1}^j) P(\sigma_1^j), \quad (5)$$

where $P_\beta(\sigma_t^j | \sigma_{t-1}^j)$ is the probability of getting a system configuration σ_t^j at time t , given that the system configuration is σ_{t-1}^j at an earlier time $t-1$. $P(\sigma_1^j)$ is the probability of choosing the initial configuration. One may obtain the probability distribution function, $P_{\beta'}(\vec{x}_t^j)$, of the path at another temperature β' using $P_\beta(\vec{x}_t^j)$ as a trial distribution. The SIS method can then be used by defining the following quantities in Eq. (4) as

$$\pi_{t+1}(\vec{x}_{t+1}^j) \equiv P_{\beta'}(\vec{x}_{t+1}^j), \quad (6)$$

$$\pi_t(\vec{x}_t^j) \equiv P_{\beta'}(\vec{x}_t^j), \quad (7)$$

$$g_{t+1}(\sigma_{t+1}^j | \vec{x}_t^j) \equiv P_\beta(\sigma_{t+1}^j | \vec{x}_t^j). \quad (8)$$

The requirement for the Monte Carlo process being Markovian implies $P_\beta(\sigma_{t+1}^j | \vec{x}_t^j) = P_\beta(\sigma_{t+1}^j | \sigma_t^j)$, and using Eq. (5), we obtain

$$w_{t+1}^j = \frac{P_{\beta'}(\vec{x}_{t+1}^j)}{P_{\beta'}(\vec{x}_t^j) P_\beta(\sigma_{t+1}^j | \vec{x}_t^j)} w_t^j = \frac{P_{\beta'}(\sigma_{t+1}^j | \sigma_t^j)}{P_\beta(\sigma_{t+1}^j | \sigma_t^j)} w_t^j, \quad (9)$$

which is as presented in Eq. (3). The initial condition in Eq. (3) is $w_1^j = 1$ because the initial system configuration is chosen from a distribution independent of temperature.

To illustrate how the reweighting algorithm is implemented, we use the ferromagnetic Ising model on a square lattice. Its Hamiltonian is given by

$$\mathcal{H} = - \sum_{\langle kl \rangle} s_k s_l, \quad (10)$$

where the sum is over nearest neighbors and s_k takes the values ± 1 . Periodic boundary conditions are used on a

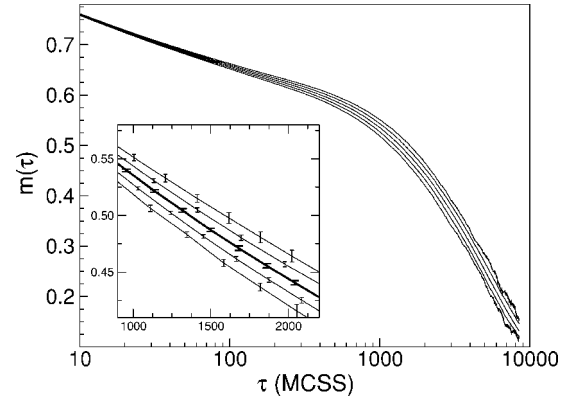


FIG. 1. Plot of magnetization for reweighted temperatures from simulations at a single temperature $T=2.270$ (bold line). From top to bottom, $T=2.268, 2.269, 2.270, 2.271, 2.272$. The system size is $L=64$. τ represents the Monte Carlo time in units of MCSS. The inset shows the region between 1000 to 2000 MCSS with representative error bars.

$L \times L$ lattice. We use the single spin-flip update with the Metropolis acceptance rate, but other update schemes are also applicable. The simulation is performed at β ; the objective is to reweight it to β' . The system configuration σ is denoted by the states of all spins, $\sigma = \{s_1, \dots, s_N\}$, where N is the total number of sites. The initial system configuration at time $t=1$ is set to $s_k = +1$ for all $k=1, \dots, N$. Hence $w_1^j = 1$ for $j=1, \dots, n$; recall that j is used for indexing different paths. For each path $\vec{x}_t^j = (\sigma_1^j, \sigma_2^j, \dots, \sigma_t^j)$,

(1) Choose a spin and flip it with probability, $A_\beta(\sigma^j | \sigma_t^j) = \min[1, \exp(-\beta \Delta E)]$. Here, ΔE is the energy change due to the spin flip.

(2) At this point, there are three possible outcomes. (a) If $\Delta E \leq 0$, the proposed spin flip is always accepted; and we obtain $w_{t+1}^j = w_t^j \times 1$. (b) If $\Delta E > 0$ and the proposed spin flip is accepted, we obtain $w_{t+1}^j = w_t^j \times \exp[-(\beta' - \beta)\Delta E]$. (c) If $\Delta E > 0$ and the proposed spin flip is rejected, we obtain $w_{t+1}^j = w_t^j \times [1 - \exp(-\beta' \Delta E)] / [1 - \exp(-\beta \Delta E)]$.

(3) Although the weights should be updated for every single spin flip move, thermal quantities may be recorded only once per N single spin-flip steps, for example, to save memory. Let τ be the time in unit of Monte Carlo steps per site (MCSS); weights w_τ^j and moments of magnetization $(m^\lambda)_\tau^j$, $\lambda=1,2,4$ (i.e., m, m^2 , and m^4 moments) are accumulated into the sums, $\sum_j w_\tau^j$, $\sum_j (m^\lambda)_\tau^j$ and $\sum_j (m^\lambda)_\tau^j w_\tau^j$.

We carried out many simulations to obtain a set of paths \vec{x}_t^j , $j=1, \dots, n$. Finally, the dynamical thermal averages for each time τ , $\langle m(\tau)^\lambda \rangle_{\beta'}$, for example, can be calculated from the accumulated sums using Eq. (2). In practice, reweighting to many temperatures $\beta'_1, \beta'_2, \dots$ were made at the same time in a single run.

Figure 1 shows the plots of the temporal evolution of magnetization for several reweighted temperatures from simulations at a single temperature $T=2.270$ (bold line) on the $L=64$ square lattice. These data were generated with three independent runs to estimate error bars; for each run, averages were taken over 2.94×10^5 samples. The effective range is about $\Delta T = 0.002$ for

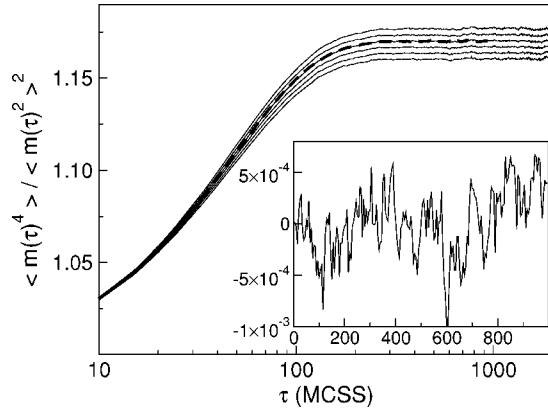


FIG. 2. Values of $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$ for reweighted temperatures from simulations at $T=2.270$. From top to bottom, $T=2.272, 2.271, 2.270, 2.269, 2.268, 2.267$. To check the range of reweighting, an additional simulation was performed at $T=2.268$ and reweighted to $T=2.270$. The dashed line shows $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$ at $T=2.270$ reweighted from $T=2.268$. The inset shows that the difference between the dashed line and solid line is about 5×10^{-4} while the error bars on $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$ are of the order 10^{-3} . The system size is $L=32$. τ represents the Monte Carlo time in units of MCSS.

$L=64$. The inset shows the region between 1000 and 2000 MCSS with representative error bars. The error bars become larger as reweighting is done at temperatures further away from the simulation temperature. Similar to the argument put forward by Ferrenberg and Swendsen [3], reweighting is effective when the distributions $P_{\beta'}(\vec{x}_t)$ and $P_{\beta}(\vec{x}_t)$ have sufficient overlaps. An additional simulation, performed at $T=2.268$, for example, yields the results consistent with the reweighted ones within statistical errors. A more detailed comparison of actual and reweighted data will be discussed shortly.

The ratio of the moments of the order parameter is used for the analysis of the phase transition [13]. Figure 2 shows plots of $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$ for several reweighted temperatures from simulations at $T=2.270$. From top to bottom, $T=2.272, 2.271, 2.270, 2.269, 2.268, 2.267$. The lattice size was $L=32$ and accuracy of reweighting was checked by performing an additional simulation at $T=2.268$. This simulation was then reweighted to $T=2.270$ and compared to the curve from the original simulation. The dashed line in Fig. 2 shows $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$ at $T=2.270$ reweighted from $T=2.268$. The inset shows that the difference between the dashed line and solid line is about 5×10^{-4} while the error bars of $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$ are of the order 10^{-3} . Averages were taken with the 1.28×10^6 samples. The systematic errors due to reweighting are smaller than the statistical errors for this temperature shift.

Equilibrium properties can be calculated using reweighting by performing the simulation up to equilibrium and beyond, and then disregarding the data at nonequilibrium. In this domain, our reweighting method yields the same results as the histogram reweighting [3] method. Figure 3 shows Binder's cumulants [13] for $L=32, L=48, L=64$, and $L=80$. Simulations were performed at one temperature for each lattice size. The crossing of curves with different sizes yields

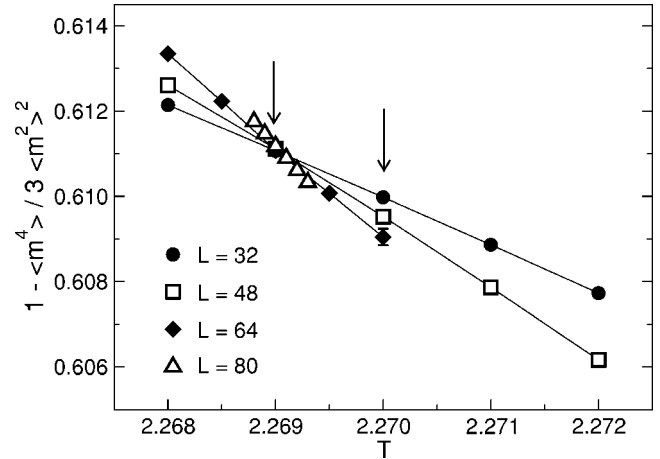


FIG. 3. Binder's cumulants for $L=32, L=48, L=64$, and $L=80$. The simulation temperatures are indicated by arrows; $T=2.27$ for $L=32, 48$; $T=2.269$ for $L=64, 80$. Error bars, when not shown, are smaller than the size of the symbols.

the determination of the critical temperature T_c . In the present case, we confirm that the exact $T_c=2.2691\dots$ is well reproduced. Simulation temperatures are indicated by arrows; $T=2.27$ for $L=32, 48$, and $T=2.269$ for $L=64, 80$. The reweighting temperature range we used is $\Delta T=0.004$ for $L=32, 48$, $\Delta T=0.002$ for $L=64$, and $\Delta T=5 \times 10^{-4}$ for $L=80$. Error bars were generated with several independent simulations, and they are smaller than the size of the symbols. This suggests that the effective reweighting temperature range is actually larger than the temperature range we used in our calculations. For each independent run, averages were taken with 1.28×10^6 samples for $L=32$, 2.59×10^5 samples for $L=48$, 1.28×10^5 samples for $L=64$, and 4×10^4 samples for $L=80$.

The dynamical finite-size scaling [14] can be used in combination with nonequilibrium relaxation [15,16]. Making use of the scaling form [17],

$$\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2 = g(\tau L^{-z}) \quad (11)$$

the dynamical exponent z can be estimated by plotting $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$ versus τL^{-z} at the known $T_c=2.2691\dots$ value (Fig. 4). The estimate of z is obtained when curves of different sizes are collapsed into a single curve. The best fit for the data collapse is obtained by choosing $z=2.143 \pm 0.063$ for all the data shown in Fig. 4. For the curves of $L=32$ and 48 , the best fit occurs at $z=2.11 \pm 0.02$. The best fit is obtained at $z=2.138 \pm 0.039$ for $L=48$ and 64 , and at $z=2.143 \pm 0.063$ for $L=64$ and 80 . We have given the error bars on z from the variance of the estimate of z by a set of independent runs. Simulations were performed at relatively small system sizes compared to more extensive simulations [17,18]. Considering the effect of corrections to scaling, our value of z is, within the error bars, approaching the values that were previously reported, $z=2.16 \sim 2.17$ [17–19].

To summarize, we have presented a reweighting method for nonequilibrium Markov processes. We have shown the basis of this method starting from the formulation of the SIS method. As a demonstration, we have used the Ising model

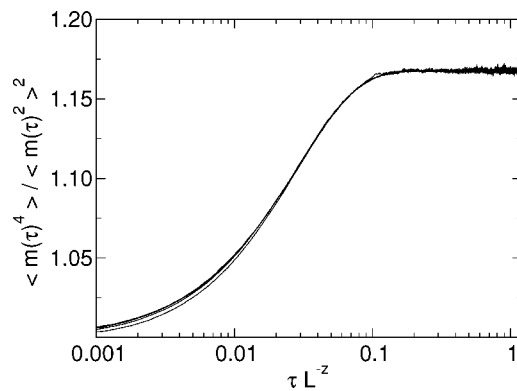


FIG. 4. Finite-size scaling plot of $\langle m(\tau)^4 \rangle / \langle m(\tau)^2 \rangle^2$ for $L=32, 48, 64$, and 80 at $T_c=2.2691\dots$. The dynamical exponent is chosen as $z=2.143$ for this plot.

on a square lattice. With the nonequilibrium simulation at a single temperature, we can determine the critical temperature and critical exponents using finite-size scaling. The nonequilibrium simulation for large enough systems [6,7] is one way

to extract dynamical and also static properties without worrying about finite-size effects. The systematic analysis of finite-size effects, the finite-size scaling [14–16], is another way of studying nonequilibrium relaxation. The nonequilibrium reweighting is useful when it is combined with the latter approach. We should note that this method is neither restricted to single spin-flip updates nor the Ising model. This method is applicable, in principle, whenever the ratio of probabilities $P_{\beta'}(\sigma_{t+1}^i | \sigma_t^i) / P_{\beta}(\sigma_{t+1}^i | \sigma_t^i)$ can be calculated numerically. It should be applicable with other Monte Carlo update schemes such as the cluster update schemes [20,21] as well as the N -fold way method [22]. We should mention that Dickman [23] proposed a similar reweighting method for the application to the contact process. However, our formalism is more extensive and general.

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