Transition Matrix Monte Carlo Reweighting and Dynamics

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We study an induced dynamics in the space of energy of single-spin-flip Monte Carlo algorithm. The method gives an efficient reweighting technique. This dynamics is shown to have relaxation times proportional to the specific heat. Thus, it is plausible for a logarithmic factor in the correlation time to specific heat. We present simulation data for relaxation time in one dimension and relate the relaxation time to specific heat. We give arguments to verify the general results.

Let us consider a single-spin-flip Glauber dynamics of the Ising model which is described in continuous time as

\[
\frac{\partial P(\sigma, t)}{\partial t} = \sum_{\{\sigma'\}} \Gamma(\sigma, \sigma') P(\sigma', t)
\]

\[
= \sum_{i=1}^{N} \left[ -w_i(\sigma_i) + w_i(-\sigma_i) F_i \right] P(\sigma, t),
\]

where \(N\) is the total number of spins, and

\[w_i(\sigma_i) = \frac{1}{2} \left[ 1 - \sigma_i \tanh \left( K \sum_{\text{nn of } i} \sigma_k \right) \right],\]

\[K = \frac{J}{k_B T},\]

is the flip rate of site \(i\), which depends on the spin value at the site \(i\) as well as the values of its nearest neighbor spins \(\sigma_k\). And \(F_i\) is a flip operator such that \(F_i P(\ldots, \sigma_i, \ldots) = P(\ldots, -\sigma_i, \ldots)\). The transition matrix Monte Carlo dynamics is defined, based on the above dynamics, by

\[
\frac{\partial P(E, t)}{\partial t} = \sum_{E'} W(E|E') P(E', t),
\]

where \(P(E, t)\) is the probability of having energy \(E\) at time \(t\), and

\[W(E|E') = \frac{1}{n(E')} \sum_{H(\sigma)=E} \sum_{H(\sigma')=E'} \Gamma(\sigma, \sigma').\]

Although Eq. (1) and (3) give the same equilibrium distribution of energy, they have totally different dynamics. We note that the transition matrix is banded along diagonal. The matrix elements are not independent—the column sum is zero due to the conservation of total probability, and the row sum satisfies \(\sum_{E} W(E'|E) P_{eq}(E) = 0\) due to the fact that the equilibrium distribution is a stationary distribution. The transition matrix also satisfies detailed balance condition, \(W(E'|E) P_{eq}(E') = W(E'|E) P_{eq}(E)\), inherited from the detailed balance in the original dynamics of spins. The detailed balance conditions put strong constraint on the matrix elements. For example, for any three energies with nonzero transition rates among them, we have

\[W(E|E'') W(E''|E') W(E'|E) = W(E|E') W(E'|E'') W(E''|E).\]
The matrix elements can be computed by Monte Carlo sampling as follows. For a configuration \( \sigma \), we consider the number \( N(\sigma, \Delta E) \) of cases that energy is changed by \( \Delta E \), for the \( N \) possible single-spin flips. Then for \( \Delta E \neq 0 \),

\[
W(E + \Delta E|E) = w(\Delta E)\langle N(\sigma, \Delta E) \rangle_{H(\sigma) = E},
\]

where the average is over all configurations having energy \( E \), and \( w(\Delta E) = \frac{1}{2}(1 - \tanh(\Delta E/(2k_B T))) \) for the Glauber dynamics. Since the quantity in the angular brackets of Eq. (6) is independent of temperature (or flip rates), once it is determined, we can use it at any temperature (or with any flip rates) for \( W(E|E') \) and consequently the equilibrium distribution at any temperature.

The microcanonical averages can be computed in any ensembles which have the property that equal energy states have equal probability. We used canonical simulations at a selection of temperatures, so that the total histogram \( H(E) \) is approximately flat. Of course, the total \( H(E) \) obtained by adding results at different \( T \) is not meaningful. However, it is perfectly correct to add statistics to \( \langle N(\sigma, \Delta E) \rangle_E \) from equilibrium simulations at different temperatures.

The single histogram method uses \( H(E) \) in a canonical simulation as an estimate to the equilibrium energy distribution \( P(E) \). Multiple histogram method attempts to overcome the problem of narrow window in the distribution. In the present method, adding simulations at different \( T \) is handled rather naturally. Such a "multiple histogram" TMMC is extremely simple and effective. In connection with the broad histogram method, we note that when \( T \) is set to \( \infty \), the detailed balance conditions reduce to the broad histogram equations. Unfortunately, the dynamics proposed in Ref. [7] is incorrect and the rest of the elements \( W_{k,k'} = 0 \) if \( |k - k'| > 1 \).

The matrix can not be diagonalized analytically in general. Nevertheless, at zero temperature, \( \gamma = 1 \), the eigenvalues can be obtained explicitly as \( \lambda_k = -2(k+1)/L - 1 \), which give us relaxation times as \( -1/\lambda_k \), with the longest relaxation time \( \tau = (L - 1)/2 \).

The TMMC for large system follows a simple and interesting dynamics. It can be shown rigorously, with the method of \( \Omega \)-expansion for master equation, that in the large-size scaling limit, the process is described by the equation

\[
\frac{\partial P(x, t')}{\partial t'} = \frac{\partial}{\partial x} \left( \frac{\partial P(x, t')}{\partial x} + xP(x, t') \right),
\]

where \( t' \) and \( x \) are properly scaled time and energy deviation from equilibrium.

\[
x = \frac{E - u_0 N}{(Nc')^{1/2}}, \quad u_0 N = \bar{E},
\]

and \( t' = bt \) with

\[
b = \lim_{N \to \infty} \frac{1}{2c' N} \sum_E W(\bar{E}|E)(E - \bar{E})^2,
\]

where \( u_0 \) is the average energy per spin and \( c' = k_B T^2 c \) is the reduced specific heat per spin. The equation is obtained by replacing \( E \) by \( x \) and expanding all the terms.
in small parameter $1/\sqrt{N}$. Details will be presented elsewhere.

The continuum limit equation describes a constrained random walk. There are two competing effects in the current $j = -\partial P/\partial x - x P$; while the first term is the usual diffusion, the second term keeps the walker at the origin. Equilibrium is obtained when $j = 0$, giving the well-known Gaussian distribution $P_{eq}(x) \propto e^{-x^2/2}$.

Equation (13) can be transformed into a one-dimensional quantum harmonic oscillator equation with the change of variable $P(x, t') = e^{-x^2/4}\phi(x, t')$. The relaxation spectrum is discrete and equally spaced (on $1/\tau$). In particular, the relaxation modes are $e^{-n^2-x^2/2}H_n(x/\sqrt{2})$, where $H_n$ is Hermite polynomials. Translating back to the original time $t$, the relaxation times are $1/(nb) \propto c$. Applying the general result, Eq. (13), to the one-dimensional Ising model, we have

$$\tau_n = \frac{1}{2n}\cosh 2K, \quad n = 0, 1, 2, \ldots$$

It is instructive to have an intuitive picture of the asymptotic dynamics, which we argue as follows.

The TMMC is equivalent to the following steps (Algorithm A).

1. Do perfect microcanonical simulation, i.e., pick a state at random among the degenerate states of current energy $E$.

2. Do one canonical Monte Carlo move, chosen a site at random.

Repeat step (1) and (2) $N$ times, where $N$ is the number of spins in the system. This is one TMMC step (sweep).

Consider the dynamics at very low temperatures. Then only two energies $E_0$ (ground state) and $E_1 = E_0 + 4J$ (first excited states) dominate. Consider $K$ such that correlation length ($\xi \propto \exp(2K)$) is about the size of the system. $P(E_0) \propto \exp(-E_0/k_B T)$, $P(E_1) \propto L^2\exp((-E_0-4J)/k_B T)$, and $P(E_1)/P(E_0) \approx L^2\exp(-4K) \approx 1$.

We now consider the time scales (from the point of view of TMMC) that a transition is made $E_0 \rightarrow E_1$, and $E_1 \rightarrow E_0$.

Let’s assume that the system is in its ground state $E_0$. Step (1) actually does nothing; in step (2), a kink pair (unsatisfied bonds) is excited with probability $\exp(-4K)$. Thus, we need $\exp(4K)$ moves to produce a kink pair. So the time scale in units of TMMC steps is $\tau \propto \exp(4K)/L \propto L$. We have used the fact that correlation length in one dimension is proportional to $\exp(2K)$ and that correlation length is comparable to system size $L$. The reverse process has a similar scale. This argument is consistent with the exact calculation.

A more general argument relating the relaxation time to the specific heat can be given, as follows: the variance of the energy distribution $P(E)$ is related to the specific heat as $\delta E^2 = c N k_B T^2$. Transition matrix Monte Carlo moves are random walks in energy confined in a region of $\delta E$. Thus the typical time for energy varying over $\delta E$ is proportional to the square of distance in energy. Therefore, time is proportional to $\delta E^2$, when we measure in steps of moves. To get $\tau$ in sweeps, we must divide by $N$. Let $a$ be the typical time for one step of walk in energy, the equation should be

$$\tau \propto a(\delta E^2/N) = a N k_B T^2 = a c', \quad (15)$$

We can give $a$ a precise meaning as $1/(c'b)$, where $b$ is given in Eq. (13). In one dimension, the unit time $a$ diverges. However, this does not happen in dimensions $d > 1$ as $T_c > 0$, and $a$ will be some finite value asymptotically independent of $N$.

We check the above results in two dimensions by extensive Monte Carlo simulations using two different methods: (1) the microcanonical/canonical algorithm $A$ described above, by computing the time correlation functions; and (2) by direct computation of $W(E|E')$ with a Wolff cluster algorithm [3]. The eigenvalues are computed with standard package [19]. While the first method is restricted to very small sizes, the second method can apply to large systems. In Fig. 3 we plot only the inverse eigenvalues. Very good confirmation of the log $L$ behavior for the relaxation time is observed.

This result has serious implication. In the standard single-spin-flip dynamics, if we add between canonical Monte Carlo moves microcanonical moves, the resulting dynamics is TMMC and still has a residue slowing down $\tau \sim \log L$ at $T_c$. It is thus difficult to imagine how this logarithmic factor can be canceled exactly in the original dynamics. In fact, such logarithmic factor is conjectured [13], while many numerical computations [21] did not seem to find it explicitly. We think that the Domany conjecture is still an open question.

One of the prediction of Eq. (11) is that the eigenvalues of $W(E|E')$ in the large-size limit are equally spaced, this is indeed the case for large systems. The eigenfunctions associated with these eigen modes are compared with numerical results. In Fig. 3 we plot the analytic results (curves) together with numerical values (symbols) from exact diagonalization of matrix $W(E|E')$ for a three-dimensional Ising model of $16^3$ at $k_B T/J = 6.0$. There are no adjustable parameters in the comparison except an overall normalization.

In conclusion, the transition matrix Monte Carlo shows a novel dynamical behavior. We find an unusual critical slowing down in one dimension. For two dimensions and higher, we conclude that correlation time is proportional to the specific heat. This is in contrast with cluster algorithms where Li and Sokal [21] showed that the specific heat is only a lower bound to the correlation time. While the TMMC artificial dynamics is of theoretical interest, the reweighting technique is very useful in practice.

3
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FIG. 3. The first four eigenmodes of the transition matrix Monte Carlo dynamics. The continuous curves are analytic results $\propto e^{-x^2/2}H_n(x/\sqrt{2})$. Symbols are from exact diagonalizations of matrix $W(E|E')$ for a three-dimensional Ising model on a $16^3$ system at $k_B T/J = 6.0$. For clarity, only every fifth data points are plotted.