Efficient Monte Carlo Simulation Methods in Statistical Physics

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15 March 2001

Abstract

The basic problem in equilibrium statistical mechanics is to compute phase space average, in which Monte Carlo method plays a very important role. We begin with a review of nonlocal algorithms for Markov chain Monte Carlo simulation in statistical physics. We discuss their advantages, applications, and some challenge problems which are still awaiting for better solutions. We discuss some of the recent development in simulation where reweighting is used, such as histogram methods and multicanonical method. We then discuss the transition matrix Monte Carlo method and associated algorithms.

The transition matrix method offers an efficient way to compute the density of states. Thus entropy and free energy, as well as the usual thermodynamic averages, are obtained as functions of model parameter (e.g. temperature) in a single run.

New sampling algorithms, such as the flat histogram algorithm and equal-hit algorithm, offer sampling techniques which generate uniform probability distribution for some chosen macroscopic variable.

1 Statistical Physics

Statistical mechanics is a theory developed at the end of nineteenth century to deal with physical systems from an atomistic point of view. In principle the properties of bulk matter, which may contain $10^{22}$ atoms, can be worked out from the motion of atoms following the basic equations of Newtonian mechanics or quantum mechanics. However, such detailed information is not available or not really necessary. A probabilistic point of view, in the form of statistical ensemble is taken. The theory is extremely economical and successful in dealing with equilibrium problems.

There are a number of equivalent formulations of the theory. But statistical mechanics in a nutshell is the following concise formula that connects statistical
mechanics with thermodynamics. First the partition function is defined as

\[ Z = \sum_X \exp \left( -\frac{E(X)}{kT} \right) \]  \hspace{1cm} (1)

where \( X \) is a “state” of the system; the summation is carried over all possible states. \( T \) is absolute temperature and \( k \) is the Boltzmann constant \((1.38 \times 10^{-23} \text{ Joule/Kelvin})\). The free energy of the system at temperature \( T \) is given by

\[ F = -kT \ln Z. \] \hspace{1cm} (2)

Free energy is a useful thermodynamic quantity in dealing with phase transitions. Other macroscopic observables are averages of the corresponding microscopic quantities over the Boltzmann-Gibbs weight \( \exp\left(-\frac{E(X)}{kT}\right) \),

\[ \langle g(X) \rangle = \frac{1}{Z} \sum_X g(X) \exp\left(-\frac{E(X)}{(kT)}\right). \] \hspace{1cm} (3)

The following three quantities are perhaps the most important ones, internal energy \( U = \langle E \rangle \), heat capacity \( C = dU/dT = \langle (E^2) - \langle E \rangle^2 \rangle / (kT^2) \), and entropy \( S = (U - F)/T = -k\langle \ln p(X) \rangle \), where the average is over the Gibbs probability density, \( p(X) = \exp(-E(X)/(kT))/Z \).

2 Monte Carlo Method

The essential task in statistical mechanics is to do the multi-dimensional integrations (for continuous systems) or summations (for discrete systems). To fix the notation and language, we briefly introduce the basics of Monte Carlo method \([2, 3, 4]\). Consider the computation of a statistical average,

\[ G = \int_{\Omega} g(X) p(X) dX = \langle g \rangle, \] \hspace{1cm} (4)

where the probability density obeys \( p(X) \geq 0 \), and \( \int_{\Omega} p(X) dX = 1 \). Suppose that we can generate samples \( X_i \) according to the probability \( p(X) \), then the integral can be estimated from an arithmetic mean over the samples,

\[ G_M = \frac{1}{M} \sum_{i=1}^{M} g(X_i). \] \hspace{1cm} (5)

The random variable \( G_M \) has mean \( G \) and standard deviation \( \sqrt{\tau \langle (g - G)^2 \rangle} / M \), \( \tau \) being decorrelation time. Thus in the limit of large number of samples, the estimate converges to the exact value.

The most general method to generate \( X \) according to \( p(X) \) is given by a Markov chain \([5]\) with a transition probability \( P(X'|X) = W(X \rightarrow X') \), satisfying the conditions stated below. This is the probability of generating a new state \( X' \) given that the current state is \( X \). Such process converges if

\[ W^n(X' \rightarrow X) > 0, \text{ for all } X' \text{ and } X, \text{ and } n > n_0. \] \hspace{1cm} (6)
The equilibrium distribution of the Markov chain satisfies

\[ p(X) = \sum_{X'} p(X') W(X' \to X). \]  \hspace{1cm} (7)

In constructing a Monte Carlo algorithm, it is convenient to consider a much stronger condition, the detailed balance

\[ p(X') W(X' \to X) = p(X) W(X \to X'). \]  \hspace{1cm} (8)

One of the most famous and widely used Monte Carlo algorithms is the Metropolis importance sampling algorithm [6, 7]. It takes a simple choice of the transition matrix:

\[ W(X \to X') = S(X \to X') \min \left(1, \frac{p(X')}{p(X)} \right) \]  \hspace{1cm} (9)

where \(X \neq X'\), and \(S\) is a conditional probability of choosing \(X'\) given that the current value is \(X\), and it is symmetric, \(S(X \to X') = S(X' \to X)\). Usually \(S(X \to X') = 0\) unless \(X'\) is in some “neighborhood” of \(X\). The diagonal term of \(W\) is fixed by the normalization condition \(\sum_{X'} W(X \to X') = 1\).

3 Cluster Algorithms

In order to facilitate the discussion we first introduce the Ising model. Ising model is an interacting many-particle model for magnets. A state consists of a collection of variables \(\sigma_i\) taken on only two possible values +1 and −1, signifying the spin up and spin down states. The spins are on a lattice. The energy of the state \(\sigma = \{\sigma_i\}\) is given by

\[ E(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \]  \hspace{1cm} (10)

where \(J\) is a constant which fixes the energy scale, the summation is over the nearest neighbor pairs. When temperature \(T\) is specified, the states are distributed according to

\[ p(\sigma) = Z^{-1} \exp \left( -\frac{E(\sigma)}{kT} \right). \]  \hspace{1cm} (11)

In a local Monte Carlo dynamics (Metropolis algorithm), one picks a site \(i\) at random, i.e., choosing a site with equal probability (this specifies or realizes \(S\)). Then, the energy increment if the spin is flipped, \(\sigma_i \to -\sigma_i\), is computed, which has the result \(\Delta E = 2J\sigma_i \sum_j \sigma_j\). The flip is accepted with probability \(\min(1, \exp(-\Delta E/kT))\). If the flip is rejected, the move is also counted and the state remains unchanged. One Monte Carlo step is defined as \(N\) moves (trials) for a system of \(N\) spins, such that each spin is attempted to flip once on average.
The local algorithm of Metropolis type has some salient features: (1) it is extremely general. Less assumption is made of the specific form of probability distribution. (2) Each move involves $O(1)$ operations and $O(1)$ degrees of freedom. (3) The dynamics suffers from critical slowing down. The correlation time $\tau$ diverges as a critical temperature is approached. We shall elaborate more on this in the following.

The statistical error, using estimator Eq. (5), is given by

$$\epsilon \approx \sigma_G \sqrt{\frac{\tau}{M}},$$

(12)

where $\text{Var}(G_1) = \sigma_G^2 = \langle g^2 \rangle - \langle g \rangle^2$ is the variance of the observable, $M$ is the number of Monte Carlo steps, and $\tau$ is the decorrelation time. We can take the point of view that the above equation defines $\tau$, i.e.,

$$\tau = \lim_{M \to \infty} \frac{M \text{Var}(G_M)}{\text{Var}(G_1)}.$$  

(13)

Perhaps it is appropriate to call $\tau$ decorrelation time, since $(\tau - 1)/2$ is sometimes called correlation time in the literature. The decorrelation time $\tau$ is the minimum number of Monte Carlo steps needed to generate effectively independent, identically distributed samples in the Markov chain. The smallest possible value for $\tau$ is 1, which represents independent sample by every step. The usual integrated autocorrelation time [8] differs from our definition by a factor of 2, $\tau_{int} = \tau/2$.

The critical slowing down manifests itself by the fact that $\tau \propto L^z$ at the critical temperature $T_c$ where a second order phase transition occurs. Here $L$ is the linear dimension of the system ($N = L^d$ in $d$ dimensions). For the local algorithms for many models and in any dimensions, $z \approx 2$. This suggests bad convergence, specially for large systems. At a first-order phase transition, where some thermodynamic variables change discontinuously, the situation is even worse — $\tau$ diverges exponentially with system sizes.

For the two-dimensional Ising model, a phase transition occurs at $kT_c/J \approx 2.269$. The magnetization is non-zero below this temperature and becomes zero above $T_c$. In addition, in the limit of large system ($L \to \infty$), heat capacity per spin and fluctuation of magnetization diverge. These intrinsic properties make computer simulation near critical point very difficult.

Cluster algorithms [10] overcome this difficulty successfully. For example, for the two-dimensional Ising model, the dynamical critical exponent defined in $\tau \propto L^z$ is reduced from 2.17 for the single-spin flip [1] to much small value for the cluster algorithm [10, 12, 13]. It turns out that a precise characterization of the Swendsen-Wang dynamical critical exponent is very difficult, due to weak size dependence of the decorrelation time. Table 1 represents a recent extensive calculation, based on the definition Eq. (13) for the total energy, rather than the usual method of extracting information from time-dependent auto-correlation functions. In this calculation, the variance of the sum of $M$ consecutive energies (c.f. Eq. [3]) are computed explicitly. Good convergence to the limiting value
Table 1: The decorrelation time $\tau$ of the Swendsen-Wang dynamics of the two-dimensional Ising model for different linear lattice size $L$ at the critical temperature.

| $L$ | $\tau$ | standard error |
|-----|--------|----------------|
| 4   | 4.04575| 0.00033        |
| 8   | 5.17696| 0.00032        |
| 16  | 6.5165 | 0.0012         |
| 32  | 8.0610 | 0.0018         |
| 64  | 9.794  | 0.004          |
| 128 | 11.723 | 0.012          |
| 256 | 13.872 | 0.009          |
| 512 | 16.29  | 0.04           |
| 1024| 18.87  | 0.2            |

The nonlocal cluster algorithm introduced by Swendsen and Wang for the Ising model (and more generally the Potts model) goes as follows: (1) go over each nearest neighbor pair and create a bond with probability

$$1 - \exp\left(-\frac{2J\delta_{\sigma_i, \sigma_j}}{(kT)}\right).$$

That is, if the two nearest neighbor spins are the same, a bond is created between them with probability $1 - \exp(-2J/kT)$; if spin values are different, there will be no bond. (2) Identify clusters as a set of sites connected by zero or more bonds (i.e., connected component of a graph). Relabel each cluster with a fresh new value $+1$ or $-1$ at random.

We note that each Monte Carlo step per spin still takes $O(1)$ in computational cost. The method is applicable to models containing Ising symmetry, i.e., the energy is the same when $\sigma_i$ is changed to $-\sigma_i$ globally.

The algorithm is based on a mapping of Ising model to a random cluster model of percolation. Specifically, we have \[14, 15, 16, 17\]

\[
Z = \sum_{\{\sigma\}} \text{exp}\left(K \sum_{(i,j)} (\delta_{\sigma_i, \sigma_j} - 1)\right) \quad (15)
\]
\[
= \sum_{\{\sigma\}} \sum_{\{n\}} \prod_{(i,j)} \left[p\delta_{\sigma_i, \sigma_j}\delta_{n_{ij}, 1} + (1 - p)\delta_{n_{ij}, 0}\right] \quad (16)
\]
\[
= \sum_{\{n\}} p^b(1 - p)^{N_d - b2N_c}, \quad (17)
\]
where $K = 2J/kT$, $p = 1 - \exp(-K)$, $\delta_{i,j}$ is the Kronecker delta, and $b$ is the number of bonds, $d$ is the dimension of a simple hypercubic lattice, and $N_c$ is the number of clusters. $\sigma_i$ is spin on the site and $n_{ij} = 0, 1$ is the bond variable between the sites $i$ and $j$. It is evident that the moves in the Swendsen-Wang algorithm preserves configuration probability of the augmented model containing both the spins and bonds.

A single cluster variant due to Wolff [18] is very easy to program. The following C code generates and flip one cluster:

```c
#define Z 4
#define L 8
double p = 0.7;
int s[L*L];

void flip(int i, int s0)
{
    int j, nn[Z];
    s[i] = -s0;
    neighbor(i, nn);
    for(j = 0; j < Z; ++j)
        if(s0 == s[nn[j]] && drand48() < p)
            flip(nn[j], s0);
}
```

In this single cluster version, a site $i$ is selected at random. The value of the spin before flip is $s_0$. It flips the spin and looks for its neighbors. If the value of the neighbor spins are the same as $s_0$, with probability $p$ a neighbor site becomes part of the cluster. This is performed recursively. It turns out that single cluster is somewhat more efficient than the original Swendsen-Wang, particularly in high dimensions. For dimensions greater than or equal to 4, Swendsen-Wang dynamics gives the dynamic critical exponent $z = 1$, while Wolff single cluster is $z = 0$ [19].

It is easy to see why the single cluster algorithm of the above works. Let us consider a general cluster flip algorithm with two bond probabilities: $P_s$ will be the probability of connecting two parallel spin sites; $P_d$ the probability of connecting anti-parallel sites. Consider the transition between two configurations $A$ and $B$, characterized by flipping a cluster $C$. A cluster is growing from a site $i$ until the perimeter of the cluster is not connected to the outside. The transition probabilities can be written down as

$$W(A \rightarrow B) = P_t \prod_{\partial C(\uparrow\uparrow)} (1 - P_s) \prod_{\partial C(\uparrow\downarrow)} (1 - P_d), \quad (18)$$

$$W(B \rightarrow A) = P_t \prod_{\partial C(\uparrow\uparrow)} (1 - P_d) \prod_{\partial C(\uparrow\downarrow)} (1 - P_s). \quad (19)$$

Note that the bond configuration probabilities are the same in the interior of
the clusters. The difference occurs at the boundary \( \partial C \), where parallel spins \((\uparrow\uparrow)\) in \( A \) becomes anti-parallel spins \((\uparrow\downarrow)\) in \( B \), or vice versa. Detailed balance requires that

\[
\frac{W(A \rightarrow B)}{W(B \rightarrow A)} = \frac{P(B)}{P(A)} = (1 - P_s)^{N_1} - N_2 (1 - P_d)^{N_2} - N_1 = e^{-\Delta E \over kT},
\]

where \( N_1 \) is the number of parallel spins on boundary of \( C \) in configuration \( A \); and \( N_2 \) is the number of anti-parallel spins on boundary of \( C \) in configuration \( A \). Since we have \( \Delta E = E_B - E_A = 2(N_1 - N_2)J \), we obtain

\[
1 - P_s = \exp \left( -{2J \over kT} \right).
\]

Although the algorithm is valid for any \( 0 \leq P_d < 1 \), it is most efficient at \( P_d = 0 \), the Coniglio-Klein \[15\] bond probability value.

A quite large number of statistical models can be treated with cluster algorithms, with varied success. Excellent performance has been obtained for Ising model, Potts models, and antiferromagnetic Potts models \[20\], XY model and general \( O(n) \) models \[18\], \( \phi^4 \) field-theoretic model \[21\], some regularly frustrated models \[22, 23\], six-vertex model \[24\], etc. Cluster algorithms are proposed for hard sphere fluid systems \[25\], quantum systems \[26, 27, 28, 29\], microcanonical ensembles \[30\], conserved order parameters \[31, 32\], etc. Invaded cluster algorithm \[33\] and other proposal \[34\] are excellent methods for locating critical points. The cluster algorithms are also used in image processing \[35, 36\].

The cluster algorithms do not help much in temperature-driven first-order phase transition – the slow convergence has been shown rigorously \[37\]. Models with frustration, spin glass being the archetype, do not have efficient cluster algorithms, although there are attempts \[38, 39, 40\] with limited success. Breakthrough in this area will have a major impact on the simulation methods.

### 4 Reweighting Methods

In this and the following sections, we discuss a class of Monte Carlo simulation approaches that aim at an efficient use of data collected, and sampling methods that enhance rare events.

The computation of free energy, Eq. (2), poses a difficult problem for Monte Carlo method. A traditional method is to use thermodynamic integration, e.g.,

\[
\frac{F(T_2)}{T_2} - \frac{F(T_1)}{T_1} = - \int_{T_1}^{T_2} {\langle E \rangle \over T^2} dT,
\]

based on the relation \( \langle E \rangle = -\partial \ln Z / \partial \beta \), where \( \beta = 1 / (kT) \).

If we can estimate the density of states (the number of states with a given energy \( E \) for discrete energy models), then we can compute free energy, as well as thermodynamic averages. The result is obtained as a function of temperature.
$T$, rather than a single datum point for a specific value of $T$, as in standard Monte Carlo simulation.

This idea has been pursued over the last decade by Ferrenberg and Swendsen \[41, 42\], Berg et al \[43, 44, 45\], Lee \[46\], Oliveira et al \[47\], and Wang \[48\]. Consider the following decomposition of summations over the states

$$\sum_{\{\sigma\}} A(\sigma) e^{-\frac{E(\sigma)}{kT}} = \sum_{E} e^{-\frac{E}{kT}} \sum_{\sigma(E)=E} A(\sigma) = \sum_{E} e^{-\frac{E}{kT}} n(E) \langle A(\sigma) \rangle_E,$$

(23)

where $\langle A \rangle_E$ is the microcanonical ensemble average,

$$\langle A \rangle_E = \frac{1}{n(E)} \sum_{\sigma(E)=E} A(\sigma).$$

(24)

Since the state space is exponentially large ($2^N$ for the Ising model with $N$ spins), and the range of $E$ is typically of order $N$, if $n(E)$ can be computed accurately, the task is done. The canonical average of $A$ is related to the microcanonical average through

$$\langle A \rangle_T = \frac{\sum_{E} \langle A \rangle_E \exp\left(-\frac{E}{kT}\right) n(E)}{\sum_{E} \exp\left(-\frac{E}{kT}\right) n(E)},$$

(25)

and free energy is computed as

$$F = -kT \ln \sum_{E} \exp\left(-\frac{E}{kT}\right) n(E).$$

(26)

### 4.1 Histogram method

Ferrenberg and Swendsen \[41\] popularized a method which in a sense is to compute the density of states (up to a multiplicative constant) in a range close to a given simulation temperature. This method is generalized as multiple histogram method to combine simulations at differential temperatures, to get the whole energy range \[42\]. We discuss here only the single histogram method for its simplicity.

During a normal canonical simulation at fixed temperature $T^*$, we collect the histogram of energy, $H(E)$, which is proportional to probability distribution of energy,

$$H(E) = c n(E) \exp\left(-\frac{E}{kT^*}\right).$$

(27)

The constant $c$ is related to the partition function, $c = M/Z(T^*)$, where $M$ is the total number of samples collected. From the above equation, we find $n(E) \propto H(E) \exp\left(E/(kT^*)\right)$. With this information, we can compute the free energy difference between temperature $T^*$ and a nearby temperature $T$. Similarly, moments of energy can be computed after the simulation, through histogram reweighting,

$$\langle E^n \rangle_T = \frac{\sum_{E} E^n H(E) \exp\left(-E/(kT) + E/(kT^*)\right)}{\sum_{E} H(E) \exp\left(-E/(kT) + E/(kT^*)\right)}.$$
The range of $E$ that the histogram data can be collected at a fixed temperature is limited by the energy distribution, which for the canonical distribution away from critical point, is of order of $\sqrt{N}$. The whole range of energy $E$ is of order $N$. This limit the usefulness of single histogram method.

4.2 Multicanonical Monte Carlo

The multicanonical Monte Carlo method has been shown to be very effective to overcome supercritical slowing down, reducing the relaxation time from exponential divergence with respect to system size to a power, at the first-order phase transitions [43]. Multicanonical ensemble flattens out the energy distribution, so that the computation of the density of states $n(E)$ can be done for all values of $E$. A multicanonical ensemble is defined to following the probability density for the states as

$$p(\sigma) = f(E(\sigma)) \propto \frac{1}{n(E(\sigma))},$$ (29)

such that the energy histogram $H(E) (\propto n(E)f(E))$ is a constant. From the histogram samples obtained by a simulation with the weight of state at energy $E$ as $f(E)$, the density of state can be computed [46] from $n(E) = H(E)/(f(E)c)$. However, unlike canonical simulation where $f(E) = e^{-E/kT}$ is given, in a multicanonical simulation, $f(E)$ is unknown to start with.

Berg proposed an iterative method to compute the weight in a parametrized form $f(E) = \exp(-\beta(E)E + \alpha(E))$, starting with no information, $f_0(E) = \text{const}$. A new estimate at iteration $n$ is then based on the results of all previous iterations. We refer to references [44, 45] for details.

5 Transition Matrix Monte Carlo and Flat Histogram Algorithm

The flat histogram algorithm offers an efficient bootstrap to realize the multicanonical ensemble, while transition matrix Monte Carlo utilizes more data that can be collected in a simulation to improve statistics.

5.1 Transition matrix

We start from the detailed balance equation for some given dynamics:

$$p(\sigma)W(\sigma \rightarrow \sigma') = p(\sigma')W(\sigma' \rightarrow \sigma).$$ (30)

By summation over the states $\sigma$ of fixed energy $E$, and $\sigma'$ of fixed energy $E'$, and assuming that the probability of the state is a function of energy only, $p(\sigma) \propto f(E(\sigma))$, we get

$$n(E)f(E)T(E \rightarrow E') = n(E')f(E')T(E' \rightarrow E),$$ (31)
where the transition matrix in the space of energy is defined as

\[
T(E \rightarrow E') = \frac{1}{n(E)} \sum_{E(\sigma) = E} \sum_{E'(\sigma') = E'} W(\sigma \rightarrow \sigma').
\]  

(32)

The matrix \( T \) has a number of interesting properties: it is a stochastic matrix in the sense of \( T(E \rightarrow E') \geq 0 \) and \( \sum_{E'} T(E \rightarrow E') = 1 \); the stationary solution of \( T \) is the energy distribution \( n(E)f(E) \); the dynamics associated with \( T \) is considerably faster than that of \( W \).

We specialize to the case of single-spin-flip dynamics for the Ising model. The transition matrix \( W \) for the spin states consists of a product of two factors, the probability of choosing a spin to flip \( S(\sigma \rightarrow \sigma') \), and the flip rate \( a(E \rightarrow E') = \min(1, f(E')/f(E)) \). We have \( S(\sigma \rightarrow \sigma') = 0 \) less the two configurations \( \sigma \) and \( \sigma' \) differ by one spin, in this case, the value of \( S \) is \( 1/N \), where \( N \) is the number of spins in the system. Using these results, we can rewrite the transition matrix as

\[
T(E \rightarrow E') = \frac{1}{N} \langle N(\sigma, \Delta E) \rangle_E a(E \rightarrow E'), \quad E \neq E'.
\]  

(33)

The diagonal elements are determined by normalization. Substituting Eq. (32) into Eq. (33), using the relation between \( a(E \rightarrow E') \) and \( f(E) \), we obtain

\[
n(E)\langle N(\sigma, \Delta E) \rangle_E = n(E')\langle N(\sigma', \Delta E') \rangle_{E'}.
\]  

(34)

This is known as broad histogram equation \[50, 51\] which forms the basis for the flat histogram algorithm presented below. Additionally, this equation also gives us a way of computing the density of states \( n(E) \) by the quantity \( \langle N(\sigma, \Delta E) \rangle_E \) obtained from spin configurations generated from any distribution \( f(E(\sigma)) \). The quantity \( N(\sigma, \Delta E) \) is the number of ways that the system goes to a state with energy \( E + \Delta E \), by a single spin flip from state \( \sigma \). The angular brackets indicate a microcanonical average:

\[
\langle N(\sigma, \Delta E) \rangle_E = \frac{1}{n(E)} \sum_{E(\sigma) = E} N(\sigma, \Delta E).
\]  

(35)

### 5.2 Flat histogram algorithm

The following algorithm \[48, 52\] generates flat histogram in energy and realizes the multicanonical ensemble.

1. Pick a site at random.

2. Flip the spin with probability

\[
a(E \rightarrow E') = \min \left(1, \frac{\langle N(\sigma', -\Delta E) \rangle_{E+\Delta E}}{\langle N(\sigma, \Delta E) \rangle_E} \right),\]

(36)

where the current state \( \sigma \) has energy \( E \), the new state \( \sigma' \) has energy \( E' = E + \Delta E \).
3. Accumulate statistics for \( \langle N(\sigma, \Delta E) \rangle_E \).

4. Go to 1.

We note by virtue of Eq. (34), the flip rate is the same as that in multicanonical simulation with a weight \( 1/n(E) \) and Metropolis acceptance rate. While in multicanonical sampling, the weight is obtained through several simulations iteratively, the quantities \( \langle N(\sigma, \Delta E) \rangle_E \) is much easier to obtain, through a single simulation. This quantity serves a dual purpose—it is used to construct a Monte Carlo algorithm (used as input), and at the same time, it is used to compute the density of states (output of the simulation). Clearly, this is circular unless approximation is made. We have considered replacing the exact microcanonical average by an accumulative average, over the history of simulation generated so far, i.e.,

\[
\langle N(\sigma, \Delta E) \rangle_E \approx \frac{1}{H(E)} \sum_{i=1}^{M} \delta_{E(\sigma_i), E} N(\sigma_i, \Delta E),
\]

where \( \{\sigma_i, i = 1, 2, \ldots\} \) is the sequence of states generated with the algorithm given above; \( H(E) \) is the number of samples accumulated at the energy bin \( E \). In case the data for computing the flip rate is not available, we simply accept the move to explore the new state. A more rigorous way of doing simulation is to iterate the simulation with constant flip rate. For example, after the first simulation, we compute a first estimate to the density of states. In a second simulation, we perform multicanonical simulation à la Lee. The data collected in the second run for \( \langle N(\sigma, \Delta E) \rangle_E \) will be unbiased. It is found that even with a single simulation, the results converge to the exact values (for \( \langle N(\sigma, \Delta E) \rangle_E \) and \( n(E) \)) for sufficiently long runs, even though a rigorous mathematical proof of the convergence is lacking.

Wang and Landau proposed recently a new algorithm that works directly with the density of states \( n(E) \). The simulation proceeds with the flip rate \( \min(1, n(E)/n(E')) \), but the value of the density of states is updated after every move by \( n(E) \leftarrow n(E)f \) and letting \( f \rightarrow 1 \) for convergence. Excellent results were obtained. A careful comparison with flat histogram method is needed.

### 5.3 N-fold way (rejection-free moves)

In Metropolis algorithm, moves are sometimes rejected. This rejection is important for realizing the correct stationary distribution. In 1975 Bortz, Kalos, and Lebowitz proposed a rejection-free algorithm. It is still based on Metropolis flip rate, but the waiting due to rejection is taking into account by considering all possible moves. The Bortz-Kalos-Lebowitz N-fold way algorithm for the Ising model goes as follows:

1. Compute the acceptance probability for one attempt of a move

\[
A = \sum_{\Delta E} \frac{N(\sigma, \Delta E)}{N} a(E \rightarrow E + \Delta E).
\]

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2. Pick an energy change $\Delta E$ according to probability 
\[ p_{\Delta E} = \frac{N(\sigma, \Delta E)}{AN} a(E \rightarrow E + \Delta E). \] (39)
flip a site belonging to $\Delta E$ with probability 1. The site is choosing from the $N(\sigma, \Delta E)$ sites with equal probability.

3. One $N$-fold-way move is equivalent to $1/A$ moves in the original dynamics. Thus thermodynamic averages are weighted by $1/A$, i.e., $\langle g \rangle = \sum_t (g_t/A) / \sum_t 1/A$, where summation is over every move $t$.

In order to implement step 2 efficiently, additional data structure is needed so that picking a spin in a given class characterized by $\Delta E$ is done in $O(1)$ in computer time.

### 5.4 Equal-hit algorithm

Combining $N$-fold way and flat histogram algorithm is easy, since the important quantity $N(\sigma, \Delta E)$ is already computed in flat histogram algorithm. The flip rate $a$ is given by formula (36). In the flat histogram algorithm, the probability that the energy of the system is $E$ is a constant, i.e.,
\[ H(E) = \langle \delta_{E(\sigma), E} \rangle \propto n(E)f(E) = \text{const} \]
\[ = \left( \langle \delta_{E(\sigma), E} \frac{1}{A(\sigma)} \rangle_N / \langle \frac{1}{A(\sigma)} \rangle_N \right). \] (40)

The averages in the second line of the above equation refer to samples generated in an $N$-fold way simulation.

In equal-hit algorithm (ensemble) [55], we require that the number of “fresh configurations” generated at each energy is a constant. More precisely equal-hit ensemble is defined by
\[ u(E) = \langle \delta_{E(\sigma), E} \rangle_N = \text{const}. \] (41)

One possible choice of the flip rate is
\[ a(E \rightarrow E') = \min \left( 1, \frac{\left( \frac{1}{A(E', N(\sigma', E - E'))} \right)}{\left( \frac{1}{A(E, N(\sigma, E'}) \right)} \right), \] (42)
where
\[ \langle \frac{1}{A} \rangle_{E,N} = \frac{\langle \delta_{E(\sigma), E} \frac{1}{A(\sigma)} \rangle_N}{\langle \delta_{E(\sigma), E} \rangle_N} \] (43)
is the inverse total acceptance rate $1/A$ arithmetic averaged over the $N$-fold way samples at energy $E$.

The histogram $H(E)$ generated in the equal-hit algorithm depends on the precise dynamics (the rate $a$) used. Since there are many possible choices of the rate, such “equal-hit ensemble” is not unique.
5.5 Determination of the density of states

While Eq. (34) gives us a way of obtaining the density of states, there are more equations than unknowns. We consider two optimization methods. The first method is based on the transition matrix itself. We define $T_{E,\Delta E} = \langle N(\sigma, \Delta E) \rangle_E / N$. Symbols with hat being unknown, and $T_{E,\Delta E}$ the Monte Carlo estimate, consider

$$\text{Minimize} \sum_{E,\Delta E} \sigma_{E,\Delta E}^2 (\hat{T}_{E,\Delta E} - T_{E,\Delta E})^2, \quad (44)$$

subject to $0 \leq \hat{T}_{E,\Delta E} \leq 1$, $\sum_{\Delta E} \hat{T}_{E,\Delta E} = 1$, and $\hat{T}_{E,1} \hat{T}_{E+1,1} \hat{T}_{E+2,-2} = \hat{T}_{E,2} \hat{T}_{E+2,-1} \hat{T}_{E+1,-1}$.

The last constraint needs more explanation. We assume that the energy level is equally spaced (as in the Ising model). Consider three energy levels, $E, E+1, E+2$. If we write down three equations of type (34), for transitions from $E$ to $E+1$, $E+1$ to $E+2$, and $E+2$ to $E$, we can cancel the density of states by multiplying the three equations together. This leaves the last equation above, and it is known as TTT identity. It can be shown that multiple T identities (four or more) are not independent, and they need not put in as constraints. For Ising model there is also one additional symmetry constraint, $T_{E,i} = T_{-E,-i}$.

When the solution for $T$ is found, we can use any of the energy detailed balance equation to find density of states $n(E)$. The TTT identity guarantees that the answer is unique whichever detailed balance equation is used.

The second method is based on optimization directly with variable $n(E)$, actually $S(E) = \ln n(E)$, by

$$\text{minimize} \sum_{E,\Delta E} \sigma_{E,\Delta E}^2 \left( \hat{S}(E + \Delta E) - \hat{S}(E) - \ln \frac{T_{E,\Delta E}}{T_{E+\Delta E,-\Delta E}} \right)^2, \quad (45)$$

subject to, for the Ising model, $\sum_{E} n(E) = 2^N$, where $N$ is the total number of spins in the system. In addition, we can put in the known fact that the ground states are doubly degenerate, $n(0) = 2$.

Figure 1 shows one of the simulation results of the density of states, using the second method. The errors by comparison with exact known values [56] are presented in the insert of the figure. The density of states $n(E)$ is determined to an accuracy of better than 2 percents in a matter of few minutes of computer time.

The flat-histogram dynamics is used to study spin glasses [57]. The dynamic characteristics is quite similar to multi-canonical method of Berg. The study of lattice polymer and protein folding is under way. For related ideas and approaches, see refs. [58, 59, 60].

6 Conclusion

The phenomenon of critical slowing down can be effectively dealt with by cluster algorithms for a large class of statistical mechanics models. We reported new
Figure 1: Logarithmic density of states, $S(E) = \ln n(E)$, calculated by transition matrix Monte Carlo method for a $16 \times 16$ two-dimensional Ising model with a total $1.1 \times 10^5$ Monte Carlo steps and the first $10^4$ discarded, using the flat-histogram algorithm and N-fold way. The insert is error in $S(E)$ with respect to exact results.

and very accurate results for the decorrelation times of the Swendsen-Wang dynamics. Large size asymptotic behavior is analyzed. For super-critical slowing down occurring in first-order phase transitions, multicanonical ensemble simulation and flat-histogram or equal-hit algorithms are very effective. Since the latter algorithms and associated transition matrix method is efficient in computing the density of states, this method can also be useful for general counting problems by Monte Carlo method.

Acknowledgements

The author thanks Prof. R. H. Swendsen for many of the work discussed here. He also thank Z. F. Zhan, T. K. Tay, and L. W. Lee for collaborations. This work is supported by a NUS research grant R151-000-009-112 and Singapore-MIT Alliance.
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