

Flat histogram method comparison on 2D Ising Model

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We examine the convergence of the Stochastic Approximation with a Dynamic update factor (SAD) algorithm applied to the 2D Ising model. Comparison with SAMC and WL methods show that SAD performs robustly and without user input knowledge of an energy range. We confirm that SAD is more powerful in the common case in which the range of energies is not known in advance.

I. INTRODUCTION

Flat histogram Monte-Carlo simulation algorithms calculate the thermodynamic properties of various systems over a range of temperatures. The first histogram method used a single canonical Monte Carlo simulation to predict properties for nearby temperatures [1]. While the method effectively samples a narrow energy range given limited by a narrow temperature range, it proves computationally inefficient at sampling large energy ranges.

Due to a canonical Monte Carlo simulation's inefficient sampling of large energies, a variety of “flat” (or “broad”) histogram methods [2–6] were developed to explore a wider range of energies. In addition to obtaining thermodynamic information for the entire energy range for a single simulation, these approaches cannot be easily trapped in a local energy minimum like a canonical simulation.

Wang and Landau introduced one of the most widely used flat-histogram Monte-Carlo algorithms that accurately determined the density of states (DOS) for a statistical system [5, 6]. For all of its power, the method unfortunately requires a priori knowledge of several user-defined parameters. Thus, for any given system under study, the user needs to determine the ideal parameters in order to apply the method. The Wang-Landau algorithm is also known to violate detailed balance (although only for brief time intervals) [7, 8]. With the violation of detailed balance, convergence of the algorithm is not guaranteed.

Because of the uncertainty of convergence for WL, many studies were undertaken to understand how the modification (or update) factor γ impacts the convergence [9–11]. The ideal choice of decreasing the modification factor helps to prevent CPU time from being wasted by continuing to perform calculations after the error in the density of states is saturated [12]. Modification factors that decrease faster than $1/t$ were found to lead to non-convergence [13]. These findings led to the formation of the $1/t$ -WL algorithm.

Liang independently considered whether WL could be treated as a special case of Stochastic Approximation whose convergence could be mathematically proven [14, 15]. In 2007, Liang et al. [15] argued that WL can be considered a form of Stochastic Approximation Monte Carlo (SAMC). Unlike WL, SAMC can guarantee convergence (if certain conditions are met). Despite the added benefit

of guaranteed convergence, the method still has a system specific user-defined variable. Such variables often create difficulty when applying Monte-Carlo methods across arbitrary systems.

Kim *et al.* introduced Statistical Temperature Monte Carlo (STMC) and the related Statistical Temperature Molecular Dynamics (STMD), an adaption of the WL method that approximates the entropy as a piecewise linear function, which improves convergence for systems with a continuously varying energy [16, 17]. STMC applied to WL requires a temperature range be specified rather than an energy range. Kim *et al.* extended this work as Replica Exchange Statistical Temperature Monte Carlo (RESTMC), which uses replica exchange of multiple overlapping STMC simulations to improve convergence [18]. Recently, Junghans *et al.* demonstrated a close connection between metadynamics, which was introduced by Laio and Parinello [19], and WL-based Monte Carlo methods, with STMD forging the connection [20].

The SAD (Stochastic Approximation with Dynamic γ) method outlined by Pommerenck et al. [21] is a special version of the SAMC algorithm that dynamically chooses the modification factor rather than relying on system dependent parameters. SAD shares the same convergence properties with SAMC while replacing un-physical user-defined parameters with the algorithm's dynamic choice.

In this work, we apply the family of weight-based flat histogram Monte Carlo methods (WL, $1/t$ -WL, SAMC, SAD) to the 2D Ising model.

II. ISING MODEL

The 2D Ising spin-lattice system is widely used as a testbed when benchmarking or comparing Monte-Carlo methods [22–24]. The 2nd order phase transition behavior and the ability to directly calculate the exact solution for finite lattices [25] make the system sufficiently interesting for such theoretical comparisons. It is also important to note that direct comparison of the other methods can be made with WL as its original implementation was done on this system [5, 6]. We test the convergence of several flat histogram methods on the periodic 2D square lattice ferromagnetic Ising model with nearest neighbor

interactions [26].

$$\mathcal{H} = - \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i s_i \quad (1)$$

The $N \times N$ spin system can take on values of $\sigma_i = \pm 1$ for up or down spins respectively. In the absence of a magnetic field ($h = 0$), We can write the Hamiltonian as follows [27, 28]:

$$\mathcal{H} = - \sum_{\langle i,j \rangle} \sigma_i \sigma_j \quad (2)$$

where the sum is over nearest neighbor spin sites. Beale showed that for finite lattices the Density of States could directly be calculated from the partition function [25]

$$Z = \sum_E g(E) e^{-\beta E} \quad (3)$$

where $g(E)$ is the multiplicity of the system which is proportional to $D(E)$. We can estimate the average deviation from the exact solution using the relation [29–31]:

$$\langle \epsilon(t) \rangle_E = \frac{1}{N_E - 1} \sum_E \left(\frac{S(E, t) - S_{\text{Beale}(E)}}{S_{\text{Beale}(E)}} \right) \quad (4)$$

As per the implementation by Wang and Landau [5], the total number of available energy states are $N - 1$.

III. FLAT HISTOGRAM METHODS

Flat histogram methods determine the density of states $D(E)$ over a broad range of energies by simulating each energy with equivalent accuracy. Flat histogram Monte Carlo methods propose randomly chosen “moves” which change the state of the system and must satisfy detailed balance. Each algorithm differs in how it determines the probability of accepting a move and in what additional statistics must be collected in order to decide on that probability.

We describe four closely related flat histogram methods which each rely on a weight function $w(E)$ to determine $D(E)$. For these algorithms, the probability of accepting a move is given by

$$\mathcal{P}(E_{\text{old}} \rightarrow E_{\text{new}}) = \min \left[1, \frac{w(E_{\text{old}})}{w(E_{\text{new}})} \right] \quad (5)$$

which biases the simulation in favor of energies with low weights. The result of weights $w(E)$ that are proportional to $D(E)$ is an entirely flat histogram. We can relate the entropy to the weights in the microcanonical ensemble, since the entropy is defined as $S(E) \equiv k_B \ln(D(E)) \approx \ln w(E)$.

Each approach uses a random walk in energy space to estimate $D(E)$. At the core of each of these approaches

is to continuously update the weights at each step of the simulation

$$\ln w_{t+1}(E) = \ln w_t(E) + \gamma_t \quad (6)$$

where t is number of the current move, $\gamma(t)$ is a move-dependent update factor, and E is the current energy. This update causes the random walk to avoid energies that have been frequently sampled, leading to a rapid exploration of energy space. The four methods differ primarily in how they schedule the decreasing of γ_t .

The Wang-Landau algorithm [5, 6, 32] explores energy space by initially setting $\gamma = 1$, and then decreases γ in discrete stages. An energy range of interest must be specified [6, 7, 33], which can require multiple simulations if unknown.

The number (“counts”) of moves ending at each energy are stored in a histogram. For a sufficiently flat energy histogram (specified by the user to typically be 0.8), γ is decreased by a specified factor of $\frac{1}{2}$ and the histogram is reset to zero. The entire process is repeated until γ reaches a desired cutoff.

Zhou et. al also showed that the WL algorithm never converges exponentially [34] and successfully bounded the statistical error between $t^{-\frac{1}{2}}$ and $1/t$ [34]. He also suggests that a modification factor of $1/t$ is optimal for WL.

The $1/t$ -WL method is a refinement of the original implementation that addresses the error saturation of WL. Belardinelli and Pereyra implemented a schedule [13] that enforced that if $\gamma < 1/t$ then the update factor is set to $1/t$ and the histogram is no longer tracked. Using this metric, the error saturation is avoided since the correct density of states is approached asymptotically as $t^{-\frac{1}{2}}$ [12]. Schneider et. al outline minor refinements to the $1/t$ -WL algorithm including N_S/t scaling and switching from standard WL to $1/t$ -WL when the update factor $\gamma < N_S/t$ [29]. As per the original $1/t$ implementation [13], the update factor is decreased once all N_S energy states are visited at least once (i.e. $H(E) \neq 0$) effectively avoiding the concept of ‘flatness’.

Another weight-based flat histogram method is the Stochastic Approximation Monte Carlo (SAMC) algorithm. SAMC has a simple schedule by which the update factor γ is continuously decreased [15, 29, 35]. The update factor is defined in the original implementation [15] in terms of an arbitrary tunable parameter t_0 ,

$$\gamma_t^{\text{SA}} = \frac{t_0}{\max(t_0, t)} \quad (7)$$

where as above t is the number of moves that have been attempted.

SAMC offers extreme simplicity and proven convergence. Provided the update factor satisfies

$$\sum_{t=1}^{\infty} \gamma_t = \infty \quad \text{and} \quad \sum_{t=1}^{\infty} \gamma_t^{\zeta} < \infty \quad (8)$$

where $\zeta \in \{1, 2\}$, Liang has shown that the weights are proven to converge to the true density of states [14, 15].

Unlike WL methods, the energy range need not be known *a priori*. The convergenc time depends only on the choice of parameter t_0 . The parameter t_0 can unfortunately be difficult to chose in advance for arbitrary systems. Liang *et al.* give a rule of thumb in which t_0 is chosen in the range from $2N_S$ to $100N_S$ where N_S is the number of energy bins [15]. Schneider *et al.* found that for the Ising model this heuristic is helpful for small spin systems, but that larger systems require an even higher t_0 value [29]. Our work also confirms this.

Pommerenck et al. propose a refinement [21] to SAMC where the update factor is determined dynamically rather than by the user. Stochastic Approximation with a dynamic γ (SAD) requires the user to provide the lowest temperature of interest T_{\min} . This is analogous to WL requiring a priori an energy range of interest; however, this may easier to identify and is more physical than the SAMC parameter t_0 . The update factor can be written in terms of the current estimates for the highest E_H and lowest E_L energies of interest and the last time that an energy in the range of interest is encountered t_L .

$$\gamma_t^{\text{SAD}} = \frac{\frac{E_H - E_L}{T_{\min}} + \frac{t}{t_L}}{\frac{E_H - E_L}{T_{\min}} + \frac{t}{N_S t_L}} \quad (9)$$

SAD only explores the energy range of interest as specified by the minimum temperature of interest $T_{\min} < T < \infty$. During the simulation the two energies E_H and E_L , are refined such that the range of energies are conservatively estimated. The weights are calculated for each energy region according to the original prescription.

1. $E < E_L$: $w(E > E_H) = w(E_H)$
2. $E_L < E < E_H$: moves are handled the same as other weight-based methods that are mentioned
3. $E > E_H$: $w(E < E_L) = w(E_L)e^{-\frac{E_L - E}{T_{\min}}}$

Each time the simulation changes the value of E_H or E_L , the weights within the new portion of the interesting energy range are updated.

IV. RESULTS

We tested the algorithms on two 2D Ising model systems. The first is a smaller simulation with a lattic size of 32 and the second has a lattice size of 128. For each system we use a reasonable root-mean-square displacement distance $\delta_0 = 0.05\sigma$ for proposed moves. The simulations explore the energy space of the systems with minimum reduced temperatures of $T_{\min} = 1$ for simulations. All simulations lead to the minimum important energy E_{\min} and maximum entropy energy E_{\max} being calculated (with the exception of the WL methods where both of these parameters are needed a priori).

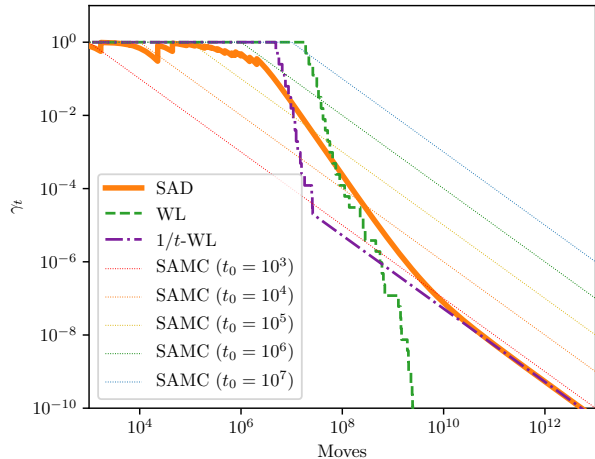


FIG. 1. The update factor γ_t versus the iteration number for the $N = 32 \times 32$ system.

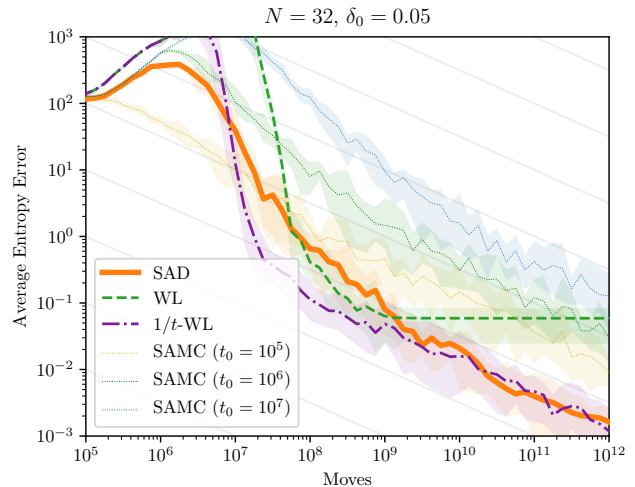


FIG. 2. The average entropy error for each MC method for $N = 32 \times 32$, $\delta_0 = 0.05\sigma$, and $T_{\min} = 1$ as a function of number of iterations run. The error is averaged over 8 independent simulations, and the best and worst simulations for each method are shown as a semi-transparent shaded area.

A. The 32×32 Ising model

For this simulation, we chose a minimum reduced temperature of 1, which corresponds to an interesting energy range from -2048 to 48 . The number of important energy states for this system is $N_S = 529$.

Fig. 2 shows the average error in the entropy as a function of time for this system with the displacement distance of $\delta_0 = 0.05$. The solid/dashed lines represent the average of the absolute value of the error in the entropy averaged over eight simulations using different random number seeds. The range of average errors for each sim-

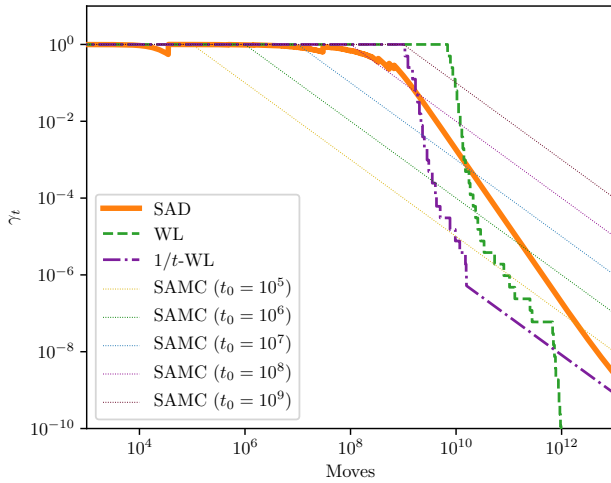


FIG. 3. The update factor γ_t versus the iteration number for the $N = 128 \times 128$ system.

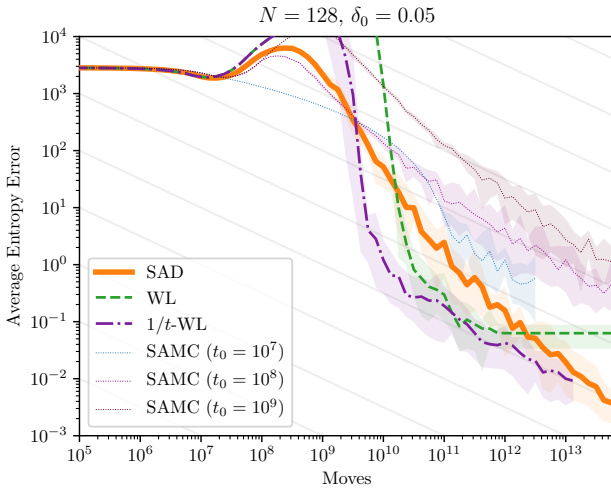


FIG. 4. The average entropy error for each MC method for $N = 128 \times 128$, $\delta_0 = 0.05\sigma$, and $T_{\min} = 1$ as a function of number of iterations run. The error is averaged over 8 independent simulations, and the best and worst simulations for each method are shown as a semi-transparent shaded ar.

ulation is shown as a shaded region around its mean error. By the time 10^8 moves have been made all but the WL simulation have begun to converge as $1/\sqrt{t}$. We then see the WL error saturate around 10^9 moves.

B. 128×128 Ising system

For this simulation, we chose a minimum reduced temperature of 1, which corresponds to an interesting energy range from -32768 to 100 . The number of important energy states for this system is $N_S = 8214$. Fig. 4 shows the average error in the entropy as a function of time for this system with the displacement distance of $\delta_0 = 0.05$. The solid/dashed lines represent the average of the absolute value of the error in the entropy averaged over eight simulations using different random number seeds. The range of average errors for each simulation is shown as a shaded region around its mean error. By the time 10^{12} moves have been made all but the WL and SAD simulations have begun to converge as $1/\sqrt{t}$. We then see the WL error saturate around 10^{12} moves. The error in the SAD method will continue to converge faster than $1/\sqrt{t}$ until the update factor approaches that of $1/t$ -WL at which point both methods will converge equivalently.

V. CONCLUSION

We have examined the convergence of SAD versus other widely used weight-based histogram methods. We have shown that Sad samples the energy space corresponding to a desired range of temperatures for a variety of system sizes. We find that both SAD and $1/t$ -WL demonstrate excellent and robust convergence. They both converge more rapidly than SAMC, and unlike WL do not suffer from error saturation. We find that for larger systems SAD reduces the updated factor more slowly (and conservatively) than $1/t$ -WL. This means that SAD will take proportionately more moves to converge to the same value as $1/t$ -WL as system size is increased. SAD requires the user to specify a temperature range of interest rather than an energy range of interest as $1/t$ -WL does. For use cases in which a range of desired temperatures is known, this will make the SAD method considerably more convenient.

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