

Intrinsic convergence properties of entropic sampling algorithms

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Abstract

We study the convergence of the density of states and thermodynamic properties in three flat-histogram simulation methods, the Wang-Landau (WL) algorithm, the $1/t$ algorithm, and tomographic sampling (TS). In the first case the refinement parameter f is rescaled ($f \rightarrow f/2$) each time the flat-histogram condition is satisfied, in the second $f \sim 1/t$ after a suitable initial phase, while in the third f is constant (t corresponds to Monte Carlo time). To examine the intrinsic convergence properties of these methods, free of any complications associated with a specific model, we study a featureless entropy landscape, such that for each allowed energy $E = 1, \dots, L$, there is exactly one state, that is, $g(E) = 1$ for all E . Convergence of sampling corresponds to $g(E, t) \rightarrow \text{const.}$ as $t \rightarrow \infty$, so that the standard deviation σ_g of g over energy values is a measure of the overall sampling error. Neither the WL algorithm nor TS converge: in both cases σ_g saturates at long times. In the $1/t$ algorithm, by contrast, σ_g decays $\propto 1/\sqrt{t}$. Modified TS and $1/t$ procedures, in which $f \propto 1/t^\alpha$, converge for α values between $0 < \alpha \leq 1$. There are two essential facets to convergence of flat-histogram methods: elimination of initial errors in $g(E)$, and correction of the sampling noise accumulated during the process. For a simple example, we demonstrate analytically, using a Langevin equation, that both kinds of errors can be eliminated, asymptotically, if $f \sim 1/t^\alpha$ with $0 < \alpha \leq 1$. Convergence is optimal for $\alpha = 1$. For $\alpha \leq 0$ the sampling noise never decays, while for $\alpha > 1$ the initial error is never completely eliminated.

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I. INTRODUCTION

The Wang-Landau (WL) algorithm is currently one of the most widely used Monte Carlo (MC) simulation methods [1–3]. Its effectiveness is based on its simplicity and versatility in estimating the density of states (DOS) $g(E)$ with high accuracy (here $g(E)$ represents the number of states or configurations with energy E , of a given physical system). Several recent studies propose improvements and sophisticated implementations of the WL algorithm [4–14]. A controversial point in the application of the WL and related methods is the saturation of the error, i.e., the difference between the simulation estimate for $g(E)$ and the exact values. In the WL algorithm the error approaches a constant value as the number of iterations tends to infinity, as first pointed out by Yan and de Pablo [15]. Several authors [5, 7, 8, 16–18] have studied the accuracy, efficiency and convergence of the WL algorithm. In particular, Zhou and Bhatt [5] presented an argument for its convergence, in apparent conflict with [15].

Numerical integration is an efficient test of convergence of MC methods [19], in part because successive points in the integration space are independent random variables. A definitive numerical demonstration of the non-convergence of the WL algorithm can be found in its application to numerical integration; the method generates a systematic error in the evaluation of integrals such as the evaluation of π [20].

The principal reason for saturation of the error in the original WL algorithm is that the refinement parameter f decreases exponentially with the number of iterations, so that in the final stages of sampling, the estimate for $g(E)$ is essentially constant. In Refs. [20–22] a modified version of the WL algorithm is introduced, in which, at long times, the refinement parameter f scales as $1/t$ instead of exponentially. This procedure, known as the $1/t$ algorithm, has been successfully applied to diverse systems [18, 23–32]. Zhou and Su [8] argued that the optimal behavior of the statistical error $w(t)$ follows $w \sim t^{-\alpha}$ with $1/2 \leq \alpha \leq 1$. Nevertheless, numerical studies show that the error in the $1/t$ algorithm decays as $\sqrt{1/t}$; to our knowledge it has not been improved upon.

Although both the WL and $1/t$ algorithms have been used to simulate many systems, several questions remain open. For instance, does the long-time scaling of the error

($w(t) \rightarrow w_\infty > 0$ in the WL algorithm, $w(t) \sim 1/t^{1/2}$ in the $1/t$ algorithm) represent an intrinsic property of the method, or does it depend on the physical characteristics of the problem under study? Although the $1/t$ algorithm owes its improved convergence to the use of a refinement factor $f \propto 1/t$ at long times, it has been found that the best way to implement this algorithm is to follow the WL prescription initially, and after some time switch to $f \propto 1/t$ [20, 21]. One may again ask whether this property is intrinsic to the algorithm, or if it depends on the system being simulated. The above questions motivate our application of the WL, $1/t$, and tomographic algorithms to a model density of states that is completely featureless: for each integer energy between 1 and L , there is one and only one state. We may then follow the convergence of the sampling in the simplest possible context, both numerically and analytically. The resulting rates of convergence are qualitatively similar to those observed in applications to physical models such as the Ising model, which possess a nontrivial density of states, thereby suggesting that the convergence properties are intrinsic to the sampling methods, in particular, to how $f(t)$ is reduced at long times. Tomographic sampling was originally implemented using, in effect, a refinement parameter f that does not change with time [14]. Here we show that convergence is improved if we instead use $f \sim 1/t$ in this method as well.

The remainder of this paper is organized as follows: In Section II, after defining the sampling procedures, the results are reported and discussed. A simple stochastic model of the sampling process is analyzed in Sec. III. We present our conclusions in Section IV.

II. SAMPLING PROCEDURES

Entropic sampling MC methods, such as the WL, $1/t$ and tomographic algorithms, typically employ a histogram $H(E)$ to refine an estimate for the entropy. Here $H(E)$ represents the number of visits to energy E during a certain iteration of the process. In these methods one also defines a dimensionless entropy $S(E) \equiv \ln g(E)$, where $g(E)$ is an estimate for the number of configurations with energy E . The goal of entropic sampling algorithms is to obtain precise estimates for $g(E)$ via Metropolis

MC sampling, using the acceptance probability $\min\{1, g(E_j)/g(E_i)\}$, where E_i and E_j denote the energies before and after a proposed transition, respectively. Since the $g(E)$ are of course unknown *a priori*, the acceptance probability is evaluated using the current estimates for the $g(E)$. As is usual in Metropolis sampling, when a trial configuration is rejected, the existing configuration is counted once again in the sequence.

In studies of entropic sampling, a recurrent question is whether convergence is limited by the specific properties of the model (such as large entropy barriers), or by the method itself, due to sampling noise. In the present study we eliminate the former possibility by studying a system with a trivial, featureless entropy: by definition, $g(E) = 1$ for each energy $E \in \{1, \dots, L\}$. We ask to what precision the sampling methods are able to recover this result. Since a perfect entropic sampling procedure would yield $S(E) = \text{Const.}$, the standard deviation of $S(E)$ represents the global sampling error. We define

$$w(t) = \sqrt{\frac{1}{L} \sum_{E=1}^L [S(E, t) - \langle S(t) \rangle]^2}, \quad (1)$$

where $\langle S(t) \rangle$ is the mean of S over all states at time t . We are interested in how the global error $w(t)$ scales asymptotically with time.

It is convenient to define Monte Carlo time as $t = n/L$, where n is the number of attempted changes of state, or *steps*. We also define the jump length, λ , as the maximum distance accessible at each step. Thus $\lambda = 1$ means that the energy E_n at step n can only differ by ± 1 from E_{n-1} , (under periodic boundaries), whereas $\lambda = L/2$ means that all energies are accessible at each step. In the former case, an attempt to visit site n means that the previously visited site was $n \pm 1$, so that the acceptance probability involves a comparison of $g(E)$ at a pair of neighboring states; in the latter case, the previously visited site can be any site in the system, with equal probability. Thus for $\lambda = 1$, visits to states E with $g(E)$ greater than their nearest neighbors are suppressed. This corresponds to local relaxation, since g will instead increase at one of the neighbors. For $\lambda = L/2$ by contrast, relaxation is global, with visiting suppressed (favored) at states with higher (lower) than average values of $g(E)$.

We now define the sampling procedures in detail. The WL algorithm is as follows:

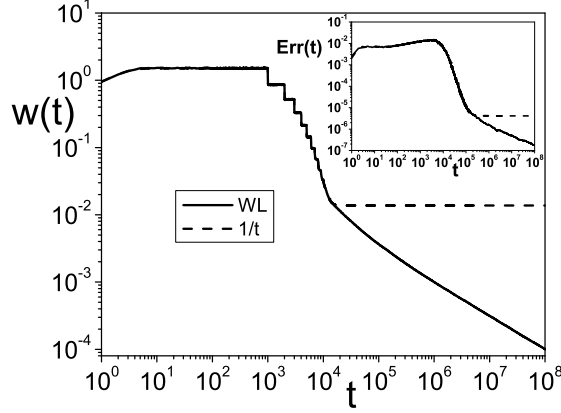


FIG. 1: Global error for the uniform energy landscape. The inset shows the error in the calculation of π using two-dimensional integration (see Ref. [20]). Data represent averages over 100 independent realizations.

i) Initially, $S(j, 0) = H(j) = 0, \forall j \in \{1, \dots, L\}$. The initial refinement parameter is $f(0) = 1$. We define a global stopping criterion of $f_{stop} = 10^{-8}$: sampling halts when $f(t) \leq f_{stop}$.

ii) A state i is chosen at random.

iii) A state j is also chosen at random between among the 2λ states nearest i , that is, from $\{i \pm 1, \dots, i \pm \lambda\}$.

iv) Let $p = \min\{1, e^{-\Delta S}\}$, where $\Delta S = S(j, t) - S(i, t)$. A random number, ξ , uniformly distributed on $[0, 1]$, is generated. If $\xi < p$, then the variables associated with state j are updated so: $S(j) = S(j) + f(t)$, $H(j) = H(j) + 1$, and the current state changes ($i \rightarrow j$); otherwise, $S(i, t) = S(i, t) + f(t)$ and $H(i) = H(i) + 1$.

v) After a fixed number of events (i.e., an MC time increment of 1000), the flatness of the histogram H is tested; if H is flat*, the histogram is reset ($H(j) \rightarrow 0, \forall j \in \{1, \dots, L\}$) [33], and the refinement parameter is reduced so: $f \rightarrow f/2$.

vi) If $f(t) < f_{stop}$, the process stops, otherwise, a new iteration begins at item iii).

The $1/t$ algorithm [20] follows steps i) - v) of the above scheme, but step vi) is replaced with:

vi) If $f \leq 1/t$ then $f \rightarrow 1/t$; thereafter, $f(t) = 1/t$ is updated at each event, and step (vi) is not used for the remainder of the study.

vii) If $f(t) < f_{stop}$, the process stops, otherwise, a new iteration begins at item iii).

For $\lambda = L/2$, these algorithms are similar to well known algorithms used in numerical evaluation of multiple integrals [19, 20].

The global error, $w(t)$, found in the WL and $1/t$ procedures, is shown in Fig. 1, for $L = 256$. The inset shows the errors corresponding to the WL and $1/t$ algorithms in the calculation of π , using two-dimensional integration (see Ref.[20]). (The latter calculation uses $I_\pi = 4 \int_0^1 \sqrt{1-x^2} dx \approx 4 \sum_{i=0}^L g(y_i)y_i$ for x and y in the first quadrant. The system size is $L = 256$ and $dy = 1/L$.) The time dependence of the global error is very similar in the two cases, suggesting that the convergence exhibits general features. We can distinguish three stages in the evolution: i) a short-time regime, from the beginning to the first plateau; ii) an intermediate regime, in which $w(t)$ diminishes $\propto \sqrt{f(t)}$ in both algorithms [5]; and iii) in the WL case, a long-time regime, in which $w(t)$ saturates. Regime (iii) is not observed using the $1/t$ algorithm.

The general features of convergence identified above also appear in simulations of the two-dimensional Ising model, when we compare the simulation estimates for $S(E)$ with the exact result for $L = 16$ [34] (see Fig. 2). This adds further support to the idea that the general convergence properties of entropic sampling algorithms are model-independent.

We also examine the error in a modified $1/t$ algorithm using $f(t) = t^{-\alpha}$ at long times. In Fig. 3 we plot $w(t)$ for $\alpha = 0.8, 1$ and 1.2 ; for $\alpha \leq 1$, $w(t) \propto \sqrt{f(t)}$, whereas for $\alpha > 1$, the global error saturates at long times. Convergence appears to be optimal for $\alpha = 1$.

As noted above, the $1/t$ algorithm is implemented using $f \rightarrow f/2$ (i.e., the WL rescaling) at each iteration, *until* $f \leq 1/t$, at which point one switches to $f = 1/t$. Numerical studies show that if we take $f(t) = 1/t$ from the very beginning (the “pure” $1/t$ algorithm), convergence is slower, and the error may saturate in some cases. It is nevertheless of interest to know if this is a general property of the $1/t$ algorithm, or if it depends on the manner in which states are sampled. The global error $w(t)$ is plotted as a function of time, for several values of λ , in Fig. 4; the full lines correspond to the

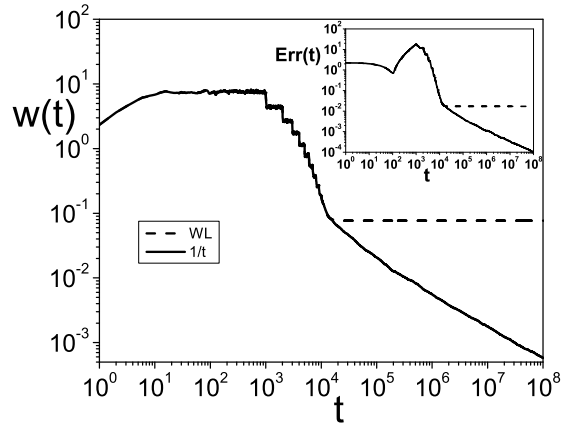


FIG. 2: Global error for $\lambda = 2$. Inset: error in the WL and $1/t$ algorithms for the 2D Ising model (see Ref.[21]). Data are the averages over 100 independent realizations.

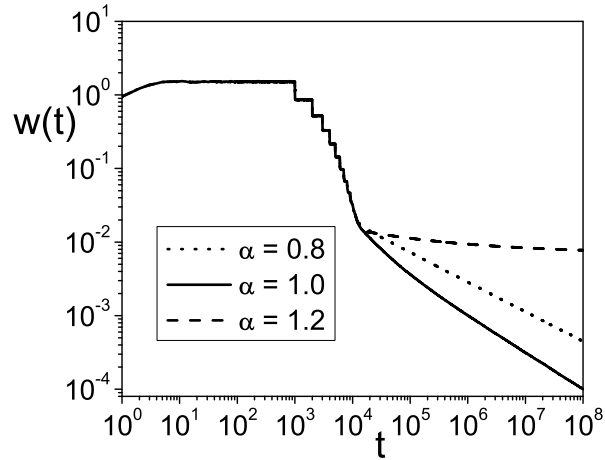


FIG. 3: Global error $w(t)$ for $f(t) = t^{-\alpha}$, with $\alpha = 0.8, 1.0$, and 1.2 . The data represent averages over 100 independent realizations.

(standard) hybrid $1/t$ algorithm (i.e., initially following the WL prescription), while the dashed lines represent the pure $1/t$ algorithm [$f(t) = 1/t$ for all times $t \geq 1$]. Figure 4a shows results for $\lambda = L/2$, that is, complete independence between subsequent pairs of states i and j (global relaxation). In this case the error decays more rapidly in the pure $1/t$ algorithm than in the hybrid algorithm. When the new state j is restricted to

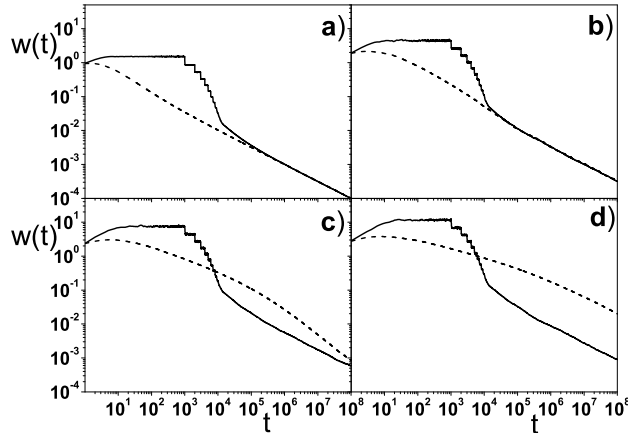


FIG. 4: Global error $w(t)$ versus time for a) $\lambda = L/2$; b) $\lambda = 4$; c) $\lambda = 2$; d) $\lambda = 1$, with $L = 256$. Dashed lines: pure $1/t$ algorithm; solid lines: modified algorithm. The data represent averages over 100 independent realizations.

the neighborhood of i (local relaxation), however, the hybrid algorithm converges more rapidly, as seen in Figs. 4b-4d, which correspond to $\lambda = 4, 2$ and 1 , respectively. The difference in convergence rates between the pure and modified $1/t$ algorithms, in the local and global relaxation cases, likely reflects the fact that the modified algorithm employs a flatness criterion, albeit only in the initial phase of sampling. This criterion has the effect of suppressing long-wavelength sampling fluctuations, which arise more readily under local as opposed to global relaxation. We note that faster convergence of the hybrid $1/t$ algorithm is also found in studies of the two-dimensional Ising model, and in the numerical evaluation of π .

We turn now to a related entropic simulation method, tomographic sampling [14]. Here configurations are sampled using the acceptance probability p of item iv) above during each iteration. An iteration consists of N_i studies beginning from different initial configurations, with each study employing a large (but fixed) number N_s , of MC steps. At the end of each iteration, the estimate for $g(E)$ is updated using $g(E, n) = [H(E)/\overline{H}]g(E, n-1)$, where the second argument of g denotes the iteration. (\overline{H} is the average of the histogram $H(E)$ over all energies visited; $1/\overline{H}$ is used as a convenient normalization factor.) We applied this procedure to the problem defined above, using

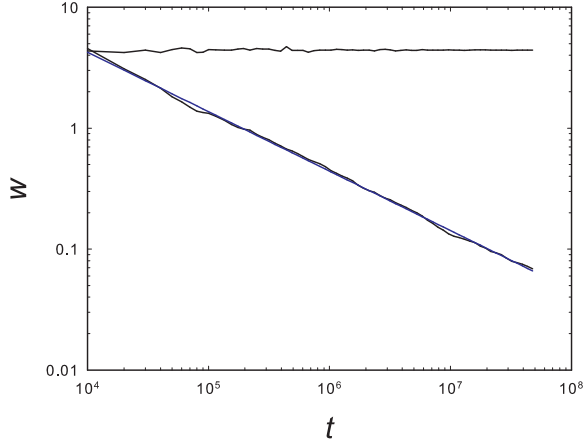


FIG. 5: (Color online) Global error w versus sampling time t for tomographic sampling using $\alpha = 0$ (upper line) and $\alpha = 1$ (lower). The straight line fit to the data for $\alpha = 1$ has slope -0.49 . Data represent averages over 50 independent realizations of the procedure.

5000 iterations, each using ten initial states, uniformly spaced over a ring of $L = 256$ sites; for each initial configuration we generate a random walk of $1000 L$ steps in state space. Initially $g(E) = 1$, $\forall E \in \{1, \dots, L\}$. Following each update of the $g(E)$ we calculate the standard deviation, w , of g over the L states. Figure 5 shows that for the procedure described above, which corresponds to $\alpha = 0$, the error $w(t)$ is essentially constant. Modifying the procedure so that at the n -th iteration, $g(E, n) = [H(E)/\overline{H}]^{1/n} g(E, n)$ (corresponding to $\alpha = 1$), we observe convergence, again with $w(t) \sim t^{-1/2}$. (Time is measured in units of lattice updates, so that each iteration corresponds to a time increment of 10^4 .)

A. Convergence of thermodynamic properties in tomographic sampling

While the preceding discussion concerns a rather idealized situation in which the number of configurations is the same for each energy, the scaling of the refinement

factor also affects the convergence of tomographic sampling in practical applications. In this method, as noted above, the estimate for $g(E)$ is updated at each iteration, with an iteration consisting of a set of studies using a large number of updates, starting from diverse initial configurations that span the range of energies. In [14] the method was applied to the Ising model in two and three dimensions, yielding good results for critical exponents. The studies used a series of five iterations, each involving 10^7 lattice updates for each of ten initial configurations, with the estimate for $g(E)$ updated using the same factor following each iteration, corresponding to the case $\alpha = 0$ discussed above.

Here we examine the quality of the results, as characterized by the statistical uncertainty of the estimates over a set of twenty independent runs, each consisting of five iterations as described above, in tomographic sampling of the Ising model on a square lattice of size $L = 20$. The quantities analyzed are two estimates for the critical temperature, T_C and T_χ (the temperatures at which the specific heat and the magnetic susceptibility take their maximum values, respectively), and the maximum values, C_{max} and χ_{max} , of the specific heat and susceptibility. Using $\alpha = 0$ the relative uncertainties in T_C and T_χ are both 4×10^{-5} , while for $\alpha = 1$ they fall to 2×10^{-5} . Similarly, the relative uncertainties in the maximum values are $\sim 3 \times 10^{-4}$ for $\alpha = 0$, compared with 2×10^{-4} for $\alpha = 1$. Interestingly, essentially the same reduction in uncertainties is found using $\alpha = 1/2$. Further studies using ten iterations reveal that, for the values of α considered here, there are no significant changes in the mean values or associated uncertainties after the fourth or fifth iteration. Although this may seem surprising given the results for the featureless entropy landscape reported above, which show faster convergence for $\alpha = 1$, and continued reduction of statistical errors with increasing numbers of iterations, it should be recalled that the distribution of configurations in the Ising model is considerably more complex than that of the uniform landscape, as is the question of the connectivity of the configuration space via single spin flip moves, as used here and in [14].

Tomographic sampling (with $\alpha = 0$) was applied to the two-dimensional Ising anti-ferromagnet in an external magnetic field in [35]. In this case, the sampling is bivariate, i.e., we estimate the number of configurations with given energy *and* magnetization; bi-

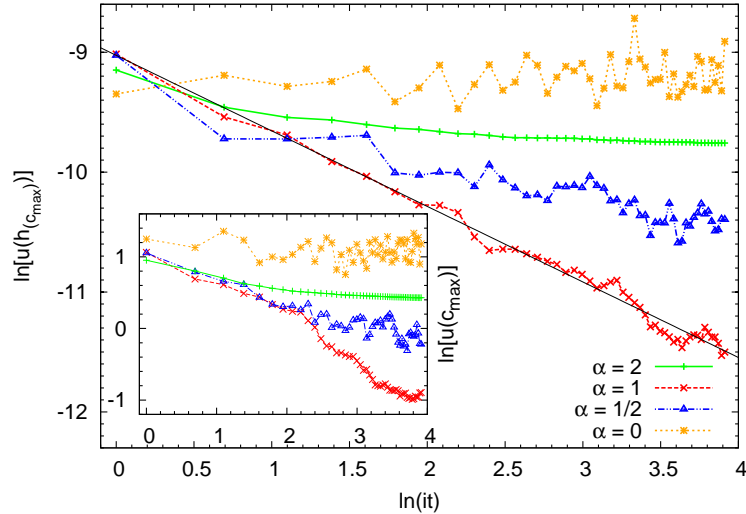


FIG. 6: Antiferromagnetic Ising model in two dimensions: variance of the tomographic sampling estimate for the external field h associated with maximum specific heat versus iteration number, for parameters as specified in text. The slope of the straight line is -0.63 . Inset: variance of estimate for the maximum specific heat.

variate sampling presents a greater challenge for entropic methods than single variable sampling. Here, we compare results using $\alpha = 0, 1/2, 1,$ and 2 . In Fig. 6, for system size $L = 20$, the variance of tomographic sampling estimates for the external field h maximizing the specific heat (at fixed temperature $T = 0.2$), is plotted versus iteration number. (Each iteration consists of 10 studies starting from different initial conditions, with each study comprising 10^7 lattice updates; the variance is calculated over a sample of 30 independent realizations.) It is again evident that the variance saturates for $\alpha = 0$, and $\alpha = 2$, and decays most rapidly (roughly $\propto t^{-0.63}$) for $\alpha = 1$. The inset shows that the maximum specific heat behaves in an analogous manner. In this study, employing a sequence of 50 iterations, using $\alpha = 1$ instead of $\alpha = 0$ reduces the final uncertainty by an order of magnitude. Despite this significant improvement, we note that uncertainties in the field value that maximizes the *antiferromagnetic susceptibility* χ are essentially independent of α . This may be because, different from the specific heat, calculating χ requires using “microcanonical” (fixed energy and magnetization) averages of the antiferromagnetic order parameter and its second moment.

III. CONVERGENCE: ANALYSIS OF A SIMPLE MODEL

In this section we analyze convergence in a highly simplified example which nevertheless appears to capture the essential features of entropic sampling. The system consists of two energy levels, each having a single state. Let $g(1, n)$ and $g(2, n)$ denote the estimates for the numbers of states at the n -th iteration of the sampling process, so that convergence corresponds to $|g(1, n) - g(2, n)| \rightarrow 0$ as $n \rightarrow \infty$. At each iteration we generate a set of N independent binary random variables $\sigma_j \in \{1, 2\}$, such that $\text{Prob}[\sigma_j = 1] = p(n)$ and $\text{Prob}[\sigma_j = 2] = q(n) = 1 - p(n)$. The number $H(n)$ of 1s in the set $\{\sigma_1, \dots, \sigma_N\}$ follows the binomial distribution,

$$\text{Prob}[H(n) = m] = \binom{N}{m} [p(n)]^m [q(n)]^{N-m} \quad (2)$$

For $N \gg 1$, $H(n)$ is well approximated by a Gaussian random variable with mean $Np(n)$ and variance $Np(n)q(n)$, so that $h(n) \equiv H(n)/\overline{H} = 2H(n)/N \simeq 2p(n) + \xi(n)$, where $\xi(n)$ is a Gaussian random variable with mean zero and variance $4p(n)q(n)/N \equiv \Gamma(n)$.

In entropic simulations one wishes to sample the probability distribution $P(\mathcal{C}) = 1/g[E(\mathcal{C})]$, where $g(E)$ is the number of configurations with energy E , and $E(\mathcal{C})$ is the energy of configuration \mathcal{C} . Using the current estimate for the number of configurations, we therefore take

$$p(n) = \frac{g(2, n-1)}{g(1, n-1) + g(2, n-1)}. \quad (3)$$

At each iteration $n \geq 1$ we generate revised estimates of $g(1)$ and $g(2)$ via:

$$g(1, n) = h(n)^{1/n^\alpha} g(1, n-1) \quad \text{and} \quad g(2, n) = [2 - h(n)]^{1/n^\alpha} g(2, n-1) \quad (4)$$

Suppose $g(1, n) < g(2, n)$. Then at the next iteration, $p > 1/2$, tending to equalize $g(1, n+1)$ and $g(2, n+1)$. This procedure tends, on average, to reduce $|g(1) - g(2)|$. In a given realization of the process, however, the sampling noise $\xi(n)$ creates a fresh imbalance at each iteration, which must then be corrected at subsequent iterations for the process to converge.

To examine the asymptotic convergence, suppose that at step n_0 , after various iterations, the difference $|g(1, n_0) - g(2, n_0)| \ll 1$. Let $g(1, n_0) = 1 + u(n_0)$ and $g(2, n_0) = 1 - u(n_0)$, so that $p(n_0 + 1) = 1 - u(n_0)/2$. At the next iteration we have

$$g(1, n_0 + 1) \equiv 1 + u(n_0 + 1) = [1 - u(n_0) + \xi(n_0)]^{1/n_0} [1 + u(n_0)] \quad (5)$$

Then to first order in the small quantities $\xi(n_0)$ and $u(n_0)$ we have

$$u(n_0 + 1) - u(n_0) = -\frac{u(n_0)}{n_0} + \frac{\xi(n_0)}{n_0} \quad (6)$$

Associating a time interval dt with each iteration, and taking a continuous-time limit, $u(n) \rightarrow u(t)$, we obtain a Langevin equation

$$\frac{du}{dt} = -\frac{u}{t} + \frac{\xi(t)}{t}, \quad (7)$$

for $t > t_0$. Here $\xi(t)$ is a white noise with intensity $\Gamma = 1/N$. Thus we have a linear Langevin equation in which both the force $-u$ and the noise are scaled by $t^{-\alpha}$. There are four cases of interest.

I. $\alpha = 0$. In this case Eq. (7) is just the Langevin equation for the velocity of a Brownian particle in one dimension. Under the deterministic evolution ($\xi = 0$), u decays to zero exponentially, but due to the noise we have $\text{var}[u] \rightarrow \Gamma/2$ as $t \rightarrow \infty$, and there is no convergence.

II. $0 < \alpha < 1$. Without noise, the error decays as a stretched exponential, $u(t) \propto \exp[-t^{1-\alpha}/(1-\alpha)]$. The noise causes the variance of u to follow,

$$\text{var}[u(t)] = \Gamma \exp[-(\frac{2}{1-\alpha}) t^{1-\alpha}] \int_{t_0}^t \exp[(\frac{2}{1-\alpha}) s^{1-\alpha}] \frac{ds}{s^{2\alpha}} \quad (8)$$

Denoting the integral by $I(t)$ and integrating by parts we have,

$$I(t) = \frac{1}{2s^\alpha} \exp[(\frac{2}{1-\alpha}) s^{1-\alpha}] \Big|_{t_0}^t + \frac{\alpha}{2} \int_{t_0}^t \exp[(\frac{2}{1-\alpha}) s^{1-\alpha}] \frac{ds}{s^{1+\alpha}} \quad (9)$$

The integrated part grows asymptotically as $\frac{1}{2t^\alpha} \exp[(\frac{2}{1-\alpha})t^{1-\alpha}] \equiv F(t)$, whereas the integral in the second term in Eq. (9) is smaller than $I(t)$, since $\alpha < 1$. Thus, as $t \rightarrow \infty$, we have $F(t) \leq I(t) \leq \frac{2}{2-\alpha}F(t)$, so that $\text{var}[u(t)] \sim 1/t^\alpha$, and the rms error of the result decays as $1/t^{\alpha/2}$.

III. $\alpha = 1$. Without noise, $u(t)$ decays algebraically, $u \sim 1/t$. Including the noise, $\text{var}[u] \sim 1/t$, and the rms error decays as $1/t^{1/2}$.

IV. $\alpha > 1$. The solution to the noise-free equation is $u = \exp[\frac{1}{(\alpha-1)t^{\alpha-1}}]$, so that even deterministically, there is no convergence. The variance is

$$\text{var}[u(t)] = \Gamma \exp[\frac{2}{(\alpha-1)t^{\alpha-1}}] \int_{t_0}^t \exp[-\frac{2}{(\alpha-1)s^{\alpha-1}}] \frac{ds}{s^{2\alpha}}. \quad (10)$$

Calling the integral $I'(t)$, it is easy to show that,

$$I'(t) \geq \frac{\exp\left[-\frac{2}{(\alpha-1)t_0^{\alpha-1}}\right]}{2\alpha-1} \left(\frac{1}{t_0^{2\alpha-1}} - \frac{1}{t^{2\alpha-1}} \right) \quad (11)$$

which implies that $\text{var}[u(t)]$ remains nonzero as $t \rightarrow \infty$.

Summarizing, there is convergence only in cases II and III, that is, for $0 < \alpha \leq 1$, leading to $\text{var}[u(t)] \sim t^{-\alpha/2}$. Increasing α within this interval, the noise-induced error decays more rapidly, but the deterministic convergence is slower. The WL algorithm corresponds, in this example, to Eq. (7) with the factor $1/t^\alpha$ replaced by one which decays exponentially, and so, as in case IV above, there is no convergence.

The foregoing analysis is readily generalized to a set of L states, each represented by a single configuration. Assuming that the random walk over configuration space is able to sample all states uniformly, the decay of each deviation $u(k) = g(k) - 1$ follows, in the linearized analysis, a Langevin equation (7), but with noise intensity $\Gamma = L^2/N$.

As a further generalization, suppose there are two classes containing different numbers of configurations, r_1 and r_2 . The target values are $g(i) = 2r_i/M \equiv \bar{g}(i)$, where $M = r_1 + r_2$ and we have maintained the normalization $g(1) + g(2) = 2$. Suppose, as before, that after a number n_0 of iterations, the estimates are close to the target values, so that $g(i, n_0) = \bar{g}(i) + u(i, n_0)$ with $|u(i, n_0)| \ll 1$. Repeating the linear analysis used

above, we verify that the $u(i)$ satisfy Eq. (7) with noise intensity $\bar{g}(i)^2/N$. The asymptotic convergence properties are therefore as found above for the case $r_1 = r_2 = 1$.

IV. CONCLUSIONS

We study convergence properties of flat histogram entropic sampling methods, specifically the Wang-Landau and $1/t$ algorithms, and tomographic sampling. There appear to be two difficulties to achieving precise results in entropic sampling. The first is associated with visiting the entire configuration space uniformly. For small systems this poses no problem, but it rapidly becomes more difficult, demanding ever longer simulation times, as the system size increases. The second difficulty, which is the main focus of present work, concerns eliminating the effects of initial errors, and, crucially, sampling noise accumulated over the iterations. Numerical studies of a model with a flat entropy landscape yield the conclusion that asymptotically, the error decays most rapidly in the $1/t$ -algorithm, with the global error decaying $\propto 1/t^{1/2}$. A modified tomographic sampling scheme, in which corrections to the estimates for the number of states $g(E)$ are weighed $\propto 1/t$, yields a similar convergence. We present evidence that this behavior is general, independent of the physical model under study. The convergence of microcanonical averages, however, remains as a topic for future study.

An important conclusion is that the error converges to a nonzero value after a certain number of iterations in the WL algorithm, and does not decrease in subsequent iterations. This point, which was noted in [18], can be understood on the basis of a simple stochastic model, which also explains the observed convergence behaviors of the error in $1/t^\alpha$ schemes.

Our results would appear to conflict with those of [5], which reports convergence of the WL algorithm. They can be reconciled by observing that the latter work demonstrates convergence as the sample size $N \rightarrow \infty$, whereas here we consider iterations with a fixed, finite N , and analyze how the dependence of the refinement factor $f(t)$ on the time or iteration number t affects convergence as $t \rightarrow \infty$.

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