Wang-Landau algorithm for continuous models and joint density of states

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We present modified Wang-Landau algorithm for models with continuous degrees of freedom. We demonstrate this algorithm with the calculation of the joint density of states \( g(M, E) \) of ferromagnet Heisenberg models. The joint density of states contains more information than the density of states of a single variable–energy, but is also much more time-consuming to calculate. We discuss the strategies to perform this calculation efficiently for models with several thousand degrees of freedom, much larger than other continuous models studied previously with the Wang-Landau algorithm.

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The Wang-Landau (WL) algorithm has been applied to a broad spectrum of interesting problems, including statistical physics models such as Ising and Potts models, spin glasses, and stochastic series expansion of quantum systems, as well as models in other areas such as complex fluids and protein molecules. These applications have been successful due to two features of this algorithm. First, the random walker of the WL algorithm is not trapped by local energy minima, which is very important for systems with complex energy landscapes. Secondly, by calculating the density of states, thermodynamic observables in a wide range of temperature, including the free energy, can be calculated with one single simulation. The efficiency of the WL algorithm has been quantitatively studied, and improvements have been proposed by several authors, which have made the WL algorithm a standard tool for discrete models. However, in some areas such as biophysics, most models have continuous degrees of freedom; and naturally, the density of states of two or more variables, in contrast to the energy alone, is of much interest. Efficient algorithms for those problems are called for.

In this letter, we discuss two generalizations of the WL algorithm: (1) physical models with continuous degrees of freedom (referred to as off-lattice models in Ref. 5), and (2) density of states of more than one variable, which we refer to as joint density of states. The joint density of states is more useful than the density of states. For example, the free energy as a function of both temperature and magnetic field can be calculated from \( g(M, E) \), the joint density of states of both energy and magnetization. For the protein system studied in Ref. 6, with \( g(\xi, E) \), where \( \xi \) is the reaction coordinate, the free energy for each \( \xi \) calculated with the EXEDOS algorithm can be obtained by integrating \( g(\xi, E)e^{-E/T} \) over \( E \). The calculation of joint density of states of continuous models clearly covers many interesting problems.

However, these generalizations are not straightforward, and there are certain intrinsic difficulties which frustrate the implementation of the simple version of the WL algorithm. First, the density of states \( g(E) \) of a continuous model goes to zero at its maximum and minimum energies, which become logarithmic singularities as the WL algorithm evaluates \( \ln g(E) \). In fact, \( \ln g(M, E) \) is usually singular on its boundary. Secondly, suppose we calculate the joint density of a 32×32 Ising model on a square lattice, which was used as a test problem by Wang and Landau. If every value of the magnetization is counted, the joint density of states \( g(M, E) \) of both energy and magnetization will cost about \( 10^3 \) times the CPU time of \( g(E) \), because \( g(M, E) \) contains about \( 10^6 \) integers. Hence such calculations have been restricted to systems of small sizes. One might use a binning scheme to deal with this problem, and may also hope that binning (discretization) provides a generalization of the WL algorithm to systems with continuous degrees of freedom. However, a simple binning scheme becomes either very costly or inaccurate even for relatively small systems. Shell et. al. used interpolation among bins to handle this difficulty. We have identified the origin of the inefficiency of the binning scheme and propose a better solution to this problem.

![FIG. 1: (a) \( \ln g(M, E) \) of a three-dimensional Heisenberg ferromagnet of size \( L = 10 \) with cutoff energy at -2.8, determined up to an additive constant. (b) The magnetization at different temperature and external field evaluated from \( g(M, E) \).](image)
We first show the result of our calculation for a three-dimensional Heisenberg ferromagnet in Fig. 1. The Hamiltonian of this model is $H = -\sum_{i<j} S_i \cdot S_j$, where the summation goes over nearest neighbors on a cubic lattice of size $L$ with periodic boundary conditions. This model has a ferromagnetic phase transition and displays global spin rotational symmetry. Here we define $E = H/L^3$ and $M = L^{-3} \sum_i S_i^z$, and $g(M, E)$ is the joint density of states of $M$ and $E$. Figure 1(a) shows $\ln g(M, E)$ for negative $E$. A region with $\partial \ln g/\partial M = 0$ below $E = -1.2$ indicates a transition to the ferromagnetic phase with a global rotational symmetry. The logarithmic divergence in $w(M, E)$ near the ground state is obvious. In the following, we use the Heisenberg ferromagnet as a prototype model to identify several features and intrinsic difficulties of continuous models.

In general, the model we study has many microscopic degrees of freedom $s = (s_1, \ldots, s_N)$, which labels the microscopic states in the phase space $\Omega$. The Hamiltonian $H(s)$ is a real-valued function of the microscopic degrees of freedom, so is the order parameter, e.g. magnetization $M(s) = N^{-1} \sum_i S_i^z$ for the Heisenberg ferromagnet. The joint density of states is defined as

$$g(M, E) = |\Omega|^{-1} \int \Pi_i ds_i \delta(E - H(s))\delta(M - M(s)), \quad (1)$$

where $|\Omega|$ is the volume of the phase space, and the integral is replaced by a summation for discrete models. We refer to a pair $(M, E)$ as a macroscopic state, and define the macroscopic phase space $\Lambda = \{ (M, E) \mid \exists s, H(s) = E, M(s) = M \}$. Obviously $g(M, E) \geq 0$ is a probability measure of $\Lambda$ induced by a priori probability measure of $\Omega$. Usually this measure is almost a $\delta$-function in $\Lambda$, dominated by overwhelmingly many states in the high temperature limit. Due to the Boltzman distribution, for finite temperature properties, we are mostly interested in the very small values of $g(M, E)$. In the following, we denote $(M, E)$ collectively with $x$. (In case of $g(E)$, the macroscopic state $x$ is specified by the energy alone.) If one tries to evaluate $g(x)$ by sampling $\Omega$ uniformly, then there is virtually no chance to sample a finite temperature macroscopic state. The WL algorithm learns $g(x)$ in the runtime with a simple strategy. In a sentence, when a trial move $x_i \rightarrow x_f$ is suggested, it is accepted with probability $A_{i\rightarrow f} = \min\{1, \exp[w(x_i) - w(x_f)]\}$, where $w(x)$ is an approximation to $\ln g(x)$, and if the move is accepted $w(x_f)$ is updated with $\gamma + w(x_f)$ otherwise $w(x_i)$ is updated with $\gamma + w(x_i)$, where $\gamma = \ln f$, and $f$ is referred to as the modification factor. Previous studies [11,13] showed that for a discrete set of $x$, $w(x)$ quickly converges to $\ln g(x)$ within some statistical error proportional to $\sqrt{\gamma}$ for $\gamma \rightarrow 0$. For a continuous system, one simply cannot update $g(x)$ point by point. Some modification of the update scheme is required along with a method to represent the continuous function $w(x)$ in the computer memory.

The simple binning scheme approximates $g(x)$ with a piece-wise constant function, which has discontinuities on the boundary of the bins. This scheme works if $g(x)$ varies very slowly in each bin, otherwise as the trial moves within each bin is not biased, the maximum point of $g(x)$ in each bin is much more likely to be sampled than other points, which actually violates the spirit of the WL algorithm——to sample every macroscopic state uniformly. Reducing the size of the bins could overcome this difficulty for small systems, but generally for the joint density of states this would result in an excessively large number of bins to sample. Bilinear interpolation among neighboring bins was used by Shell et. al. [13] to prevent the random walker from being trapped in one bin. However, to capture the curvature of a 2D surface, a large number of bins are still necessary. We will give an estimation of this number in later discussions. Alternatively, we have adopted an update scheme similar to the kernel density estimation (KDE), which is consistent with the continuous nature of $g(x)$. In our simulations of joint density of states, we select a localized positive continuous kernel function $k(x) \geq 0$, and scale it by two constants $\gamma$ and $\delta$: $k(x) \rightarrow \gamma k(x/\delta)$. If the random walker arrives in $x_0$, then the continuous histogram $w(x)$ is updated by

$$w(x) \rightarrow w(x) + \gamma k((x - x_0)/\delta), \quad (2)$$

and we express the acceptance rate as

$$A_{i\rightarrow f} = \min\{1, \exp[\ln \alpha \{w(x_i) - w(x_f)\}]\}, \quad (3)$$

where we have inserted a constant $\ln \alpha$ so that $w(x)$ converges to $\log_\alpha g(x)$. The continuity of $w(x)$ ensures that the random walker is always properly biased. This update scheme is similar to the method of Ref. [13], where the potential is updated by Gaussian kernels in a molecular dynamics simulation. In addition to the Gaussian kernel function $k(x) = \exp(-|x|^2)$, we also implemented the Epanechnikov kernel $k(x) = [1 - |x|^2]_+$. Little difference has been seen in the calculations with different kernel functions. By slightly modifying the approach in Ref. [5], we can prove that this update scheme converges.

Thus the single modification factor in the original WL algorithm is replaced by a triplet $(\alpha, \gamma, \delta)$. In our simulations, we have used numbers between 0.0001 and 0.01 for $\gamma$ and $\delta$ corresponding to about 1/200 of the width of the energy window or the magnetization window. Unlike the original WL algorithm, we do not reduce $\gamma$ to extremely small values in the simulation, neither do we change $\delta$ in the simulation. We have the freedom to change $\alpha$ provided that $w(x)$ is properly rescaled. A small $\alpha$ actually does not improve the accuracy of the calculation.

From Ref. [3], we know if we start from an unbiased initial $w_0(x) = 0$, $w_T(x)$ (where $T$ labels the number of Monte Carlo steps) grows from the region of large $g(x)$, and extends to unexplored region of small $g(x)$. $w_T(x)$ can be written as:

$$w_T(x) = \left[ C(T) + \log_\alpha g(x) + r_T(x) \right]_+,$$
where $C(T)$ is an increasing function of $T$ only, $r_T(x)$ is a bounded error term controlled by the triplet $(\alpha, \gamma, \delta)$. $w_T(x)$ also increases monotonically in the simulation, and remains zero in the unexplored region. One cannot expect it to be flat as in the original WL algorithm for discrete models. The simulation should be stopped by other criteria, e.g. the visited area reaches a low energy cut-off. Then we continue the simulation with reduced $\gamma$ to improve the accuracy in the visited area. If the result is accurate, $w_T(x)$ increases uniformly in the visited area. $T$ is estimated by counting the number of kernel functions to build up $w_T(x)$:

$$T = \left[ \int \gamma k(x/\delta)dx \right]^{-1} \int_{\Lambda} w_T(x)dx. \tag{4}$$

However we find that the initial accumulation in which $\Lambda_T = \text{supp}\{w_T(x)\}$ expands to $\Lambda$ takes a very long time for joint density of states of two variables. The expansion of $\Lambda_T$ slows down as the area of $\Lambda_T$ increases. The reasons are two-fold. First, the simulation samples the macroscopic states within $\Lambda_T$ uniformly, giving rise to a uniform growth there. This uniform growth takes a considerable CPU time, while only about a fraction $|\Lambda_T|^{-1/2}$ of Monte Carlo steps on the boundary of $\Lambda_T$ happen to extend the simulation to the unexplored area. Secondly, close to the singular boundaries of $\Lambda$, $\nabla \log \alpha g(x)$ becomes very large, requiring a very small $\delta$ (high resolution in the kernel function) to capture the large derivative.

To avoid repeated sampling of the visited region $\Lambda_T$, and to push the simulation to the unexplored region, we find it is most efficient to introduce a global update of $w_T(x)$: when $w_T(x)$ is a good estimate of $\log \alpha g(x)$ inside $\Lambda_T$, we update $w_T(x)$ with the following formula:

$$w_T(x) \rightarrow w_T(x) + \kappa \exp \left[ \frac{-\lambda}{w_T(x) - \omega} \right] \Theta(w_T(x) - \omega), \tag{5}$$

where $\Theta$ is the Heaviside step function. Basically, $w_T(x)$ is shifted up by an amount of $\kappa$ where $w_T(x) > \omega$, and the exponential function removes the resultant discontinuity. Here $\omega$ is required to be positive because the above local update scheme requires a minimum number of visits to give a correct estimation of the density of states.

As a result of this global update, the random walker is confined close to $\partial \Lambda_T$, only when the accumulation on the boundary exceeds $\kappa$, is the random walker likely to come back to the interior of $\Lambda_T$. Then a short global sampling using Eq. (2) covers up possible artifacts that result from the global update. Figure 2 illustrates one cycle of calculation with the global update. Ideally, the initial accumulation is decomposed into a number of cycles. In each cycle, the simulation works on a particular subset of $\Lambda$. Let $\Lambda_0 = \emptyset$, $\lambda_0 = \max \{ \log \alpha g(x) \}$, $\Lambda_n = \{ x | \log \alpha g(x) > \lambda_0 - n\kappa \}$ for $n > 0$. The series of sets $\{\Lambda_n\}$ converges to $\Lambda$. In $n^{th}$ cycle of our calculation with the global update Eq. (5), the random walker estimates $g(x)$ in $\Lambda_n - \Lambda_{n-1}$, which roughly requires

$$T_n = \left[ \int \gamma k(x/\delta)dx \right]^{-1} \int_{\Lambda_n - \Lambda_{n-1}} \left[ \log \alpha g(x) - \lambda_n \right]dx$$

Monte Carlo steps. By comparison with Eq. (1), we see that instead of filling up the bulk of $w_T(x)$, the simulation only fills up a thin surface layer of $w_T(x)$ of thickness roughly given by $\kappa$. Consequently, the algorithm with the global update saves a huge amount of Monte Carlo steps. Compared with distributing the random walkers to a number of "windows" [1, 5, 9], the global update has the advantage of automatically selecting the "windows" on the frontier of the simulation and avoiding the boundary errors [1]. Figure 2 shows that the global update saves 90% of the CPU time in a typical simulation, where we plot $t$ as a function of maximum histogram $W \equiv w(0, 0)$. Without the global update, since the increment in $W$ is due to the uniform accumulation of samples inside the visited area $\Lambda_T$, therefore $dt/dW \propto |\Lambda_T|$. From Fig. 1 we can tell that $\Lambda_T$ mainly grows towards lower energy. Hence we expect approximately $|\Lambda_T| \approx aW + b$, which results in a leading quadratic dependence $t \propto W^2$ in Fig. 3. With the global update, both the prefactor and the exponent of this relation are reduced. The short global samplings at the end of each cycle of the global update result in $T \propto W^\lambda$, with $\lambda \approx 1.55$ in Fig. 3.

We summarize the algorithm as the following: A calculation from scratch is divided into an initial accumulation stage and a refining stage. In the initial accumulation stage, (1) we start the calculation with $w(x) = 0$, using local updates Eq. (2). (2) As soon as $w(x) > \omega$ for some $x$, we apply the global update Eq. (5), and continue the accumulation with local updates. $w_T(x)$ initially increases on the boundary of $\Lambda_T$. (3) After it resumes a uniform growth over $\Lambda_T$, we start the next cycle with

![FIG. 2: A cycle of the simulation with global update. (a) original $w_T(x)$, (b) $w_T(x)$ after the global update, (c) the increment accumulated beginning with the $w_T(x)$ in (b), (d) sum of (b) and (c) gives a new $w_T(x)$ in the end of this cycle.](image-url)
an another global update. The refining stage starts when $w_T(x)$ expands to the entire $\Lambda$ or certain cut-off one assumes. Then we reduce $\gamma$ (and $\delta$ if necessary) to continue the simulation with local updates only. When $w_T(x)$ resumes a uniform growth, we can further refine the result with reduced $\gamma$ or continue with the current parameters to decorrelate the statistical error and average over multiple uncorrelated results of $w_T(x)$.

We calculate the thermodynamic quantities from $g(M, E)$ with numerical integral. Fig. 1(b) shows the magnetization of Heisenberg ferromagnet as a function of external field and temperature. The specific heat in Fig. 4 shows a typical peak at $T_c$ of Heisenberg models. We also compare our results with that calculated with the original WL algorithm performed with a large number of bins. They only differ slightly at low temperatures where both results show small errors. This error comes from the binning or interpolation scheme used to represent the continuous $g(E)$ or $g(M, E)$ (not from the numerical integration). Actually, given that the standard deviation of the canonical distribution of the energy is $\sigma_E = \sqrt{T^2C_v/L^3} \approx 0.036$ for $L = 10$, $T = 1$, and $\sigma_E \approx 0.1$ for $L = 5$, the numerical integration requires enough data points within $\sigma_E$ to be accurate. This criterion applies to both our kernel function updates and the bilinear interpolation scheme 3. A larger $\sigma_E$ explains why the error is very small for $L = 5$ in Fig. 4. In case of $L = 10$, the internal array we used to store $g(M, E)$ has an energy resolution of 0.0012, which is comparable to the bin size (0.001) of the original WL algorithm we used for $g(E)$. Consequently, they show errors of comparable sizes. One can conclude that for larger systems, the resolution in each macroscopic quantity is required to increase as $\sqrt{N}$ to maintain the accuracy in the numerical integral, where $N$ is the number of degrees of freedom.

In summary, we have extended the WL algorithm to treat continuous systems and their joint density of states, proposed kernel function local updates and a global update to increase the efficiency of the algorithm.

Our new strategies have potential applications to many complex systems with thousands of degrees of freedom. In particular, the kernel function update benefits from the continuity of the model; and the global update effectively drives the random walker to unexplored area, so that extreme values of macroscopic variables can be searched. If the calculations of $g(M, E)$ we presented were performed with the original WL algorithm, the CPU time used would have increased roughly by a factor of ten.

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FIG. 3: Comparison of CPU time used by the calculations of $g(M, E)$ with and without the global update for an $L = 5$ Heisenberg model of ferromagnet, $\omega = 0.5$ is used. The dashed line is a guide for the eye.

FIG. 4: Specific heat of the Heisenberg ferromagnet of size $L = 10$, and 5, with comparison to the results from the original WL algorithm performed with a large number of bins.

\[\begin{align*}
\text{With global update} & \quad \text{Local update only} \\
- & \quad - \\
& \quad - \\
& \quad - \\
\end{align*}\]

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