# Comments and implementation of the Wang–Landau algorithm

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## Background

The Wang-Landau algorithm based on the Monte Carlo method is proposed by Fugao Wang and David Landau [1] to calculate density of the states(DOS) efficiently. This method constructs the DOS through non-Markov random transitions, traversing all possible states. After reviewing Wang-Landau algorithm, the analysis of the results through the implementation in Python for 2D Ising model is shown in this short report.

## The Wang-Landau algorithm

The Wang-Landau algorithm can be classified as an entropy modeling method, in which the walk in the energy space is used to study the DOS, and the access probability to all energy states is equal. This algorithm solves the problem of selecting the appropriate transition probability to obtain the uniform access to the energy state required for entropy modeling, thus obtaining the DOS: $g\ (E)$. The algorithm is described below.

First, define a function $g(E)$ and set it to unity for all $E$. Define also an histogram $H(E)$ and set it to zero for all E. Start with a random initial state. Update $g(E)$ and $H(E)$ as follows :

$$g(E_0)\ =\ g(E_0)\ \times f;\ H(E_0)\ =\ H(E_0)\ +\ 1$$

Each time the new $g(E)$ and $H(E)$ are updated, the histogram parameter $f$ is taken by steps: $f_{i+1} = \sqrt{f_i}$. And $f_0 = e \approx 2.71828$. Till $f_{final} = e^{10^{-8}} \approx 1.00000001$. In principle, $f_0$ can be any real number greater than 1, and it is best to decrease monotonically to 1. Some authors, see for example [2, 3], have found that it beneficially changes $f$ non-monotonically for initial steps.

The histogram of energy would become flat at least over the range of energy after a few Wang-Landau iteration runs. The flatter the histogram, the closer $g(E)$ is to the true unknown DOS. But as the paper said, the phrase "flat histogram" means that histogram $H(E)$ for all possible $E$ is not less than 80% of the average histogram.

Once we know the estimated DOS $g(E)$ then we can calculate the Gibbs free energy:

$$F(T) = -k_B T ln(Z) \ = -k_B T ln(\sum_E g(E) e^{-\beta E})$$

And entropy, etc. ( $T \in [0, 8]$ )

$$S(T) = \frac{< E >_T - F(T)}{T};\ < E >_T \equiv \sum_E E g(E) e^{-\beta E} \Big/ \sum_E g(E) e^{-\beta E}$$

## Results and comments

Due to the complexity of some systems, for instance compounds, biomolecules, polymers, etc., the calculation of the DOS is impossible in most cases. But the Wang-Landau algorithm provides a high-precision method for evaluating DOS. As the lack of condensed matter physics

knowledge and real data. The analysis and comments will focus on the efficiency, advantages and disadvantages of the algorithm itself.

## A. Time Cost Analysis

This test explores the effect of different L and different MCsweeps on the results. Figure 1 shows the simulation time for different $L \times L$ lattices. And the time cost rises very rapidly as L increases. In Wang-Landau's paper, $6.1 \times 10^6$ MCsweeps was used for $256 \times 256$ lattice after their acceleration, while it costs around 20 mins in my simulation. Since the number of MC sweeps defines the number of iteration cycles in a sense, Figure 2 shows that it is linearly related to the time cost.

During calculations, Wang-Landau algorithm has a disadvantage because it must reduce the modification factor $f$: from $f_0 = e^1$ to $f_{final} = e^{10^{-8}} \approx 1.00000001$. In fact, when the value of $g(E_i)$ is $10^8$, the DOS $g(E_i) * \mathrm{f_{final}}$ in this algorithm is the same as the DOS $g(E_i) + 1$ in entropy sampling. Therefore, this method has the advantage of quickly constructing a rough estimator for DOS, but near the end stage, the algorithm is very close to pure entropy sampling which is very time-consuming.

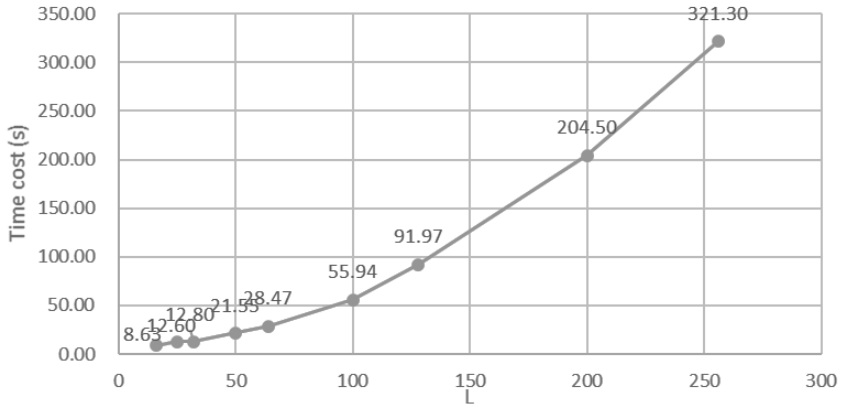


Figure 1 Time cost with different L (MC sweeps = 10^6)

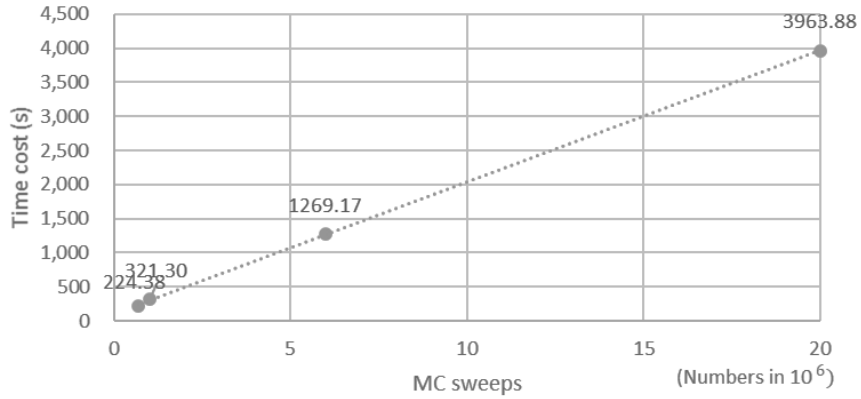


Figure 2 Time cost with different MC sweeps (L = 256)

In addition to the slowing down feature, the algorithm seems to perform badly on continuous degrees of freedom systems. These and other related issues have attracted the attention of several authors, see for example [4] and propose remedial measures.

## B. Implementation Results

After generating a random $L \times L$ 2D Ising lattice, we calculate the lattice energy, and then

cycle MCsweeps times to obtain the final $\ln(g(E))$ and the Hist. Based on that, we can also get the figure of $F(T)/N$, $C(T)/N$ and $S(T)$. Figure 3 shows the results of $50 \times 50$ and $256 \times 256$ under 0.8 flatness of the Hist.

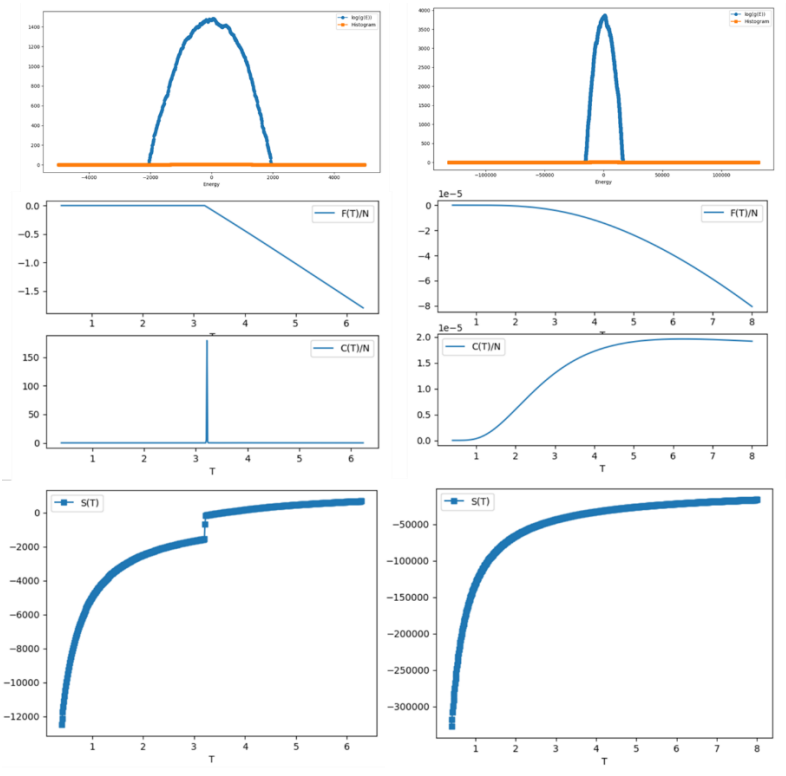


Figure 3 L = 50 (left) and L = 256 (right) plot

Overall, the algorithm and this implementation both have room for improvement. As the chain generated is not Markovian, some critics said it's not that clear how to guarantee the convergence of g(E). Also there're "Boundary Effects" [5]. But some other researchers have given an proof of the convergence of the Wang-Landau algorithm.

## References


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[3] P.Poulin, F.Calvo, R.Antoine, M.Broyer, and, P.Dugord, Performances of Wang-Landau algorithms for continuous systems, Physical Review E 73, 56704 (2006).

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[6] C.Zou, and R.N.Bhatt, Understanding and Improving the Wang-Landau Algorithm, Physical Review E 72, 25701(R) (2005).