Comparison of the Metropolis and Wang Landau algorithms for computing the Ising model

1 Introduction

The Ising model is a system in statistical physics that can be used to investigate phase transitions using computational algorithms. A simple instance of the Ising model might be a two dimensional lattice of atoms, each of which can be in one of only two possible states, There is an interaction energy between every atom and each of its nearest neighbors that can be expressed by the following Hamiltonian

$$H = -J \sum_{i,j} S_i S_j$$

where $S_i = \pm 1$ is the state of the atom at site i , $\sum_{ij}$indicates the sum over the four nearest neighbours, and J is a constant with units of energy.

The Ising model may describe a ferromagnetic system, in which case S_i is the magnetization of atom i , $J > 0$, and neighbouring spins are at a lower energy when aligned. If the lattice is allowed to equlibriate at a certain temperature then the total interaction energy and magnetization will, on average, reach steady values. It is observed that at sufficiently low temperatures the atomic spins are generally all aligned, resulting in the lattice showing an overall magnetization. At sufficiently high temperatures the spins are generally at random and the lattice has no overall magnetization. In two or more dimensions there is a certain critical temperature at which a phase transition occurs between these two regions of different magnetization.

The Ising model in two dimensions was analytically solved by Lars Onsanger in 1944 who showed that the phase transition occurs at a temperature given by

$$k_B T/J \; = \; 2/\ln(1+\sqrt{2}) \; = 2.269185...$$

The Ising model may also be investigated using computational algorithms. The first technique commonly applied was the Metropolis algorithm[1], which directly simulates fluctuations in the lattice using a Monte-Carlo process. In successive steps atoms in the lattice are selected at random and their spins may be flipped according to certain rules that take into account the potential change in lattice energy and the temperature. By operating the algorithm with suitable averaging over a range of temperatures, the characteristics of the Ising model can be measured. In addition, the Metropolis algorithm allows the lattice and its fluctuations to be visualized either as snapshots at certain temperatures or as a continuing animation.

The Metropolis algorithm is a very elegant and broadly used computational technique, but an alternative approach offering higher computational efficiency was proposed by Wang and Landau in 2001[2]. The Wang Landau algorithm is also based on a Monte-Carlo process, but this time the fluctuations of the Ising model are not simulated directly. Rather, a random walk technique is used to count how many alternative configurations of the lattice are available at each possible energy level, i.e. the density of states as a function of energy. Once the density of states has been determined, a numerical integration is performed over all the possible energy levels to calculate the averages of magnetization and energy.

Since the original algorithm was originally published various studies have looked at its effectiveness and at potential improvements. Zhou and Bhatt[3] gave a proof of the convergence of the Wang Landau algorithm and suggested a optimization strategy. Schutz and Landau[4] investigated how the density of states could be established by conducting multiple random walks over adjacent restricted energy ranges without incurring boundary

effects. Lee, Okabe and Landau[5] derived an expression for the residual error of the Wang Landau algorithm and as a result identified the central role of the histogram accumulated during the density of states calculation in the overall accuracy of the method. Recently, Caparica and Cunha-Netto[6] conducted an extensive study of the impact of various implementation adjustments on the accuracy and precision of the algorithm. A central element of their method was to run the algorithm multiple times and obtain the histogram of the location of the peak of the specific heat capacity.

- Basic overview of the project work
- Hint at results

2 Theory

2.1 Solving the Ising model

Although Onsanger's solution for critical temperature of the two dimensional Ising model is available, it may still be more straightforward to approach the problem of solving the Ising model by using a computer to generate numerical solutions rather than by following the theoretical approach. For the Ising model in three dimensions or more, only numerical solution are available.

The number of possible configurations of an Ising lattice is very large, $2^{L^D}$for a D dimensional lattice spanning L atoms in each direction. For this reason it is not feasible for a compuational method to evaluate each configuation directly (Table 1). Instead, the Metropolis and Wang Landau algorithms take a random walk through the space of alternaltive lattice configurations (the state space) and make measurements on a sample basis. Accurate determinations for the characterictistics of the Ising model can be had once sufficient measurements have been accumulated. This general approach is called a Monte-Carlo method.

The key quantities that the algorithms should determine across the range of temperatures under investigation include the average magnetization, the average interaction energy, and the average heat capacity per atom. Magnetization and interation energy can be measured directly from the lattice. The heat capacity is related to the energy, E, by

$$C = \frac{k_B}{T^2}\left(\left\langle E^2\right\rangle - \left\langle E\right\rangle^2\right)$$

The critical temperature is observed to occur at the point where the heat capacity reaches a maximum, so by evaluating the heat capacity at each temperature the algorithms can also determine the critical temperature of the model.

2.2 The Metropolis algorithm

The Metropolis algorithm is a direct simulation of the physical system. It sets up a lattice at a given termperature and follows its fluctuations in discrete steps of time. The algorithm proceeds as follows:

1. Set the current temperature
2. Create a new lattice in the initial configuration. In a "hot start" the lattice spins are initially set at random. In a "cold start" the lattice spins are initially aligned
3. Select one candidate spin in the lattice at random and calculate the energy change, $\triangle E$, that would result from flipping that spin
4. Apply the following rules to determine whether to flip the candidate spin. If $\triangle E < 0$, then flip. If $\triangle E > 0$, then flip with probability$p = e^{-\triangle E/k_B T}$
5. Periodically measure the average magnetization, $\langle m\rangle$, the average energy, $\langle E\rangle$, and the average energy squared, $\left\langle E^2\right\rangle$, for the lattice
6. Return to step 3 until sufficient measurements have been accumulated for the current temperature
7. Return to step 1 until the relevant range of temperatures has been examined

Dimensions, D	Lattice span, L	Available states	Available energy levels
2	8	1.8×10^{19}	65
2	16	1.1×10^{77}	257
2	32	1.8×10^{308}	1025
3	8	1.3×10^{154}	769
4	8	1.0×10^{1233}	8193

Table 1: Total number of available energy levels for different Ising lattices

2.3 The Wang Landau algorithm

The Wang Landau algorithm effectively detemines the partition function of the system and then uses it in a numerical summation to calculate the lattice characteristics. Consider two expressions for the partition function, Z, as follows

$$Z = \sum_{\sigma} e^{-E(\sigma)/k_B T} = \sum_{E} g(E) e^{-E/k_B T}$$

In the first case the partition function is computed over each available state, σ. As previously metioned, the total number of available states will be 2^{L^D}, which is too many to evaluate. In the second case the partition function is computed over each available energy, E , and makes use of the density of states, $g(E)$. It can be shown by considering the configurations of a lattice that the total number of available energy levels is

$$1 + \frac{1}{2} D.L^D$$

which is a much smaller quantity than the total number of states (Table 1).

The Wang Landau algorithm determines the density of states through a random walk process. At each step the probability of moving from the current configuration to a new candidate configuration is *inversely proportional* to their relative density of states. A histogram is calculated to track the number of visits to states at each energy level. When the histogram become flat it indicates that the density of states has been properly determined to within the given level of accuracy. Since the density of states is not initially known, the starting condition for all E is $g(E) = 1$. An adjustment factor is added to increase each density of states each time a certain energy is visited.

The algorithm proceeds as follows:

1. Set$g(E) = 1$ for all E and set the initial value of the adjustment factor, f
2. Create a new lattice in the initial configuration with lattice energy E_1 . Hotstart and coldstart are as for the Metropolis algorithm
3. Select one candidate spin in the lattice at random and calculate the lattice energy, E_2,that would result from flipping that spin
4. Flip the spin with probability, $p = \min(g(E_1)/g(E_2), 1)$
5. The current energy of the lattice is labeled E_1
6. Update the density of the current state with $g(E_1) = g(E_1) * f$
7. Update the histogram that records visits to the available energy levels with $H(E) = H(E) + 1$

8. Periodically test the histogram for flatness using a certain flatness criterion, say 80%
9. Return to step 3 until the histogram satisfies the flatness criterion
10. Reduce the adjustment factor, f , and zero the histogram with $H(E) = 0$, for all E
11. Return to step 3 until the adjustment factor is below a predefined final value
12. Normalize the density of states by recognizing that the lowest energy configuration has a density of states of 2, (i.e. all spins aligned in either one of two ways)
13. Use a numerical summation with the partition function and the calculated density of states to determine the average values of energy, magnetization, and heat capacity. For example the average energy of the lattice at a certain temperature is given by$\langle E \rangle = \sum_E E.g(E)\, e^{-E/k_B T}$

3 Computational implementation

4 Results

5 Discussion

References

[1] Metropolis, N., Rosenbuth, A.W., Rosenbuth fvM.N., Teller, A.H., Teller, E., J. Chem. Phys. 21, 1087 (1953)

[2] Wang, F., & Landau, D. P. (2001). An efficient, multiple range random walk algorithm to calculate the density of states, 30602, 1–4.

[3] Zhou, C., & Bhatt, R. N. (2003). Understanding and Improving the Wang-Landau Algorithm. Physical Review E - Statistical, Nonlinear and Soft Matter Physics, 72(2 Pt 2)

[4] Schulz, B. J., Binder, K., Müller, M., & Landau, D. P. (2003). Avoiding boundary effects in Wang-Landau sampling. Physical Review E - Statistical, Nonlinear and Soft Matter Physics, 67(6 Pt 2)

[5] Lee, H. K., Okabe, Y., & Landau, D. P. (2005). Convergence and Refinement of the Wang-Landau Algorithm. Computer Physics Communications, 175(1)

[6] Caparica, A., & Cunha-Netto, A. (2012). Wang-Landau sampling: Improving accuracy. Physical Review E, 85(4), 1–9.