Comparison of the Metropolis and Wang Landau algorithms for 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, commonly labeled spin up and spin down and taken as the magnetization. There is an interaction energy between every atom and each of its four nearest neighbors that is equal to -J where the two neighboring spins are aligned, or +J where they are opposite. Allowing the lattice to equlibriate at a certain temperature will result in certain average values of magnetization and energy per atom. Ising models in two or more dimensions undergo a phase transition at a certain critical temperature, below which the spins of the lattice are generally all aligned and above which they are generally at random. The physics of this phase transition are applicable to a wide range of phenomena and therefore of much interest.

Although the Ising model was analytically solved in two dimensions by Lars Onsanger in 1944, it is still commonly 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, whereby in successive steps atoms in the lattice are selected at random and their spins may be flipped, according to certain rules. After a sufficient number of iterations, the lattice will have reached equilibrium and its magnetization and energy can be calculated. The rules to determine whether or not a candidate spin is flipped at each step are as follows: allow all flips that lower the energy of the lattice but selectively accept flips that increase the energy of the lattice at random, with a probability in each case proportional to the Boltzmann factor for the relevant increase in energy and the given temperature.

By operating the algorithm with suitable averaging over a range of temperatures, the physical 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), providing some opportunity for intuitive insight.

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 Carol 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.

The random walk process is conducted so that the probability of moving to a new state with a given energy, E, at each iteration of the Monte Carlo process is *inversely proportional* to the density of states, g(E), at that energy. The density of states is not initially known and the starting arrangement is $g(E) = 1$ for all energies. Each time a certain energy is visited, g(E) is multiplied by a certain factor, $f > 1$. The random walk is finished when the accumulated count of visits to energy levels appears as a flat histogram, thus indicating that the random walk with $p = 1/g(E)$ verifies the correspondence of g(E) to the actual density of states. Once a flat histogram is obtained, the exercise is repeated with a smaller value of f to improve the precision of g(E). In the second step, the numerical integration over all energies, the density of states is multiplied by the Boltzmann factor at the given energy and temperature to give the probability that the system could be found at that particular energy after normalization. By repeating the integration for a range of temperatures the physical characteristics of the Ising model can be measured.

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 an example optimization strategy whereby the modification factor, f, is started at around Exp(4) and reduced by dividing by a large factor ~10 at each stage. 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. They observed that after a certain number of iterations the variation in the histogram will become saturated and at such point the algorithm should proceed to the next smaller modification factor, f.

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 for the 2D Ising model and obtain the histogram of the location of the peak of the specific heat capacity. The histogram shows a Gaussian distribution, of which the width indicates the relative precision of the algorithm under different circumstances, and the center relative to the known analytic solution indicates the accuracy. (This technique has been heavily borrowed in the present study.) Their specific conclusions included a number of optimization suggestions, including that the density of states should only be updated with the modification factor, f, after a number of spin-flip trials equal to the size of the lattice, rather than at every trial.

2 Method

References

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