Monte Carlo Simulation of 2D Ising Model

André Melo 4519302
Matteo Domenighini 4512154

Delft University of Technology

Abstract

The aim of this report is to present the results obtained using Monte Carlo simulation for the Ising model. Two different algorithms have been implemented to simulate the behaviour of the system: the Metropolis Monte Carlo algorithm and the Hoshen-Kopelman cluster finding algorithm. Both algorithms have been used to extrapolate relevant physical quantities, such as the magnetization, the magnetic susceptibility and the specific heat. Finite-size scaling has also been used in order to calculate the critical exponents. For the Metropolis algorithm, we tried to find a proof of the critical exponent universality by considering second neighbour interaction. The algorithms have been compared: the Hoshen Kopelman revealed itself to be better suited for (...)

I. Introduction

The Monte Carlo algorithms are a type of algorithms in which "random" numbers play an essential role [1]. This method has been widely and successfully implemented in the past decades to simulate the behaviour of physical systems in order to extrapolate information regarding their static properties.
The Hoshen Kopelman algorithm is a cluster finding algorithm that has been implemented as a non-recursive alternative to the Swendsen-Wang algorithm. It is based on the more famous Union-Find algorithm.

In section II the interaction model and the working principles of the two algorithms are outlined. In section III the numerical results obtained for specific heat, magnetization, magnetic susceptibility, Binder cumulant and critical exponent are reported. In section IV, the accuracy and speed of the two algorithms are compared.

II. Methods

While implementing the models and algorithm outlined in this section, we have considered $k_B = 1$, $J = 1$ and a unitary distance between the lattice sites.

I. Ising Model

The Ising Model consister in a lattice of size $L \times L$ in which every lattice site is associated with a spin. The Hamiltonian of the system in absence of an external magnetic field is described by

$$H = -J \sum_{\langle ij \rangle} \mathbf{s}_i \mathbf{s}_j \tag{1}$$

where $\mathbf{s}_i$ represents the spin associated with the ith site. We consider $J > 0$, which means that the system favours the parallel alignment of adjacent spins. The partition function for the system is given by

$$\mathcal{Z} = \sum_{\mathbf{s}_i} e^{-\beta H(\mathbf{s}_i)} \tag{2}$$

which is dependent on the temperature of the system, contained in β.

II. Metropolis Monte Carlo Algorithm

The Metropolis Monte Carlo algorithm is an algorithm in which the information regarding different distributions of a system is stored in a Markov chain.

III. Hoshen-Kopelman Algorithm

III. Results

I. Magnetization

In the Ising model one defines the magnetization of the system as:

$$m = \frac{1}{L^2} \left\langle \sum_i s_i \right\rangle \tag{3}$$

However the cluster flipping operations of the HK algorithm make the sum in 3 oscillate considerably, so the magnetization is approximated as:

$$m = \frac{1}{L^2} \left\langle \left| \sum_i s_i \right| \right\rangle \tag{4}$$

II. Heat capacity

The heat capacity can be directly related to the system's energy fluctuations:

$$C_v = \frac{\langle E^2 \rangle - \langle E \rangle^2}{L^2 T} \tag{5}$$

III. Binder cumulant

The Binder cumulant Q is defined as:

$$Q = 1 - \frac{\left\langle (\sum_i s_i)^4 \right\rangle}{3 \left\langle (\sum_i s_i)^2 \right\rangle^2} \tag{6}$$

It can be shown that Q has a universal value at the critical point. Therefore one can estimate βJ_c by determining the intersection point of Q for different lattice sizes.

IV. Finite size scaling

As a system approaches a critical phase transition the behaviour of its physical quantities are described by power laws. The exponents corresponding to these power laws are called the *critical exponents*. For the Ising model we have:

$$\chi \sim |T - T_c|^{-\gamma} \tag{7}$$
$$C_v \sim |T - T_c|^{-\alpha} \tag{8}$$
$$\xi \sim |T - T_c|^{-\nu} \tag{9}$$
$$m \sim |T - T_c|^{\beta} \tag{10}$$

In 1994 Lars Onsager calculated (ADD REFERENCE) the 2D Ising Model partition function from where the exact critical exponents can be found:

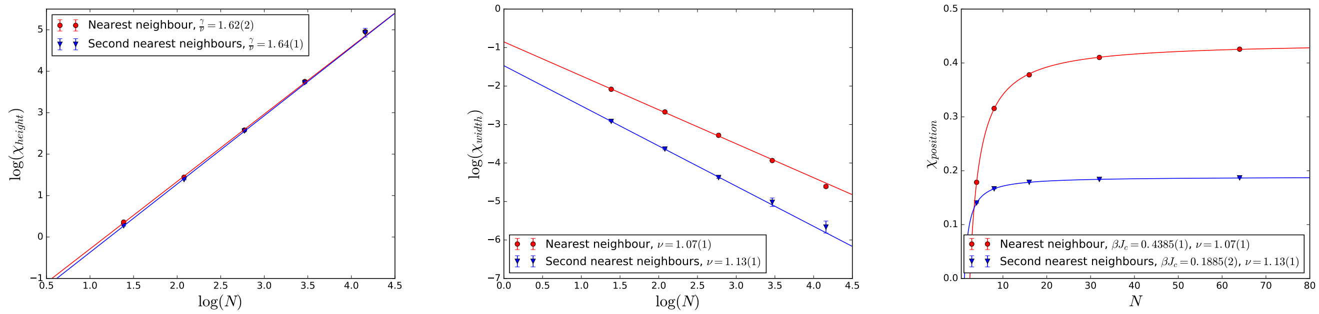
$$\gamma = \frac{7}{4} \tag{11}$$
$$\alpha = 0 \tag{12}$$
$$\nu = 1 \tag{13}$$
$$\beta = \frac{1}{2} \tag{14}$$

These exponents are said to be *universal* due to the fact that they remain invariant under certain changes in the Hamiltonian. Systems governed by different Hamiltonians but with the same critical exponents are said to belong to the same *universality class*.

It is important to note that analytical exponents are actually obtained by taking the system size LxL to be infinite. For a finite system then all the thermodynamic quantities will be a smooth function of temperature – we will not see a divergence at the critical point but a smooth peak. However as we increase the system size we observe that the size, width and position of this peak change according to a set of equations called the scaling laws. Suppose we have a thermodynamic quantity A with critical exponent σ (i.e. $A \sim |T - T_c|^{-\sigma}$ close to T_c). Then we have that:

- The peak height scales as $L^{\sigma/\nu}$
- The peak position scales as $L^{-\nu}$
- The peak width also scales as $L^{-\nu}$.

These three quantities (NUMBER OR WORD?) were tracked for the magnetic susceptibility ξ for different values of L (PLOT SAYS N) by fitting the peaks to a Gaussian function. We considered a system only with first neighbour ferromagnetic interactions (governed by the Hamiltonian in EQUATION) and a system with second neighbour ferromagnetic interactions were also considered (the coupling constant was taken to be the same for all interactions). The results are shown in Figure 1 and in Figure 2. The critical exponents were found to be very close to the exact results for the 2D Ising model ($\frac{\gamma}{\nu} = 1.75$, $\nu = 1$). Furthermore one also sees that although both systems exhibit different critical temperatures the critical exponents are very similar, indicating that both systems belong to the same universality class.



(a) *Height* **(b)** *Width* **(c)** *Positions*

Figure 1: *Scaling behaviour .*

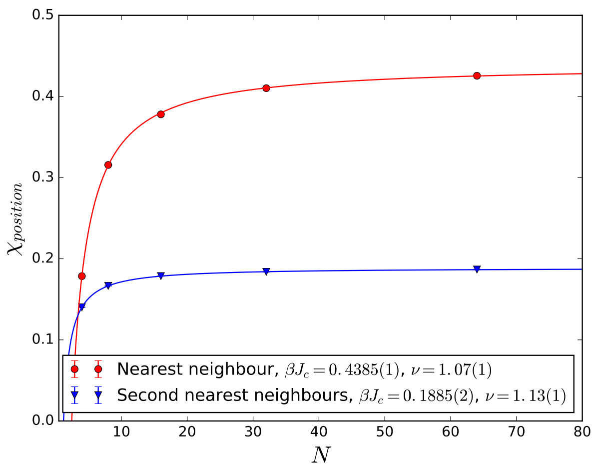


Figure 2: *Position*

Besides the scaling relations outlined the value of the magnetization at T_c is expected to satisfy the following scaling relation (ADD REFERENCE):

$$m(T_c) \propto L^{\beta/\nu} \tag{15}$$

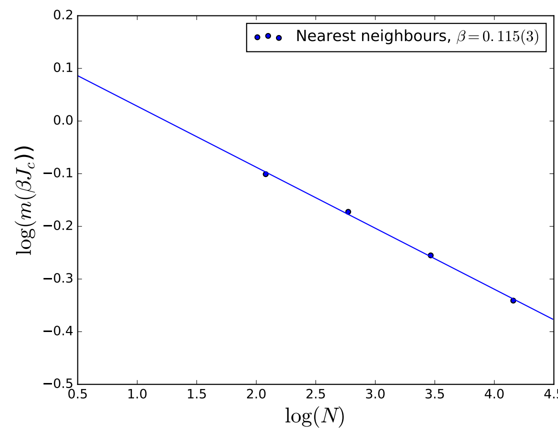


Figure 3: *asdasdasd*

IV. Conclusion

lalila

A. Appendix - Data blocking

References

[1] J.M.Thijssen, *Computational Physics*, Cambridge University Press, 2nd Edition, 2007.