UNIVERSITÀ DEGLI STUDI DI TORINO

Fisica dei Sistemi Complessi

Tecniche di analisi numerica e simulazione

Monte Carlo simulations of the Ising model on lattices and power law networks

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Contributions

M.P. put forward the original idea and directed the theoretical part.

A.S. devised the class structure and directed the programming part.

A.S., M.P., C.P. wrote the code and performed the simulations.

M.P., A.S., C.P. analyzed the data.

M.P. wrote the paper.

Abstract

The Ising model is a paradigmatic example of interactions in complex systems. Though it was initially conceived as a mathematical model for ferromagnetism, it has been used in socio-economic contexts as well. We developed object-oriented `C++` software in order to simulate the Ising model and its variations on various topologies. We found the expected results in the case of a two-dimensional lattice and pronounced finite-size effects on networks whose degree distribution is a power law. Thanks to the extreme versatility of our software, further investigations are easy to be made.

1 Introduction

Many results of statistical mechanics come from systems whose microscopic constituents interact trivially or do not interact at all (Pathria (1988), Chapter 12). If one considers stronger interactions, phase transitions associated with singularities in the physical quantities and zeros of the partition functions (Lee and Yang 1952) emerge. The usual example of phase transitions is the Ising model. It was invented by Wilhelm Lenz (1920), and the one-dimensional solution was found by his PhD student Ernst Ising a few years later. In one dimension the model displayed no phase transition. The exact two-dimensional solution was found by Onsager (1944), with an order-disorder transition at

$$T_C = \frac{2}{\ln(1+\sqrt{2})} \frac{J}{k_B} \tag{1}$$

where T_C is the critical temperature, J is the coupling constant and k_B is the Boltzmann constant. From then on, many variations on the Ising model have been proposed. As a famous example, spin glasses (Mézard *et al.* 1987) are basically Ising models where the coupling constant J is a random variable. Recently, studies of Ising models on complex networks have been performed (Barrat *et al.* (2008), Chapter 5) and a rich behaviour has been discovered. Also, Ising models have been used to model opinion dynamics (Castellano *et al.* 2009) and Random Field Ising Models have been proposed for economic choices (Bouchaud 2013).

In order to understand our results, a short explanation on the Ising model and on the Monte Carlo techniques to simulate it is given in Section 2. We shortly present our software in Section 3 and our results in Section 4. The conclusion follows.

2 The Ising model

In the standard assumptions, particles with a certain spin (up or down) are located on the N nodes of a lattice (sites) and interact with their nearest-neighbours, i.e. those particles with whom they share an edge (bond). For simplicity, spin up is identified with a value $s_i = +1$, spin down is $s_i = -1$ (spins are measured in units of $\hbar/2$). The Hamiltonian of a given configuration S is given by

$$H(S) = -\sum_{\langle ij \rangle} J_{ij} s_i s_j - \mu \sum_i B_i s_i \tag{2}$$

The first term is a summation over all pairs of interacting spins; if the behaviour of the material is ferromagnetic $J_{ij} > 0$ and concordant spins give a negative contribution to the Hamiltonian. The lowest energy level is associated with all spins concordant. So far, the Hamiltonian has $\mathbb{Z}_2$ symmetry, and spontaneous magnetization cannot arise:

$$\overline{M} = \frac{1}{N} \sum_{i=1}^{N} s_i = 0 \tag{3}$$

If one adds the second term, which is simply the potential energy due to an external magnetic field B, this explicitly breaks the $\mathbb{Z}_2$ symmetry. Even if one does not consider this term, two remarkable facts arise: as the number of sites $N \to \infty$ there is spontaneous symmetry breaking; if the temperature is above T_C (Curie temperature) the behaviour of the model is paramagnetic.

These facts can be explained using the canonical ensemble of statistical mechanics. Every configuration is given a probability

$$P(S) = \frac{e^{-\beta H(S)}}{\mathcal{Z}} \tag{4}$$

with $\beta = \frac{1}{k_B T}$ and $\mathcal{Z}$ the partition function. The configuration with the minimum Hamiltonian, i.e. the equilibrium one, is also the most likely. By making use of mean-field arguments and simplifying assumptions, one can get a self-consistent equation:

$$\langle S \rangle = \tanh\left(\beta J \langle S \rangle\right) \tag{5}$$

In Figure 1 $\langle S \rangle$ as a function of T is shown. At $T = 1$ the system undergoes a phase transition, from the ferromagnetic phase ($T < 1$) to the paramagnetic one ($T > 1$).

The Ising model may be studied on a generic graph. We are interested in networks whose degree distribution is a power law:

$$p_k = C k^{-\gamma} \tag{6}$$

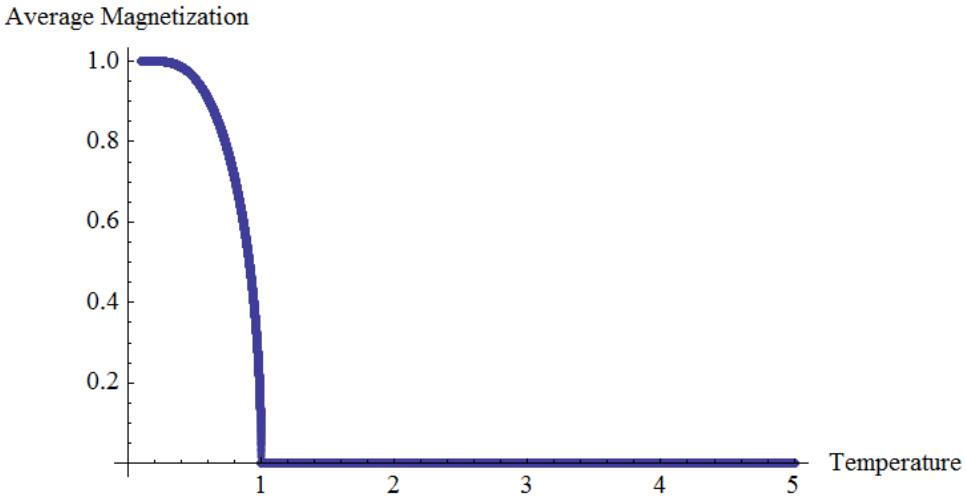


Figure 1: Numerical solution of Eq. (5) for any T between $T = 0$ and $T = 5$ with step $\Delta T = 0.0001$. T is in units of J/k_B

p_k is the probability mass that a node has degree k, C is a normalization constant and γ is called "power law parameter" and controls the slope of the power law. In Figure 2 it is possible to see that the power law parameter has a strong effect on the critical temperature. Leone *et al.* (2002) use a replica approach and find an analytic expression for T_C as a function of γ and k_{min}, the minimum node degree. For $\gamma < 2$ only ferromagnetic behaviour exists ($T_C \to \infty$): there are many nodes with high degree and they "freeze" the system. Notice that when $k_{min} = 1$ there is a percolation threshold: for $\gamma > \gamma^\star$, where $\gamma^\star$ is the solution of $\frac{\zeta(\gamma^\star - 2)}{\zeta(\gamma^\star - 1)} = 2$, $\gamma^\star \approx 3.47875$, the network does not percolate, i.e. there are many connected components: on average the magnetization is zero.

As mentioned in Section 1, exact analytical treatment is given only in the lattice case for one or two dimensions. If the topology of the graph is different, the dimensionality is higher or interactions are between 2-3 dimensional spins (XY and Heisenberg models) rather than spins which just assume values $s_i = \pm 1$, mean-field assumptions are needed. The risk with mean field assumptions is apparent in Figure 1. When $J/k_B = 1$ from Eq. (1) it is expected $T_C \approx 2.269185$, but one finds $T_C = 1$. Simulations are then needed both in cases in which analytical treatment is not possible at all and in cases in which it is necessary to check the effect of the simplifying assumptions. This is precisely what we did in Section 4.2.

Monte Carlo simulations of the Ising model are performed through the Metropolis Algorithm (MA). MAs belong to a more general class of algorithms, Monte Carlo Markov Chains (MCMCs), which are used when the probability distribution of the Monte Carlo inputs is unknown. In our case, the partition function $\mathcal{Z}$ in Eq. (4) is a summation over 2^N terms and cannot

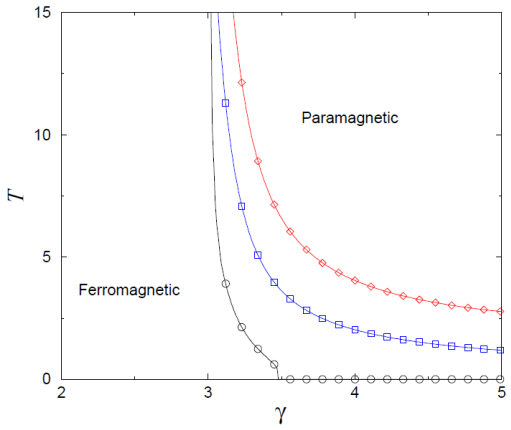


Figure 2: Critical temperature as a function of the power law parameter. The black line is for $k_{min} = 1$, the blue line for $k_{min} = 2$, the red line for $k_{min} = 3$. From Leone *et al.* (2002)

be computed even if the graph is small. The idea of MCMCs is to sample such a probability distribution by making use of an ergodic Markov Chain. The MA satisfies the detailed balance condition (needed for ergodicity) in such a way that $\mathcal{Z}$ cancels out. In practice, one takes a starting configuration S with Hamiltonian $H(S)$ and modifies it, such as to obtain S' with $H(S')$. Then, the probability to accept the new configuration is

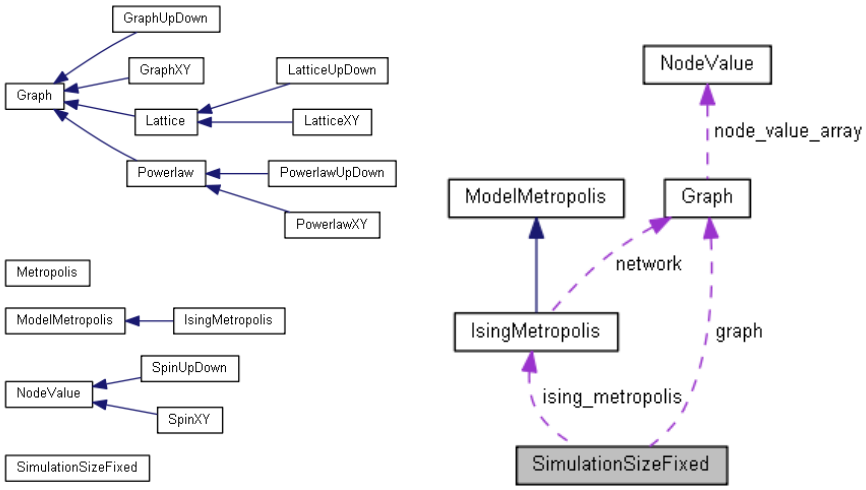
$$P(S \to S') = \min\left\{1, e^{-\beta[H(S')-H(S)]}\right\} \tag{7}$$

If $H(S') < H(S)$ the new configuration is accepted with certainty: this is a step towards the equilibrium state (which is just the most likely in statistical mechanics). If $H(S') > H(S)$ the new configuration may be accepted: this should prevent the system to get stuck in local minima. The key term in Eq. (7) is β: if β is high, T is low and it is less likely that higher energy configurations will be accepted; if β is low, T is high (there is a lot of noise) and almost any new configuration is accepted. Intuitively, in the first case the system will rush towards the equilibrium state; in the latter case it will just "wander around" the phase space.

3 The software

We carefully planned the object-oriented structure of our code in order to allow for the best reusability of its parts. In Figure 3a it is possible to inspect the classes and the inheritance relations. In a nutshell, we divided the classes into two categories: those inheriting from the parent classes `Graph` and `NodeValue`, and those defining the Metropolis Algorithm. The class

`SimulationSizeFixed` performs the simulation: in Figure 3b it is possible to see the relation of its attributes to the other classes.



(a) Hierarchy Diagram (b) Collaboration Diagram

Figure 3: These diagrams have been generated by Doxygen

Thanks to the class `Graph` we do not need to disambiguate between `Lattice` or `Powerlaw` graphs (polymorphism), and it is enough to define their own methods. It is worth to mention the accurate technique we used to create the power law graph. We generate a degree sequence with the discrete inverse transformation method applied to Eq. (6) and then we rewire link stubs following the configuration model (Newman 2010, Chapter 13), restarting every time we create a self-loop or a double edge. In `IsingMetropolis` we correct for the MA autocorrelation problem by computing autocorrelations and choosing only uncorrelated values. Finally, since we defined `NodeValue` as an abstract class, we implemented the UpDown ($s_i = \pm 1$) as well as the XY spin (2-dimensional) with a few lines of code, and other extensions can be made as readily.

4 Results

In Section 4.1 the standard results for an Ising model simulation on a 2-dimensional lattice are reported; in Section 4.2 we describe our findings on the Ising model on power law networks. Almost all the plots have been obtained by Root[1] macros we programmed.

[1] https://root.cern.ch/

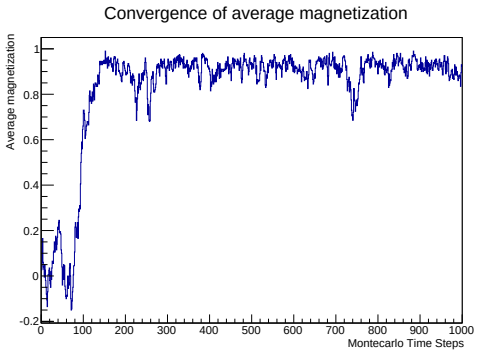


Figure 4: The simulation converges after approximately 200 Monte Carlo steps

4.1 Lattice

We ran every simulation for $N_{MC} = 10000$ Monte Carlo steps, which conventionally correspond to $N \cdot N_{MC}$ Metropolis steps. From Figure 4 it can be seen that the convergence of the MA occurs much in advance. However, that depends on the size of the lattice: for a 150×150 lattice it takes about 3000 Monte Carlo steps to reach convergence. For 200 temperature values in the range $0 < T < 5$ we computed the average magnetization $\overline{M}$ as defined in Eq. (3) and averaged over uncorrelated Monte Carlo steps, and we repeated this operation for $N = 100, 225, 324, 400$.

In Figure 5 we report our results for $N = 225$. For a comparison, consider Figure 1. Apart from the noisy points around $T = 0.5$, which may be due to local minima the MA was not able to escape from, the plots are similar. There are two main differences:

- In Figure 5 the phase transition is smoother. This is due to finite-size effects.
- The critical temperature is now close to the exact value from Eq. (1), rather than to the value found from Eq. (5).

In order to account for finite-size effects, we used the Binder Cumulant method (Binder 1981). In Figure 6 we plot $U_4 = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}$ as a function of T. The lines are parabolic fits, and they cross in a point whose T-coordinate is remarkably close to the exact value of the critical temperature, as expected.

Finally in Figure 7 we report the spin cluster rank-density plot at the critical temperature (spin clusters have been identified by a Breadth First Search). In line with the literature, it seems to follow a power law. For a visual intuition of what is going on, consider Figure 8: in Fig. 8a the system is at the critical temperature and a cluster structure emerges; in Fig. 8b the noise is too strong and the behaviour of the system is chaotic.

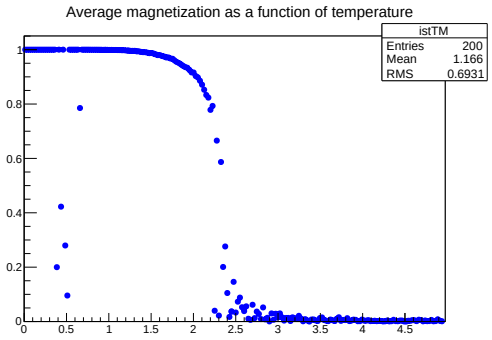


Figure 5

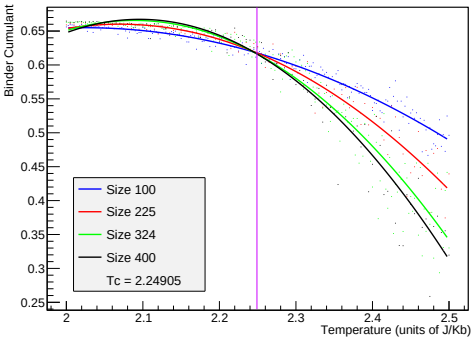


Figure 6: Binder cumulant as a function of temperature

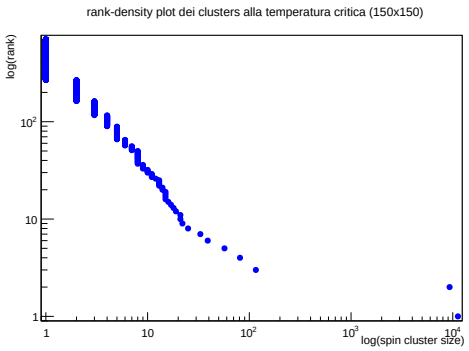
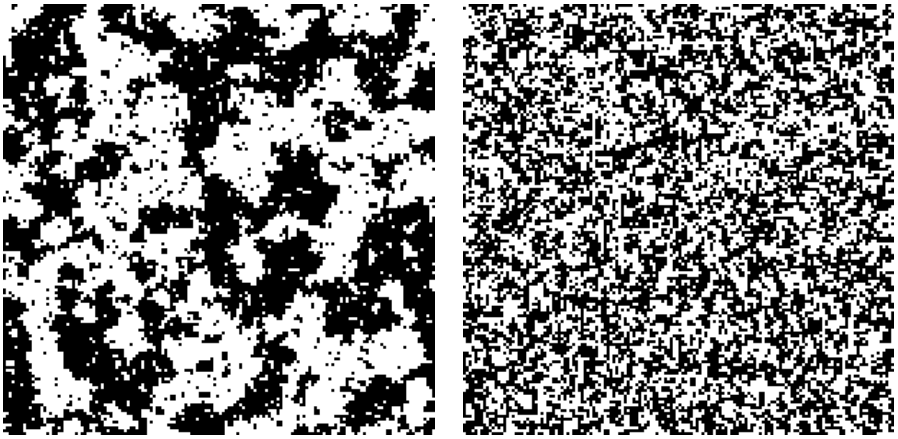


Figure 7



(a) $T = 2.25$ (b) $T = 4$

Figure 8

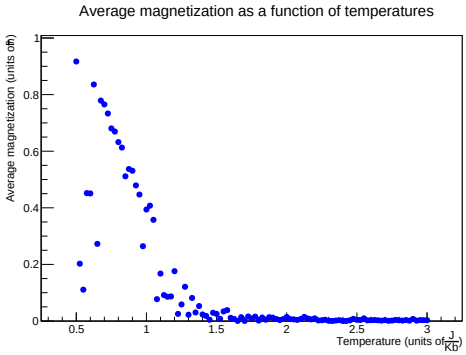


Figure 9: Parameters are $k_{min} = 1$ and $\gamma = 3$

4.2 Power law network

In Figure 9 we report the same plot as in Fig. 5, but on a power law graph rather than on a lattice. Nonetheless, there is a phase transition.

By varying the parameters k_{min} and γ we obtained the phase diagram as in Figure 10. The critical temperatures have been computed by fitting the data with an exponential function and considering a threshold $\overline{M} = 0.1$. The comparison with Figure 2 is rather good, but the role of finite-size effects is stronger than in the lattice case: our preliminary results showed that the critical temperature varies considerably with the size, so the difference with the theoretical results which assume $N \to \infty$ comes as no surprise. Notice that when $\gamma < 3$ Leone *et al.* (2002) found $T_C \to \infty$: for some values $\gamma \approx 2$ we numerically obtained the same result, the compiler stating that T_C was a `NaN`.

Finally, as it can be seen in Figure 11, also in the power law network

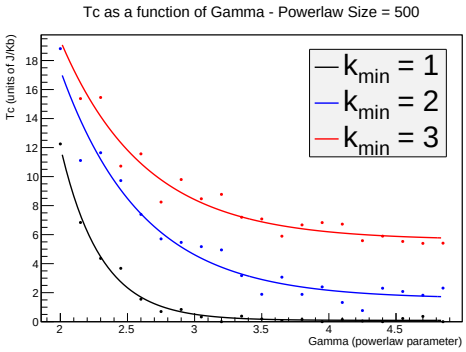


Figure 10

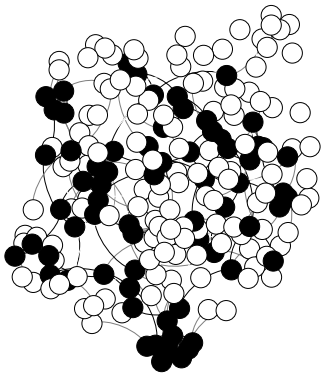


Figure 11: Visualization of the power law network. Black nodes are spins up, white nodes are spins down

case spin clusters exist.

5 Conclusion

We performed Monte Carlo simulations of the Ising Model through the Metropolis Algorithm. First, we considered the case of lattices of various size in order to check if our program was running properly, and we were able to obtain many results known in the literature. Then, we considered networks whose degree distribution was a power law. Though finite-size effects are noteworthy, our results show that the main conclusions of Leone *et al.* (2002) hold.

Almost any kind of Ising model can be simulated by our software with a few modifications. For instance, one could study Ising models on small-world

networks or Erdős-Rényi random graphs by simply defining how to create the networks. Moreover one could modify the Hamiltonian computation to account for random terms, and by these means study disordered systems. Our code is already set up for the XY model, which we may simulate on power law networks.

6 Bibliography

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