TIF150 ITCS mini project

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Information Theory analysis on 2D spin systems

Contents

1 Introduction

The aim of this project is to apply Information Theory analysis on a 2D spin system in order to get an expression for its entropy as a function of the temperature.

An ad-hoc-made "mathematica" small program (by kind concession of professor K. Lindgren) computes the analytical function of the entropy and its value at the simulated temperatures, as mean of comparison, to prove the validity of the results.

Another way to compute the entropy is adopted, using an approximation derived from the (known) magnetization of the grid. The main differences with the block entropies are discussed, pointing out where and why the approximation doesn't catch all the important properties of the system.

All the formulae used for the information theoretical approach are taken from the lecture notes ([1]) of the course and from [3]. For the statistical physics part and the Ising model details can be found in [2].

2 Background knowledge

The Ising Model

The simulation consists of implementing the Ising model and solve it with a Monte Carlo Markov Chain method.

The energy of the system is taking into account the spin interaction (J, positive for a ferromagnetic material) and the spin moments of the atoms (in this case we assume there is no external field):

$$H = -J \sum_{<i,j>} S_i \, S_j, \tag{1}$$

where $< i, j >$ means i and j are nearest neighbors. The sum runs over all the atoms in the lattice.

For every fixed temperature, the Markov Chain modelled represents the states accessible to the system, i.e. the possible combinations of spins up and down. Starting with a completely random configuration, the chain will be driven to an equilibrium state thanks to the Metropolis algorithm applied. It consists of proposing some changes in the state of the system and accept it with a certain (energy based) probability. More specifically, each proposed change is made by flipping a random spin and computing the change in energy it caused ΔE. If the $\Delta E \leq 0$, the change is always accepted, otherwise it is accepted with probability

$$P = e^{-\frac{\Delta E}{k_b T}}. \tag{2}$$

(to see details check [2]).

After a certain number of iterations (empirically set to ensure convergence according to the parameters of the model), when the Markov Chain is describing a typical equilibrium configuration for the system at the fixed temperature, the collection of useful data can start.

As any scientific experiment, data are always more reliable if they come out from a statistic. Furthermore, in order to have a good statistics all the samples of data to average from should be independent, and this is ensured by letting the system update some more times before collecting statistics again. All the samples are stored and the final reliable value will be an average of them.

Block entropy

The "statistic samples" that the program computes are the block entropies, for certain block lengths, according to the theory (see [1]):

$$S_{B^{(i)}} = \sum_m P(B_m^{(i)}) \sum_x P(x|B_m^{(i)}) log \left(\frac{1}{P(x|B_m^{(i)})} \right), \tag{3}$$

with $P(B_m^{(i)})$ the probability of finding block m of length i. m runs over all the possible blocks of length i, while x is the possible spin value of the atom under consideration. Here i=1,2,3,4.

Each block consists of 2*i units: starting from position of atom x, block 1 will contain its left and down neighbor; block 2 contains two consecutive units at the left x: its down neighbor (also present in block 1) and the unit at the right of the down-neighbour of x; and so on.

The reason for this block structure is investigated in [3].

Since each site has a spin that can only assume two states, +1 and -1, the blocks we are considering are just all the combinations of these two values. Hence, there are 2^2 possible blocks of dim 1, 2^4 different blocks of dim 2, and so on.

The probability of a block appearing is computed statistically from the system, once it has reached the equilibrium configuration for a given temperature.

Entropy approximation through magnetization

Starting from Boltzmann's formula:

$$S = k_b \; log(\Omega). \tag{4}$$

Where k_b is the Boltzmann's constant and Ω is the volume of the phase space of the system, in a discrete case the number of microstates accessible to the system.

Each temperature in this model gives unequivocally and symmetrically one (or, more precisely, two equally probable) magnetization, i.e. it determines an average fixed number of spins pointing up and down in the lattice, which are easily counted. From any fixed temperature in the model, hence, and knowing the total number of spins in the system N, $N_+(T)$, $N_-(T)$, respectively number of spins pointing up and down, can be found:

$$m(T) = N_+(T) - N_-(T), \tag{5}$$

the average magnetization. Note that also $N_+(T) + N_-(T) = \mathrm{N}$ holds and that we can write

$$N_+(T) = \frac{(N + m(T))}{2} \quad and \quad N_-(T) = \frac{(N - m(T))}{2}.$$

To give that magnetization there will always be on average the same number of spins pointing up and down, that comes in different arrangements of $N_+(T)$ and $N_-(T)$ spins. The number of available microstates for every fixed temperature will then be the number of all the possible ways this can happen:

$$\Omega_{m(T)} = \binom{N}{N_+(T)} = \frac{N!}{N_+(T)!N_-(T)!}. \tag{6}$$

Now considering these big numbers (infinite) approximations are needed: using Stirling's formula

$$N! \sim \; N^N \; e^{-N} \tag{7}$$

it becomes

$$\Omega_{m(T)} \sim \left(\frac{1 + m(T)}{2}\right)^{-N(\frac{1+m(T)}{2})} \quad \left(\frac{1 - m(T)}{2}\right)^{-N(\frac{1-m(T)}{2})} \tag{8}$$

Finally, combining eq.s (4) and (8) we get a reasonable expression that MATLAB can compute:

$$s(T) = -\left(\frac{1 + m(T)}{2}\right) log\left(\frac{1 + m(T)}{2}\right) - \left(\frac{1 - m(T)}{2}\right) log\left(\frac{1 - m(T)}{2}\right) \tag{9}$$

Note that the s from eq. (9) is the normalized entropy, obtained dividing by N the derived S expression.

It is now useful to understand when this approximation gives reliable values: since it is only based on the magnetization, and since the magnetization has a sharp drop to 0 at the curie temperature, this entropy estimation will be the same maximum value (log2=0.6931, meaning random spin configuration for the system) for a range of temperatures going from the transition to infinity. Indeed, looking at reality, this is a too simplified version: the system will not show randomness sharply at Tc. It will instead show some kind of patterns arising, leading smoothly to a more chaotic configuration. This feature, that can't be shown from the approximation, is well captured from the information theory analysis. See Further tests section for more specific examples.

3 Implementation

The program

For this simulation the parameters are set to J=k_b=1, $S_i = \pm 1$. With these settings the transition temperature is computed to be at Tc=2.2. The grid of atoms is set to 80x80. 3 million of burn in iterations are used to ensure convergence, and 50000 iterations between two sampling procedures.

First all, once defined the parameters of the model, i.e. grid dimensions, number of burn in iterations and the number of iterations to perform for independent sampling, the atoms in the lattice are numbered and a position in the grid is assigned to them (matrix "grid-pos", of dimensions "grid-dim"=total number of atoms in the lattice by 2, x and y coordinates). This indices are used in the same way in a vector called "spin-list", where each element represents the spin of a specific atom. According to this same disposition, for each numbered atom a list of nearest neighbours is defined ("nn-list"), containing in each row the numbers of the 4 nearest neighbours of the index of the atom of the corresponding row. This list is constructed such to implement boundary conditions, which means that, for example, the nearest neighbours of the atom positioned at the up right corner will be: the one at the top left corner (right neighbor), the one at the down right corner (up neighbor), the one on the same edge just a row lower (down neighbor) and the one at the left of the corner (left neighbor).

All the possible surrounding blocks of dimension 1, 2, 3 and 4 (block i contains i neighbours in left and down direction) are constructed and stored. After the burn in, all the atoms of the lattice are scanned one by one and their surroundings compared to the blocks stored, computing the rate of appearance of each block.

For each temperature there are 20 samplings for the block entropies and their average is stored and plotted as the final value.

Results

In the table below are reported the results obtained with the above described settings. 10 different temperatures are investigated. The block entropy for block i is named SBi, i=1,2,3,4. The entropy computed with the approximated formula based on the magnetization is indicated with Sm, while S is the entropy computed from the analytical formula with mathematica:

Table 1. Entropy as function of temperature and values computed

T	SB1	SB2	SB3	SB4	Sm	S
0.2	0	0	0	0	0	0
0.8	0.0299	0.0258	0.0241	0.0232	0.1331	0.0005
1.2	0.0537	0.0412	0.0385	0.0376	0.2632	0.0108
1.7	0.1236	0.1090	0.0131	0.0991	0.5986	0.0711
2.1	0.2536	0.2367	0.2286	0.2173	0.6791	0.1936
2.5	0.4502	0.4381	0.4322	0.4158	0.6907	0.4369
2.9	0.5343	0.5269	0.5222	0.5057	0.6931	0.5290
3.5	0.5948	0.5907	0.5867	0.5703	0.6931	0.5922
5.0	0.6486	0.6468	0.6431	0.6275	0.6931	0.6488
10.0	0.6824	0.6814	0.6776	0.6626	0.6931	0.6828

It follows the plot of the block entropy result (figure [1]):

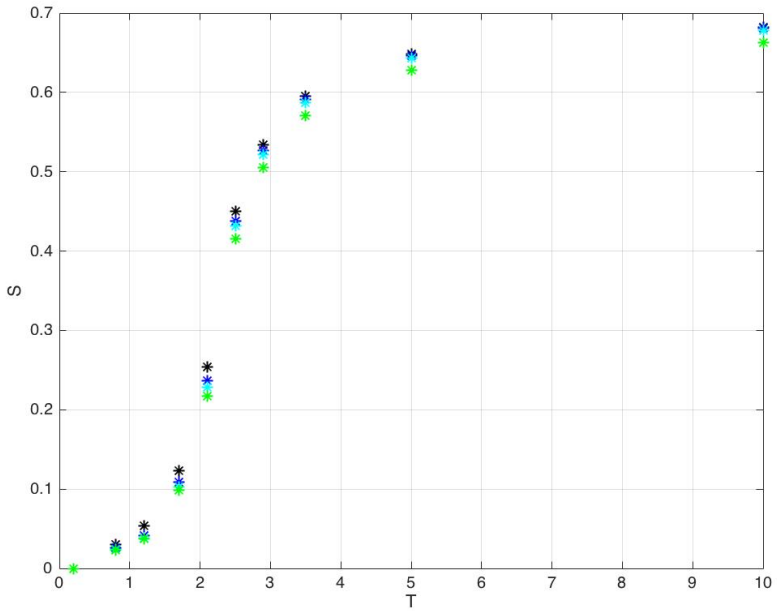

Figure 1. Block entropy as a function of temperature. The values reported are showing SB1 in black, SB2 in blue, SB3 in cyan, SB4 in green.

Some examples of the system at T=0.8 (figure [2]), T=2.1 (figure [3]) and T=10.0 (figure [4]).

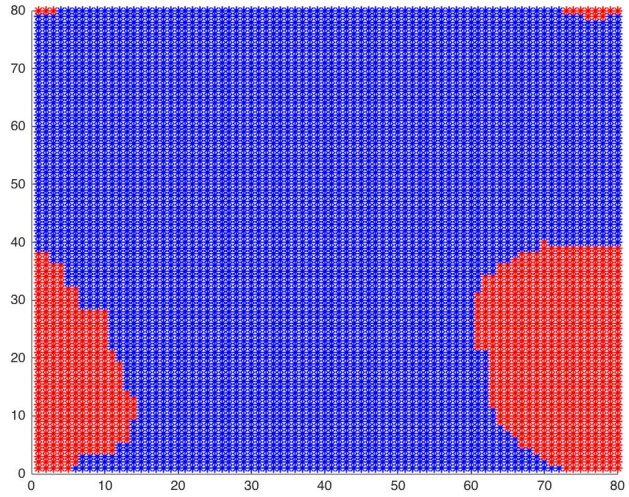

Figure 2. Spin system at temperature T=0.8, example of equilibrium state.

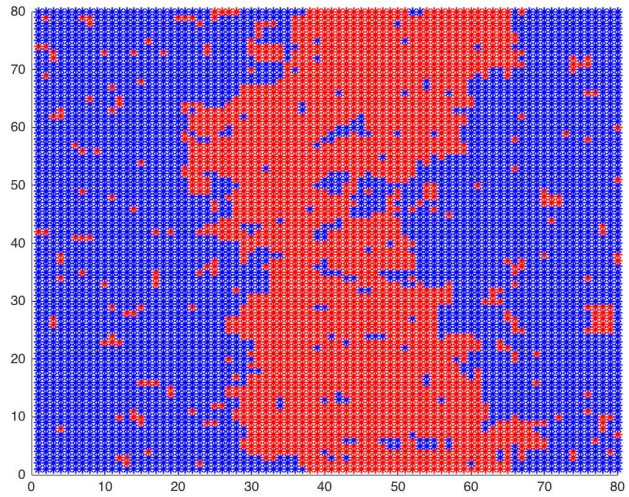

Figure 3. Spin system at temperature T=2.1, example of equilibrium state.

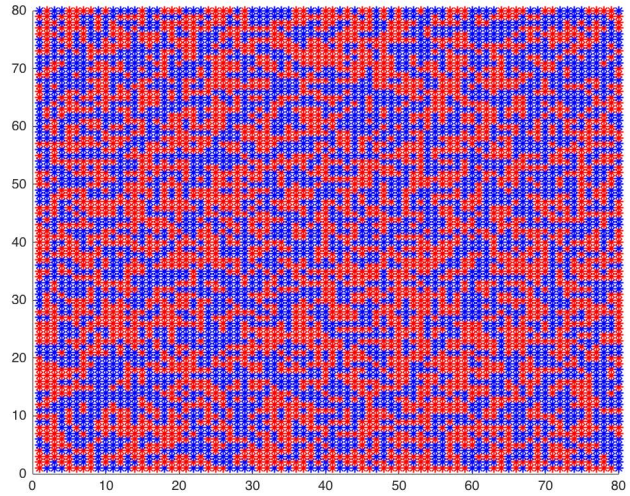

Figure 4. Spin system at temperature T=10.0, example of equilibrium state.

4 Further tests

More interesting properties of the information theoretical approach are found when just playing around with the configuration of spins: when the statistic is taken on a system with specific spin patterns, the block entropy changes dramatically according to the block dimension.

One example is given in fig. [5]: the spins are set alternatively up and down, so that Sm=0.6931 (=log2, max entropy), but the block entropy shows there is a certain order in the structure: SB1=0.0188, SB2=0.0185, SB3=0.0183, SB4=0.0181.

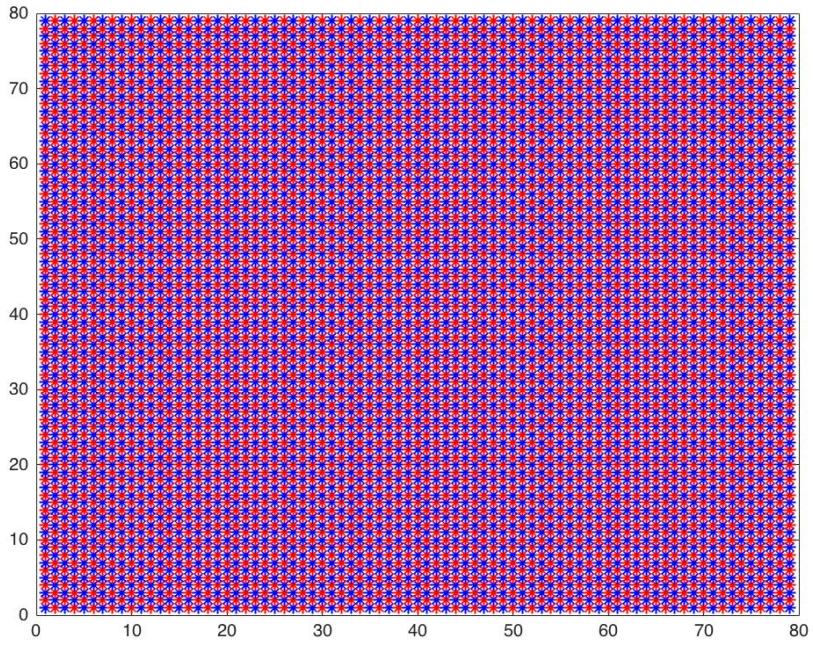

Figure 5. Particular case: arrangement defined in an alternate single spin pattern.

A similar, more dramatic, example is shown in fig. [6]: the spins are chosen to be in the same amount pointing up and down, hence magnetization=0, Sm=0.6931, but then the computed block entropies are SB1= 0.6335, SB2=0.0329, SB3=0.0070, SB4=0.0070.

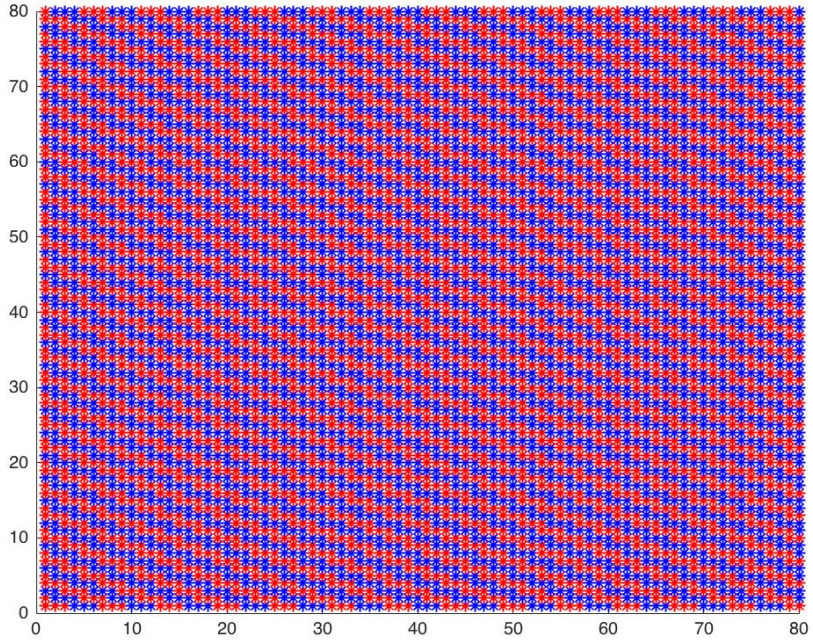

Figure 6. Particular case: arrangement defined in a diagonal pattern.

Particularly in this last case, the information gained tells that for a single element neighbourhood the pattern is not obvious, but taking into account 3 or 4 neighbours every time the recursiveness is more evident, and the block entropy per bigger blocks drops sharply.

5 Conclusions

Simulations are common and important tools in physics, especially when testing approximations, exploring complex systems, studying collective properties or behaviors that arise from micro and single particle dynamics developments. But, apart from the utility in new discoveries and/or for a better understanding of the system under consideration, these applications usually offer a good starting point for new researches and curiosity. With all these considerations in mind, together with the fact that it is extremely funny, I chose to focus on 2-D spin systems from an Information theory point of view.

It was satisfactory to find that the program was computing entropy with actual good agreement with the theoretical value (most of the times), and it was surprising to discover new properties of block entropy, like the "pattern recognition" in particular spin configurations when playing with it. This specific case brought to light that in the critical phase of the system (close to the curie temperature), when disorder is allowed, the system evolves maintaining patterns, and in that phase a lot of spatial information is stored. Having more time, I would have gone deeper into this, investigating the relation between spatial information and temperature, and using more block lengths, and playing with more elaborate spin configurations to detect patterns.

References

[1] Kristian Lindgren, *Information theory for complex systems*, Lecture notes, January 20, 2014.

[2] Roger Bowley, Mariana Sànchez, *Introductory statistical mechanics*, Second edition, University of Nottingham.

[3] Kristian Lindgren, *On the equivalence between stochastic baker's maps and two-dimensional spin systems*, Complex Systems Group, Department of Energy and Environment, Chalmers University of Technology, June 2010.