

Complexity and critical behavior

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Systems exhibit a variety of different features in physical quantities when undergoing a phase transition. In this project we choose magnetic systems as a typical candidate that exhibits a phase transition and try to understand the critical behavior using the Ising model with nearest neighbor interaction. Traditionally physicists have studied and understood how various quantities such as the magnetization, heat capacity, susceptibility etc. behave close to the critical point. In this report we study the behavior of Ising models as a function of temperature in one and two dimensions. Further, we explore how various measures that we learned about in the course such as entropy rate, excess entropy and statistical complexity vary with temperature for the Ising model in one dimension and setup the problem to study the variation of these quantities during a phase transition when we go from one to two dimensions.

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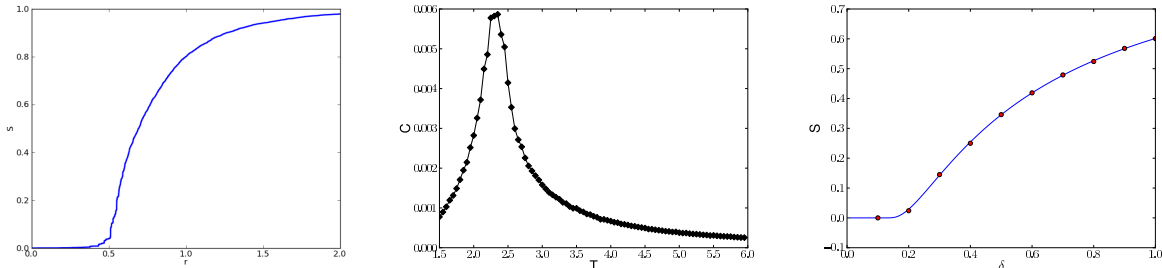


FIG. 1: The figure shows physical quantities of different systems that undergo a phase transitions. Left: Fractional size of the giant component as function of edge density for an Erdos-Reyni random graph. Middle: Heat capacity of a 16×16 lattice as function temperature. The characteristic peak is around the critical temperature. Right: Fractional size of the giant component as function of the probability (δ) of adding an edge in a growing graph where a node is added at every time step and an edge is added with probability δ .

I. INTRODUCTION

A variety of different real world systems exhibit critical behavior. Some of the more prominent examples of such systems are certain metals that exhibit spontaneous magnetic order when the temperature is lowered, even in the absence of a magnetic field, networks where a giant component emerges at a particular point as the edge density of the network is increased. Fig. 1 shows three different systems that exhibit a phase transition. The phase transition is usually characterized by several interesting behavior of physical quantities. For example, in magnetic systems, around the critical point the magnetization grows as a power-law in the difference between the current temperature and the critical temperature, the susceptibility and the heat capacity typically diverge at the critical point i.e. the system is extremely sensitive to changes in the physical quantities at the critical point. The above behavior in the physical quantities are considered to be an indication of the change in the spatial organization in the system. We expect the measures of complexity to be able to pick up this change and exhibit behavior that is characteristic of the phase transition.

One of the simplest and most celebrated models of phase transitions is the Ising model [1–3]. The model captures several interesting features of the phase transitions even with just nearest neighbor interactions. We shall study the Ising model in one and two dimensions and examine the various complexity measures in order to understand how these quantities behave while the system undergoes a phase transition.

II. THE ISING MODEL

The hamiltonian for the Ising model with nearest neighbor interaction is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i \quad (1)$$

We shall restrict ourselves to nearest neighbor interactions since they are sufficient to explain phase transitions in two dimensional systems. The S_i represents spins that can take the value $+1$ (-1) if they are aligned with (against) the magnetic field whose magnitude is given by

B . The first term in the Hamiltonian represents the interaction between the spins. The term suggests that if the two spins are aligned the energy is lowered by J units. Similarly the energy is reduced by B units when a spin is aligned with the magnetic field.

The system tries to minimize its Free energy which is given by

$$F = U - TS \quad (2)$$

Consider the case when $T = 0$. At this temperature the free energy is entirely dependent on the internal energy and is minimum when the internal energy is minimum. Therefore at this temperature all spins would be aligned with each other. Let us now consider the temperature is infinity. Here the free energy is governed by the entropy and the stable state at this temperature is one in which the spins are randomly oriented independent of each other. Clearly the system is organized quite differently between these two temperatures. The temperature at which there is a transition between these two states, if it exists, is known as the critical temperature (T_c).

Apart from the internal energy (U), the various physical properties that are traditionally studied are:

- Magnetization $M = \frac{\sum_i S_i}{N}$ where N represents the total number of spins in the system,
- Susceptibility $\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{T}$,
- Heat Capacity $C = \frac{\langle U^2 \rangle - \langle U \rangle^2}{T^2}$,
- Two point correlations $\langle S_i S_j \rangle - \langle S \rangle^2 = e^{-l(i,j)/\zeta}$,
- Correlation length ζ .

III. MONTE CARLO SIMULATIONS

The Ising model is studied numerically using Monte Carlo simulations. The underlying basis of these simulations is the principle of detailed balance and the fact that our system is ergodic. The simulations in the report are performed using the heat bath algorithm. One sweep of the algorithm is when on an average each spin in the system is considered to be flipped. The spin is flipped in if it lowers the energy i.e. $\Delta U < 0$ of the system, and if $\Delta U > 0$ it is flipped with the probability given by:

$$P(S_i = -S_i) = \frac{\exp(-\beta\Delta U)}{1 + \exp(-\beta\Delta U)}. \quad (3)$$

We start the system from a random initial configuration and let the system reach equilibrium. Once this is achieved, at the end of each sweep the internal energy and magnetization of the system is recorded. Various thermodynamic quantities can be obtained from the various moments of these two physical quantities as detailed in the previous section. The two point correlations are also computed at the end of each sweep and averaged over many sweeps.

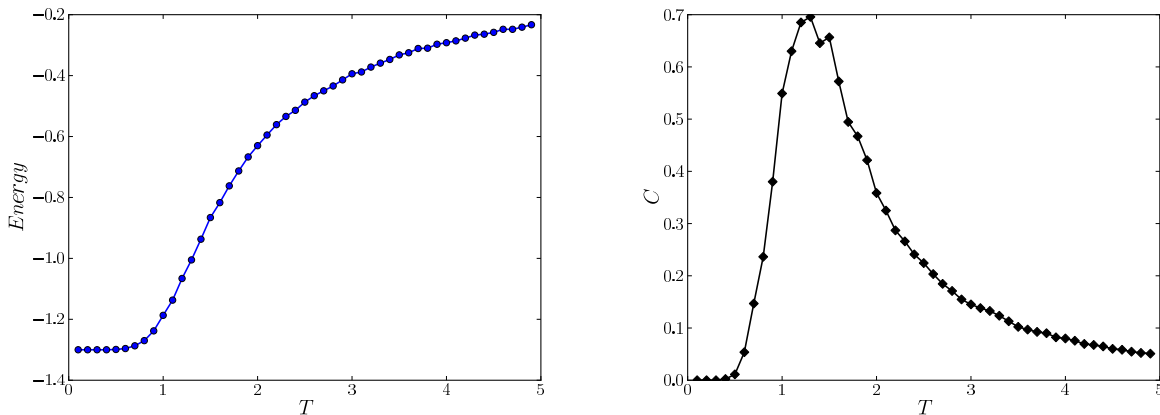


FIG. 2: The figure shows the variation of the internal energy (left) and the heat capacity (right) with temperature of a system of 1-D spin chain with $B = 0.3$.

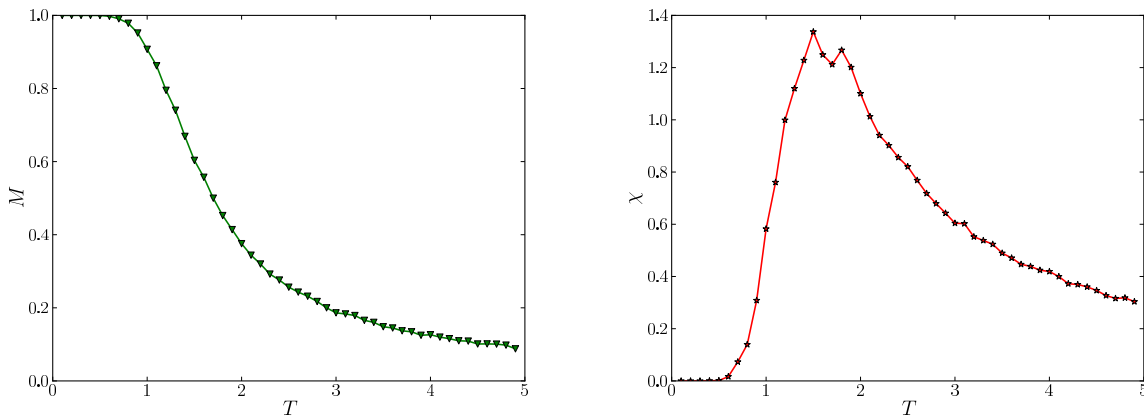


FIG. 3: The figure shows the variation of the Magnetization (left) and the susceptibility (right) with temperature of a system of 1-D spin chain with $B = 0.3$.

IV. ONE DIMENSIONAL SPIN SYSTEMS

We study the behavior of the 1-D spins systems with nearest neighbor interactions. We start by reporting the observed properties of the traditionally studied physical quantities and then explore the ϵ -machine presentation of 1-D spin configurations and the measures of complexity. We consider the 1-D spin chain of length L represented by the Hamiltonian

$$\mathcal{H} = -J \sum_{i=1}^L S_i S_{i+1} - B \sum_i S_i \quad (4)$$

with periodic boundary conditions. As the length $L \rightarrow \infty$ the boundary condition will not play a significant role. The thermodynamic properties of the system is studied using Monte-Carlo simulations. Fig. 2 and Fig. 3 show how the various thermodynamic properties vary with temperature when the magnetic field is fixed at $B = 0.3$.

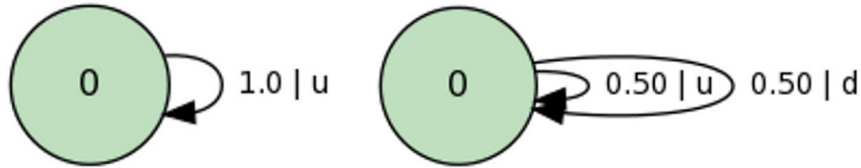


FIG. 4: ϵ -machine presentation of the 1-D spin chain at (left) $T = 0$ and (right) $T = \infty$.

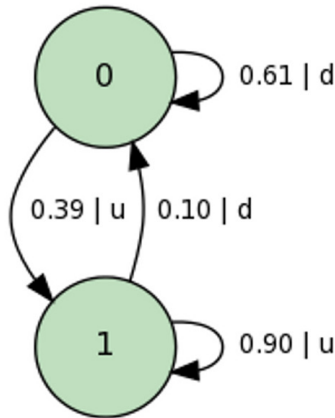


FIG. 5: The recurrent component of an ϵ -machine presentation for a spin chain with $T = 1.5$ and $B = 0.3$.

It must be noted that one dimensional system does not show phase transition at a non-zero temperature due to the fact that in order to have disorder in the system the energy cost is just twice the pair-wise interaction thereby making it extremely easy for the system to be disordered.

Let us now examine the computational mechanics of the 1-D spin chain. Let us denote a spin oriented along the magnetic field with ‘u’ and spin oriented against the magnetic field with the symbol ‘d’. We can thus represent the spin chain with a string of length L with the binary alphabets ‘u’ and ‘d’. Given the set of alphabets to the left we would like to be able to predict the next alphabet. Let us start by thinking about the ϵ -machine presentation for the spin chain at zero temperature. At this temperature all spins are aligned with the magnetic field therefore the spin chain can be represented by a string of repeated ‘u’s. Now consider the case when the temperature of the system is infinite. When the temperature is really large each spin is independent of its neighbors and thus the ϵ -machine presentation would be just the fair coin. Fig. 4 shows the ϵ -machine for these two scenarios.

Let us now consider the case of finite temperatures. Since we consider only the nearest neighbor interaction it is easy to see that the probability of next spin being in the up or down state would only depend on the last spin. Thus for any finite temperature the system has a Markov order of one. The recurrent part of ϵ -machine presentation always has two states for any finite temperature and only the transition probabilities vary as the temperature is varied. Fig. 5 shows a typical example of an ϵ -machine presentation for finite temperatures.

We have thus understood how to construct ϵ -machine presentations for the one dimensional spin chain and we can now focus on various measures of complexity that can be easily obtained from these presentations. Fig. 6 shows the entropy rate, statistical complexity and

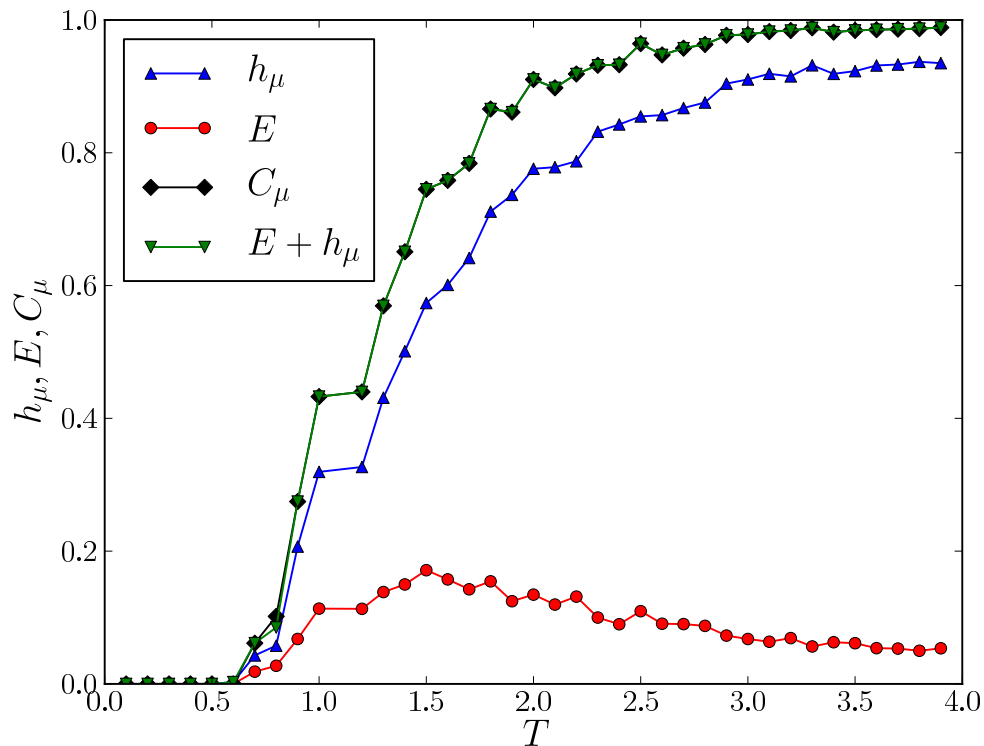


FIG. 6: Figure shows how various measures of complexity vary with temperature for a 1-D spin chain with the value of magnetic field set to 0.3.

the excess entropy of the system varies with temperature. Although not seen in the figure, the statistical complexity of the system increases asymptotically until $T = \infty$ where the process can be represented by a fair coin and C_μ abruptly drops to zero. It is important to note that the green curve which is the sum of the excess entropy and the entropy rate falls exactly on top of the black curve that represents the statistical complexity. In general it can be shown that [5]

$$C_\mu = E + Rh_\mu, \quad (5)$$

where R represents the range of interaction. In our case since we consider just the nearest neighbor interactions $R = 1$. Further one can see that excess entropy E is different from other physical quantities as the temperature at which it reaches a maximum is different from where other physical quantities such as the heat capacity or susceptibility reaches a maximum. We have thus examined the measures of complexity for the system of 1-D spin chains with nearest neighbor interactions. However the 1-D spin chain does not exhibit a phase transition and we would have to move from one to two dimensions in order to study how these measures behave during a phase transition.

V. TWO DIMENSIONAL SPIN SYSTEMS

In this section we study the behavior of the Ising model on a square lattice with nearest neighbor interactions. Unlike the one dimensional case, this system exhibits a phase

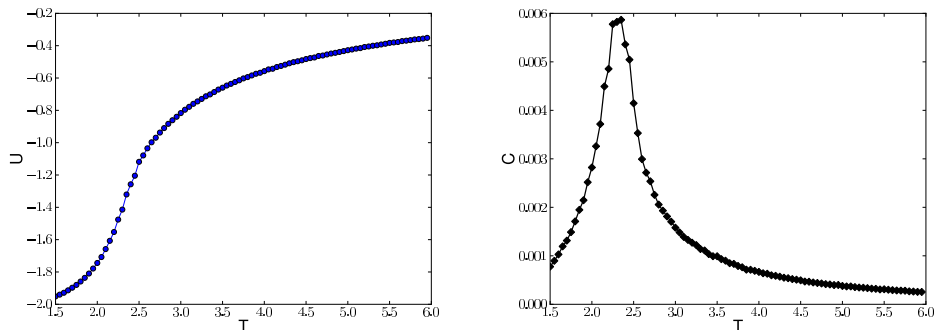


FIG. 7: The figure shows the variation of the internal energy (left) and the heat capacity (right) with temperature for a 16×16 square lattice.

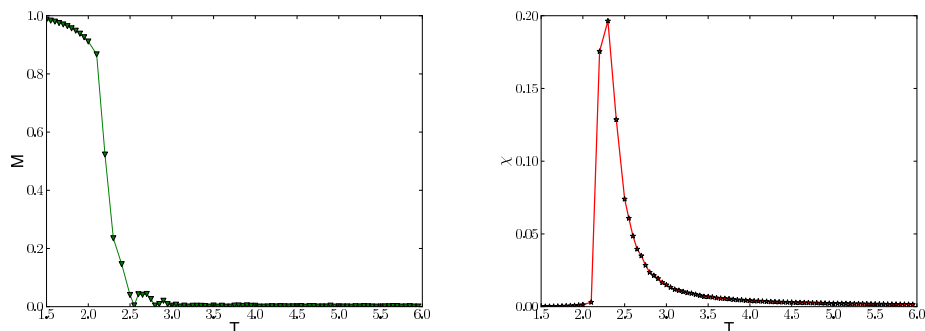


FIG. 8: The figure shows the variation of the magnetization (left) and the susceptibility (right) with temperature for a 16×16 square lattice.

transition at a non-zero temperature of $T_c/J = 2.26$. The fact that there is non-zero critical temperature can be attributed to the fact that there are many paths from one spin to another and isolating one spin unlike in the one dimensional case does not really shield the next spin from previous spins. Fig. 7 and Fig. 8 show how various thermodynamic properties, obtained from Monte Carlo simulations, vary with temperature. Note that both the susceptibility and the heat capacity have a maximum around the critical temperature. As we increase the system size these two quantities diverge suggesting that the system is extremely susceptible to small fluctuations when it is critical.

The computational mechanics of two dimensional systems is not straight forward. One of the most important reasons for this is the fact that there is no natural order in which we can read the spins in such as left to right in the one dimensional case. Sampling of spins through a one dimensional path results in measuring properties of not only the system but also of the path [7]. Therefore there is a need to adapt the various quantities defined for one dimensional systems to that of two dimensions. We start by defining

$$h_\mu = \lim_{(N,M) \rightarrow \infty} \frac{H(N, M)}{NM} \quad (6)$$

where the limit is taken such that the aspect ratio N/M is a fixed constant. The excess entropy also needs to be adapted to two dimensions. We first recall that in one dimension

we had three different definitions of excess entropy namely,

- Convergence

$$E_c = \sum_{L=1}^{\infty} h_{\mu}(L) - h_{\mu} \quad (7)$$

- *Subextensive*

$$E_s = \lim_{L \rightarrow \infty} H(L) - h_{\mu}L \quad (8)$$

- Mutual information

$$E_I = \lim_{L \rightarrow \infty} I[S_{-L} \dots S_{-2}S_{-1}; S_0S_1 \dots S_L] \quad (9)$$

and all three definition turned out to be the same [6]. However in two dimensions these three quantities are different from each other and can be adapted as follows:

- Convergence

$$E_c = \sum_{M=1}^{\infty} (h_{\mu}(M) - h_{\mu}) \quad (10)$$

- *Subextensive*

$$H(M, N) = E_s + E_s^x M + E_s^y N + h_{\mu}MN \quad (11)$$

- Mutual information

$$E_I = \lim_{M, N \rightarrow \infty} I[(M, N)\text{block}; (M, N)\text{block}] \quad (12)$$

The statistical complexity in one dimension was defined in terms of the stationary distribution of our ϵ -machine presentation. However we do not (yet) have an equivalent presentation for 2-D systems. The direction for future study is to compute how entropy rate and various excess entropy vary close to the phase transition and also attempt an ϵ -machine presentation for these processes that would lead us to a notion of statistical complexity in two dimensions.

VI. CONCLUSION

In this report we examined how phase transitions exhibit interesting physical properties and devoted our effort to reviewing tools that would help us understand the behavior of measures of complexity in these systems. In particular we focused on the Ising model and discussed its behavior in one and two dimensions. We studied computational mechanics of the one dimensional spin chain and established how these measures might provide useful insights about the physical system. Further, we presented the problems encountered when going from one to two dimensions, briefly outlined possible ways to adapt the various measures to two dimensions and set the stage for studying the critical behavior of the various measures of complexity in two dimensional systems.

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