Connectivity of Undirected Graphs and Phase Transitions in the Ising Model

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We explore the effect of several graph theoretic properties associated with connectivity on phase transitions in the Ising model setting. The model simulates a heat-bath dynamic setting on ferromagnetic ordering, expanding on prior work done on very structured undirected and directed graphs. The simulations show that the existence of phase transitions is intimately related to connectivity, and that the density of edges has implications on the critical temperature required for the phase transition. We also look into approximating the Ising universality class by relaxing conditions on undirected lattices.

I. INTRODUCTION

The Ising model is a popular abstraction of a system of microstates in statistical mechanics, whether it be modeling the interactions of spins in the presence of a magnetic field to studying phase transitions of water in different temperatures and pressure. Its broad applications makes it extremely desirable to understand and refine. Traditionally, the network is taken to be a very uniform and symmetric graph, such as a two-dimensional lattice. This is a well-studied system, and in 2015, Lipowski et al. considered heat-bath dynamics in a directed graph setting, looking at triangular, square, and cubic lattices [1]. They show that even with the introduction of directed edges, the model still undergoes phase transitions and may even belong to the Ising universality class.

A natural next step, then, is to tackle understanding dynamics in a less structured setting. In this paper, we use random undirected graphs to explore the effect of graph connectivity on critical temperature of phase transitions on the ferromagnetic Ising model. In particular, we focus on graphs that have certain graph-theoretic properties that are measures of how connected a graph is. We begin by retaining some structure in the regular graph setting. Then, we move to Erdős–Rényi graphs, which can be viewed as the simplest sort of random graphs. Finally, we look at algebraic connectivity to quantify the notion of connectivity in the most general way, and study its relation to phase transitions.

II. BACKGROUND

The particular physical setting we are interested in is ferromagnetic ordering in the heat bath dynamics paradigm. Similar to Lipowski et al., [1], we begin with N nodes (numbered $1, \dots, N$) with spin represented as $s_i = \pm 1$. Each node i will have a set of neighbors $\mathrm{adj}(i) \subseteq [N] \setminus \{i\}$, where the neighbor relation is symmetric. Define the transition probability t_i as

$$t_i = 1 + \exp(-2n_i/T)$$

where $n_i = \sum_{v \in \mathrm{adj}(i)} s_v$ and T is the temperature of the system. At each time step, we have N update steps. Each update step picks a node i uniformly at random, and sets its spin to 1 with probability t_i and -1 with probability $1 - t_i$. The magnetization of the system after T time steps is

$$\frac{1}{T}\left(\frac{1}{N}\sum_{i \in [N]} s_i\right)$$

That is, it is the sample mean of the average spin of the graph. This provides a concrete metric to describe our system.

In order to quantify the complexity of the graph, we introduce the notion of a regular graph. A graph is **d-regular** if each node i has exactly d neighbors. In terms of the preceding formalism, $|\mathrm{adj}(i)| = d$ for all $i \in [N]$. To generalize this notion of neighbors, we define the **degree** of node i to be the number of neighbors; alternatively, it is the number of edges that contain i. Therefore, we can rephrase a d-regular to be a graph where each node has degree d.

An **Erdős–Rényi** graph is a graph on N vertices with an edge between nodes i, j (for $i \neq j$) with probability p. This is usually written as the random variable $G(N, p)$. This graph is at the core of studying random graphs due to its simplicity and the existence of certain critical probabilities, similar to that of the percolation threshold in the Ising model 2. In particular, there is a famous result that for $p = 1/N$ we see a transition from fairly sparse graphs (with components of size $O(\log N)$) to a graph with one large connected component, called the giant component. Again, there is a very clear parallel between this and the percolating cluster in the Ising model view.

Finally, the **algebraic connectivity** of a graph is concept that comes from spectral graph theory 3. Spectral graph theory is a field that bridges together graph theory and linear algebra, with the main focus on what is called the *Laplacian* matrix, L. This is an $N \times N$ matrix, with entries as follows:

$$L_{i,j} = \begin{cases} |\mathrm{adj}(i)| \text{ if } i = j \\ -1 \text{ if } j \in \mathrm{adj}(i) \\ 0 \text{ otherwise} \end{cases}$$

In the undirected case, L is symmetric so we immediately get its eigenvalues are real by Spectral theorem. Spectral graph theory looks at these eigenvalues (and corresponding eigenvectors) to connect computational trends with graph properties. The second smallest eigenvalue, λ_2, is the **algebraic connectivity** of a graph. It generally represents how well connected a graph is. It can also be a measure of the synchronizability of a network, which is very desirable if we want to study ferromagnetic ordering.

III. METHODS

We use the standard Monte Carlo approach to simulating the Ising model. The general approach will follow what is described in the previous section: for each time step, select a random node i uniformly at random and set its spin according to the physical dynamics of the system. This is applied N times within the time step so that each node is updated on average 1 time. The initial state of the system will be all spin up, or $s_i = 1$.

We also follow the approach of Lipowski et al. by first allowing the system to reach a steady state, and then computing the magnetization of the system over subsequent time steps. The temperature is then varied to get a plot of temperature vs. magnetization. To quantitatively determine a phase transition, we deem a drop of more than 0.1 in magnetization over a temperature gradient to qualify as phase transition. The temperature at which this happens will be our critical temperature, T_c.

In order to generate graphs, we make use of the **NetworkX** package freely. In particular, there are built in methods to generate Erdős–Rényi graphs and regular graphs with specified degree. We can then convert these graphs to our own custom graph class and then perform the above Ising model simulation.

IV. RESULTS AND DISCUSSION

All code can be found in this repository.

A. d-Regular Graphs

The first experiment fixes the number of nodes in the graph at $N = 100$ and considers regularity in the range $d \in [5, 45]$. This allows us to look at a somewhat structured graph with higher density of neighbors than that of a traditional lattice. As seen in Figure 1, we do observe phase transitions in the regular graph case. The critical temperature seems to increase as the degree increases, which could be attributed to the increasing connectivity of the graph. To check if it falls under the Ising universality class, we attempt to fit the magnetization, m, to $|T - T_c|^\beta$, which we see in Figure 2. We expect a β value of around 0.125, the theoretical value for an Ising model, but we see high variance in the β value. As a result, we conclude that dense, regular graphs are not good representatives of Ising models, despite the existence of a phase transition.

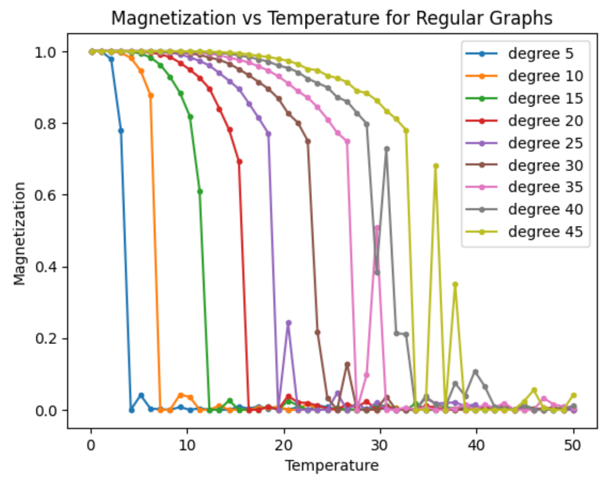

FIG. 1. Ising Magnetization for Regular Graphs ($N = 100$)

B. 4-Regular Graphs

The other (perhaps more physically realistic) experiment done on regular graphs fixed the degree at 4 and varied the number of nodes instead. The degree was chosen based on the two-dimensional lattice, which has average degree close to 4. These graphs should be less rigid than these lattices in structure, but shouldn't stray too far away from them. Indeed, in Figure 3 we see much more regularity in the fitted β values: they seem to vary in the $[0.11, 0.125]$ range, which is close to the theoretical value of 0.125.

After plotting the theoretical values against the experimental and fitted values, we see the difference is minimal (Figure 4). This suggests that in the 4-regular case, we obtain a strong approximation of the Ising universality class, despite the relaxation in graph structure.

C. Erdős–Rényi Graphs

In the $G(N, p)$ case, we look at the existence of phase transitions around the critical probability $1/N$. Here, we choose $N = 500$ and run simulations on graphs generated with p close to $1/500 = 0.002$. Figure 5 plots these results, and we can see that for $p > 0.002$, there seems to be a phase transition. For $p < 0.002$, the graphs do not indicate a strong phase transition but instead we see ordering achieved quite quickly, despite lower temperatures.

I believe this is connected to the idea that for $p < 1/N$, the largest component is of size $O(\log N)$ [2]. This means that achieving the steady state needs to be done on several systems of much smaller size, which should

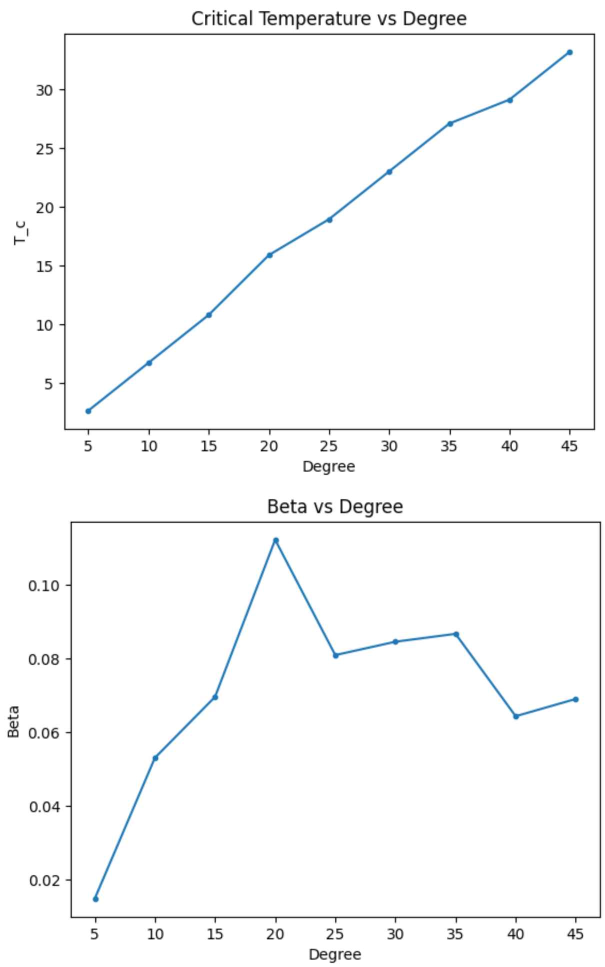

FIG. 2. Critical temperature T_c and fitted β value for $N = 100$

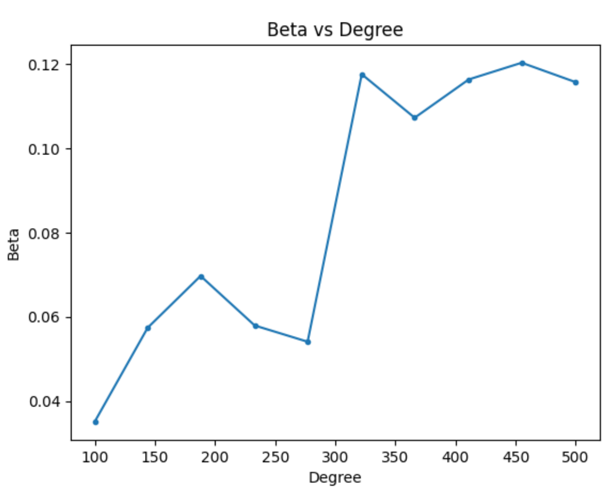

FIG. 3. Critical temperature T_c and fitted β value for 4-Regular Graphs

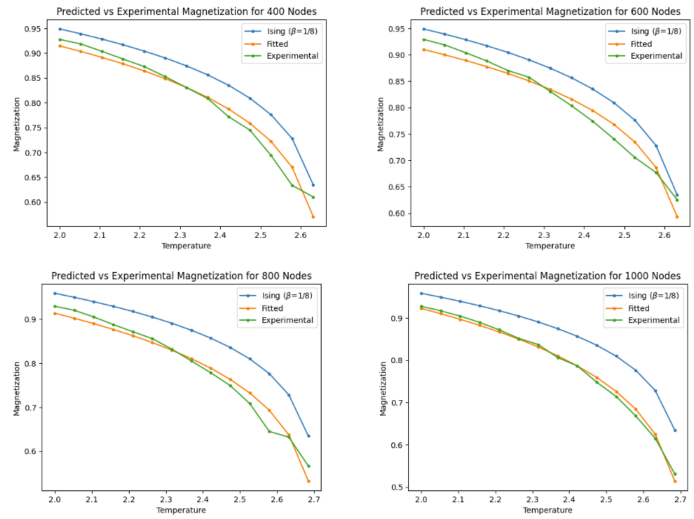

FIG. 4. Ising Universality Class vs Experimental and Fitted Magnetization

occur much faster than for $p > 1/N$. As a result, on a global level, there is a lack of a phase transition. The practical implication here is that we should only care about random graphs that are connected: otherwise, the system fragments into smaller subsystems.

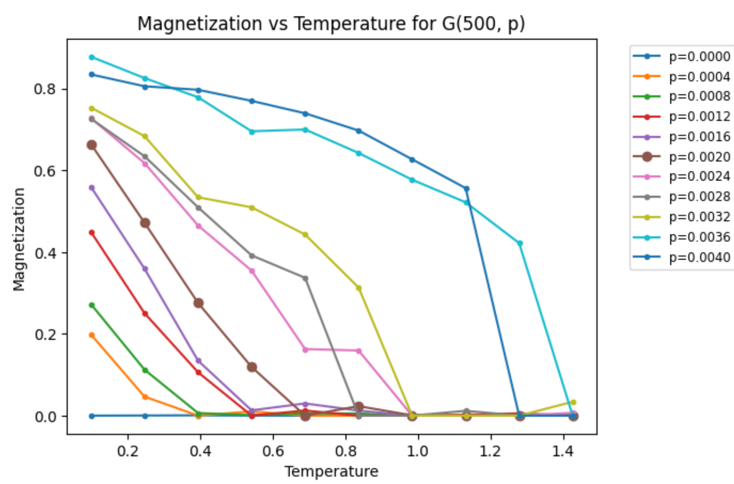

FIG. 5. Magnetization of $G(500, p)$

D. Algebraic Connectivity (λ_2)

In this experiment, we fix $N = 100$. In order to sample random values of λ_2, we found that randomly generating p in $G(100, p)$ gave quite uniform results for λ_2. The values are then conditioned to be positive in order to guarantee the graph is connected [3]. Magnetization for larger (strongly connected graphs) versus smaller (sparser) values of λ_2 are plotted in Figure 6. Again, we see increasing critical temperatures as the connectivity increases. The existence of such temperatures at smaller values indicate that the phase transition exists for positive λ_2, which supports the conclusion from looking at Erdős–Rényi graphs with $p < 1/N$. Furthermore, the trend of the critical temperature increasing with degree in the regular graph experiment is consistent with the increasing value of λ_2. This conclusion offers an improvement on the previous result, since we now drop the regularity condition entirely and focus on a very general metric of connectivity instead.

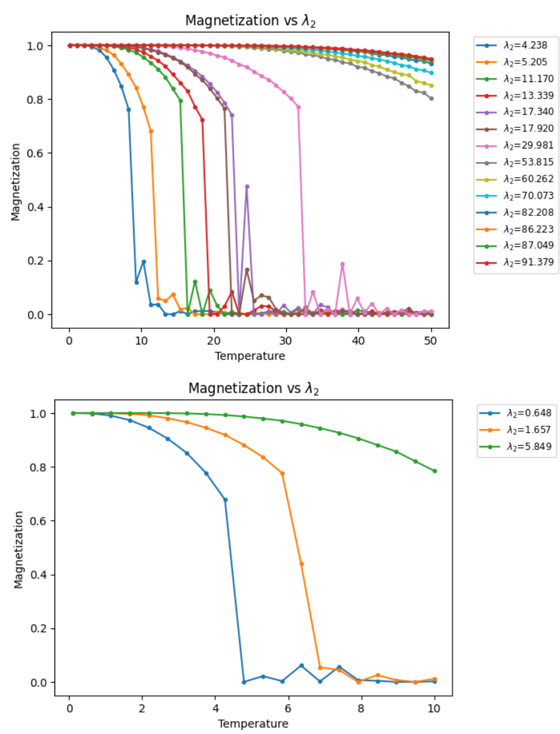

FIG. 6. Magnetization for larger and smaller algebraic connectivity

V. CONCLUSIONS

The experiments provide a strong indication that there is a positive correlation between the (algebraic) connectivity of the graph and the critical temperature of the modeled system: we observe this trend with increases in regular graph degrees, expected number of edges in random graphs, and λ_2. From a physics perspective, this could be explained due to the nature of mean field theory. The larger the number of neighbors a node has, the more effects of spin it experiences. The simulation accounts for each of these effects on the node (in expectation), resulting in a stronger force on the node to stay in equilibrium. This requires more energy to flip it from the initial state. Combining this with the fact that we want every state to flip, it makes sense that the critical temperature will have to increase significantly as the number of neighbors, an indicator of connectivity, also increases. As a result, we can see that the λ_2 metric can be used as an indicator for certain behaviors in different Ising models.

A minor conclusion that can also be drawn is that using connected, undirected graphs in the Ising model setting will exhibit phase transitions. This suggests that the model is surprisingly flexible and is not necessarily bound to very structured networks.

Finally, the brief experiment on 4-regular graphs also suggests the Ising universality class can apply to a much larger set of graphs than simply lattices and other rigid structures. I believe an interesting extension of this work would be to continue relaxing these conditions in a way that is physically significant. Planarity seems to be a natural choice, and it seems that there are already ways to randomly generate planar graphs, allowing simulations to be as unbiased as possible 4. Another extension could be to look at graphs with small cliques, which bridges the gap between phase transitions and disconnected graphs. Several small cliques allow for smaller communities within a graph that may have a sparser set of edges between them, providing us with a set of graphs that are considered densely connected but only in concentrated areas of the graph.

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