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Final Project

PHYS 422

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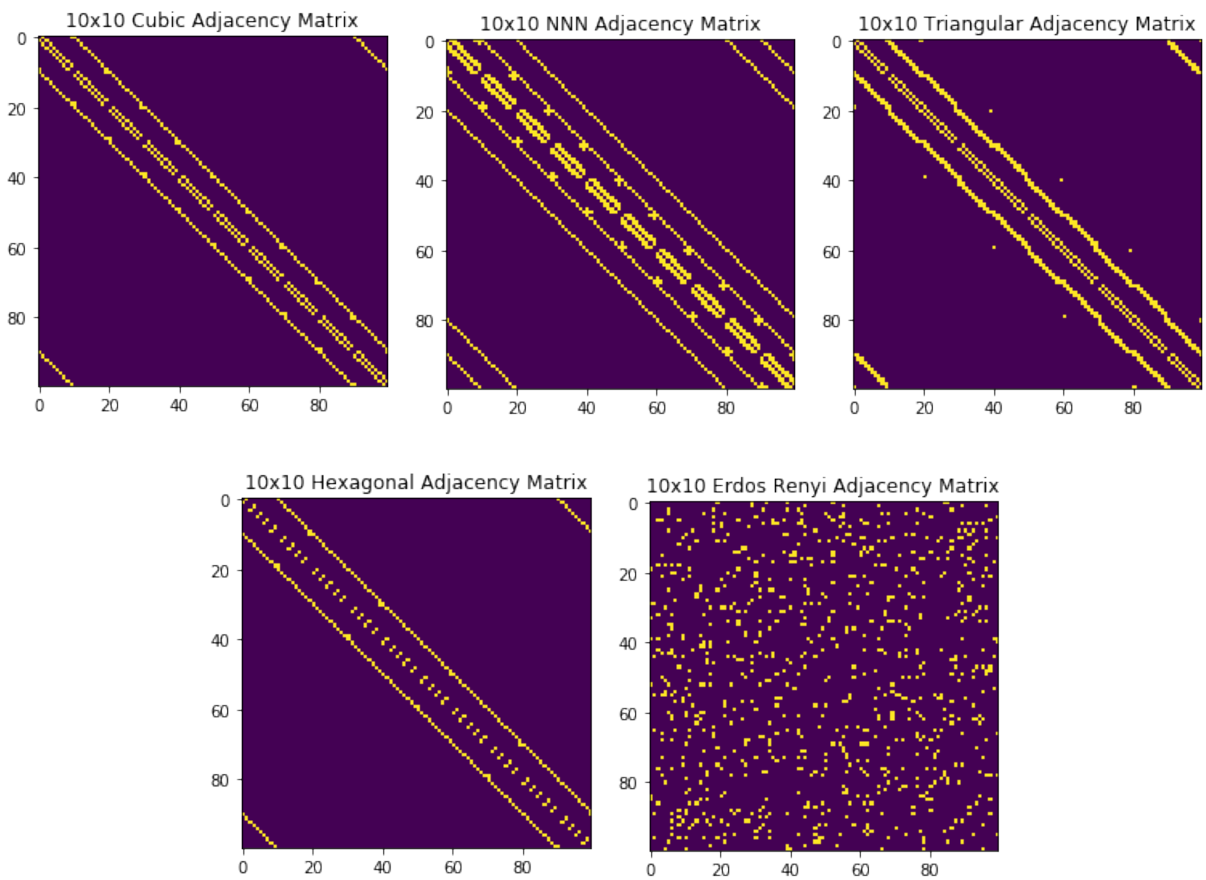
Connectivity in the Two-Dimensional Ising Model

The Ising model functions as a tool to simulate ferromagnetism, which reveals a multitude of physical qualities about magnets. In its simple form, the Ising model simulates ferromagnetism by representing a number of sites (or electrons), σ_i, as "spin up" or "spin down," plus one for up and minus one for down, thus, the total magnetization of the system in just the sum of the different sites. The real usefulness of this representation begins when we implement the metropolis algorithm. The metropolis algorithm chooses a site at random and flips it (changes it from 1 to -1 or -1 to 1) with a probability based on the current energy or Hamiltonian, $E = -J\sum_{ij}^{N}\sigma_i\sigma_{i+1}$, and the temperature of the system. For every random site chosen, if the total energy of the system will decrease by flipping the site, the site will flip; if the energy is greater, the site will flip with probability of $p = e^{-\beta\Delta E}$; and if the energy will not change by flipping the site, the site will flip with probability .5. This process is the core of the Ising model and allows us to explore large and complex systems easily with the help of a computational aid. My project uses Python 3 as the computational aid and explores how different types of connectivity affect average energy, average magnetism, heat capacity, magnetic susceptibility and ultimately the critical temperature.

My project explores the most common two-dimensional lattices: square, triangular, hexagonal and next nearest neighbor, as well as the less common Erdos-Renyi lattice, in an effort to better understand how changes in connectivity affect critical temperature. In two dimensions, the square lattice consists of four neighbors per site, the triangular lattice consists of six neighbors per site, the hexagonal lattice consists of three neighbors per site, the next nearest neighbor (NNN) lattice, which includes nearest neighbor, consists of 8 connections per site, and the Erdos-Renyi lattice consists of a random number of connections per site. The Erdos-Renyi lattice, $G(n, p)$, uses an algorithm to determine which sites of the n sites are connected based on a probability p. Higher values of p result in more connections, and lower values of p result in fewer connections; a p value of 0 will result in a completely disconnected graph. According to Wikipedia, for Erdos-Renyi lattices such that $G(n, 2\ln(n)/n)$, as n goes to infinity the probability of the lattice being connected goes to 1. Using this information, I chose $n = 100$ and $p = 2\ln(n)/n \cong .092103$ in an effort to guarantee connectedness while still keeping the total number of connections low. The average number of connections can be determined by the following formula: $average\ edges\ per\ site = \frac{\binom{n}{2}p}{n}$. For our given values the average connections per site comes out to be approximately 4.56, which situates this graph between the square lattice and the triangular lattice in terms of average connectedness. Later we'll examine how average connectivity affects critical temperature.

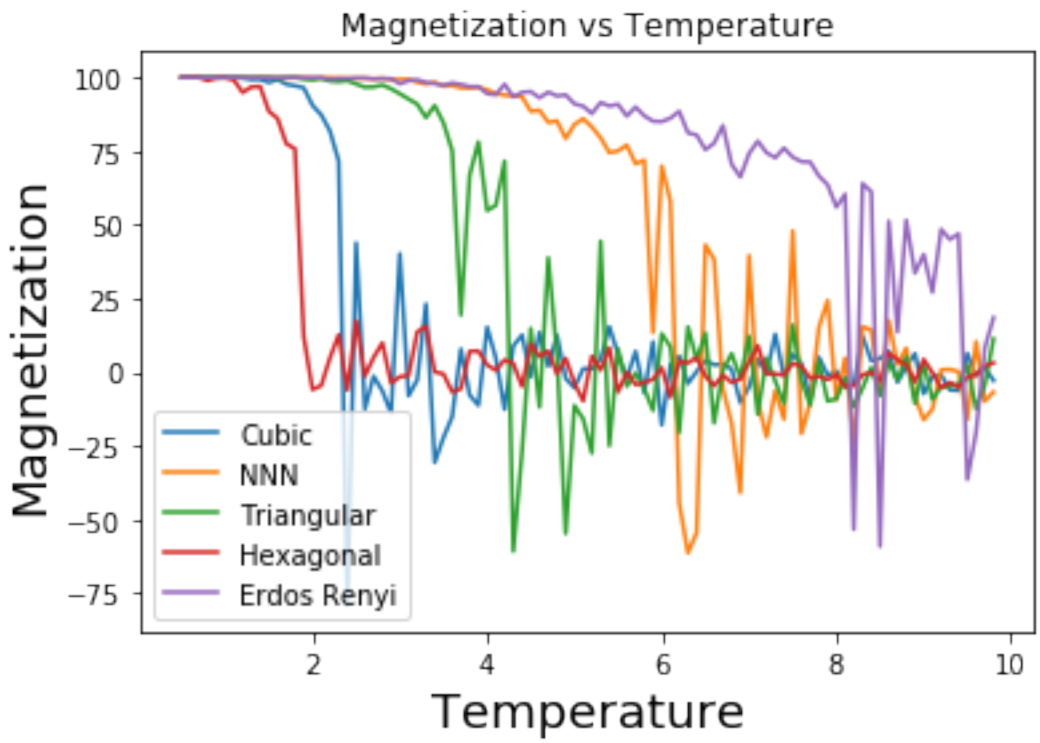
The largest obstacle to finding the critical temperature efficiently with the Ising model was finding a way to represent these different connectivity types with adjacency matrices. An adjacency matrix is a concise way of describing how every site in the Ising model is connected. Adjacency matrices are diagonally symmetric, two-dimensional arrays that represent each connection as a "1" and each non-connection as a "0." Each row or column in an adjacency matrix describes an individual site, and the numbers in that row or column represent the site's connection to every other site. Using adjacency matrices saves time, increases generality, and increases computational efficiency since adjacency matrices work in every dimension and only require one computation per Ising model simulation. Without an adjacency matrix, one could be forced to recalculate every connection in the system after every iteration since the metropolis algorithm calculates the change in energy based on how connected sites are influence. Recalculating the connection for each iteration in the metropolis algorithm would get extremely computationally expensive with higher dimensions and larger numbers of sites. Instead, the adjacency matrix for a given connectivity is calculated once and the connections for a given site are easily referenced through each iteration, even as the system changes. In addition to their computational benefits, adjacency matrices also provide a helpful graphical representation of connectivity and one can quickly see the average number of connections.



These pictures represent the adjacency matrices for the different types of connectivity I chose to explore, where yellow pixels represent a connection and purple pixels represent a non-connection.

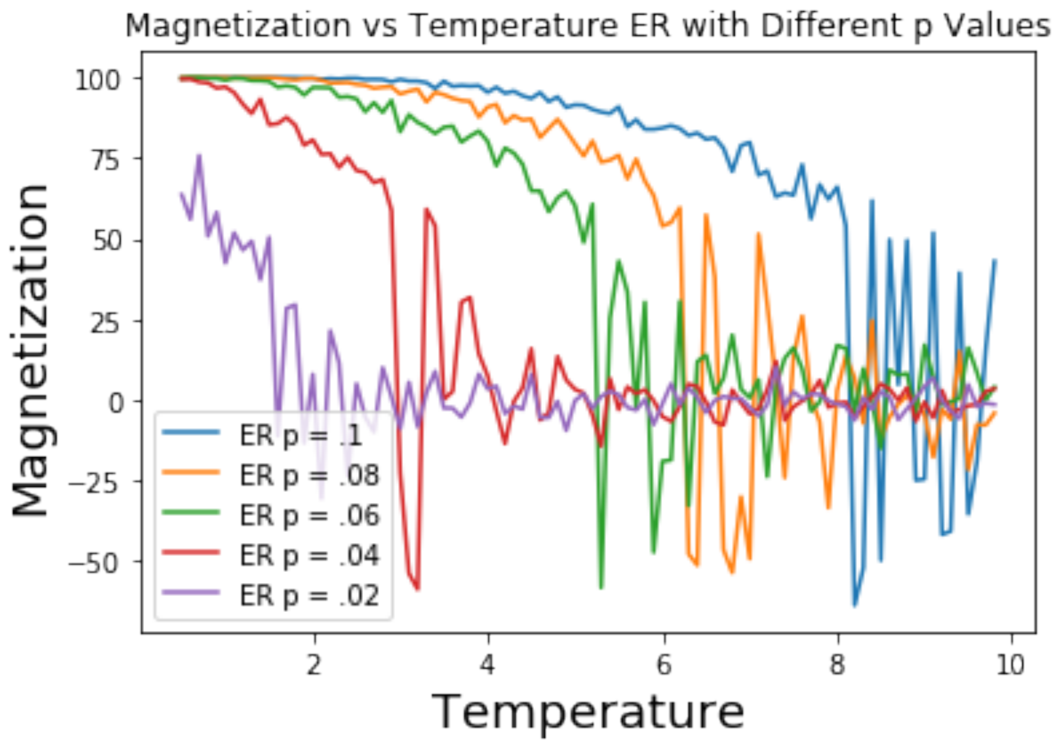
Here we can see the symmetry of the connections, since the connection sites are undirected the graph is diagonally symmetric and since no site is connected the matrix must have zeros along the diagonal. The 10x10 hexagonal adjacency matrix (the forth figure above) consists of three connections per site and has the fewest average connections per node of the above connectivity graphs. This information can be understood at a glance since the other four graphs have noticeably more yellow than the hexagonal adjacency matrix.

Armed with these adjacency matrices, analysis on the affects of connectivity and critical temperature can begin. For square, triangular, and hexagonal lattices, one can solve for the critical temperature mathematically. Stephen L. Eltinge's paper, "Numerical Ising Model Simulations on Exactly Solvable and Randomized Lattices," offers the mathematically computed values for these lattices, which served as a reference point when analyzing the graphical results. Eltinge calculates the following critical temperatures for the square, triangular and hexagonal lattices: $T_c^{square} \approx 2.269$, $T_c^{triangular} \approx 3.641$, and $T_c^{hexagonal} \approx 1.519$. While the NNN lattice is not solved mathematically in Eltinge's paper, we can infer from the trend (sites with more connections have higher critical temperatures) that the critical temperature is above 3.641 since each site has 8 connections, which is a larger number of connections per site than the square, triangular, and hexagonal lattices. Indeed, as the physical quantities of these matrices are calculated and graphed, the relationship between connections per site and critical temperature appears to be proportional if not somewhat linear. To see the relationship between the critical temperature and the number of connections per site we'll look at all the lattice's average magnetization values as temperature increases from .5 to 10 by increments of .1. The average magnetization drops and then oscillates near zero after the lattice's critical temperature has been reached. This is because the aligned state is unstable after the critical temperature, so we'll see drastic drops in magnetization at different temperatures, which correspond the specific lattice's critical temperature.



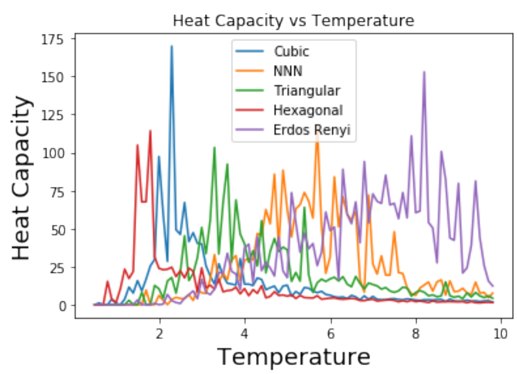
As anticipated by Eltinge's work, the critical temperature for the hexagonal lattice (with three connections per site) is around 1.5, the critical temperature for square (or cubic) lattice (with four connections per site) is around 2.3, and the critical temperature for the triangular lattice (with six connections per site) is around 3.6. Also as expected, the critical temperature for the NNN lattice (with 8 connections per site) is around 5.5, which is greater than the hexagonal, square, and triangular lattices. The Erdos-Renyi graph exhibits more complicated behavior given its non-regular connectivity and demonstrated a higher critical temperature than expected given its average of 4.56 connections per site.

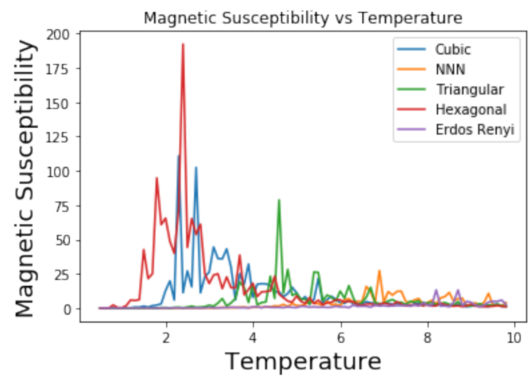
Given the unexpected critical temperature of Erdos-Renyi lattice in relation to the regularly connected lattices, I explored how a linear increase in p affects the critical temperature. I conjectured that despite the irregularity of the lattice's connections, the lattices with more average connections would have higher critical temperatures. My conjecture was affirmed most clearly again by the average magnetization versus temperature graph.

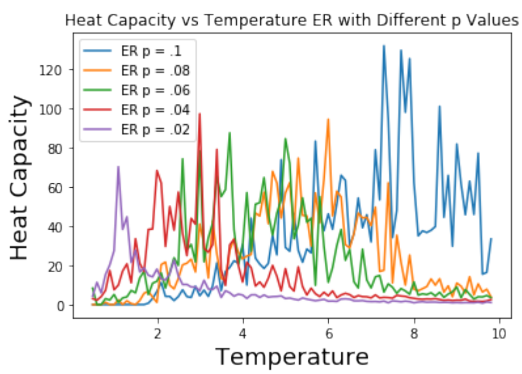


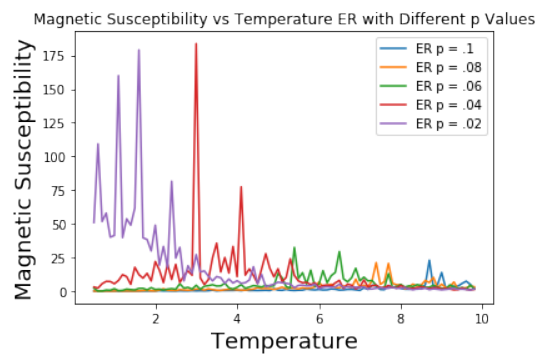
Here we can see how higher p values (which correspond to more connections per site) result in higher critical temperatures, which aligns with my prediction.

If we look at how the energy, and thus magnetization is calculated, we can better understand why more connections result in higher critical temperatures. The magnetization is calculated by summing the magnetization of each site, and the magnetization of each site is determined by how a flipped site changes the total energy of the system. If a site is on average connected to more sites and every site starts out as 1, the change in energy will most likely be positive if the site is flipped. If the change in energy is more likely to be positive, the system will be more likely to change with a probability of $p = e^{-\beta \Delta E}$, which is the lowest possible probability for small values of temperature. As a result, the more average connections a site has, the more likely that system is to remain initially unchanged as temperature increases. Since the heat capacity and the magnetic susceptibility are calculated by the variance of the energy and the magnetization respectively, we can look at how these quantities change as connectivity increases.









Once again, the graphical data demonstrate how the increased connectivity results in higher critical temperatures, but they also reveals that decreased connectivity results in spikes in heat capacity and magnetic susceptibility at lower temperatures. Since a high variance corresponds to data being very different from the average, the spikes in the heat capacity and magnetic susceptibility values directly correlate to the dramatic drops in average magnetization we saw earlier and thus predict when a system's average magnetization will begin to break out of the initially aligned state and oscillate about zero.

Based on the experimental data and analysis we can confidently conclude the correlation between increased connectivity and higher critical temperatures. The analysis of how the Ising model alters a system as temperature increases provides strong evidence to support this claim and the graphical data corroborates the analysis. With more time, this project could be continued by implementing parallel tempering to increase computational efficiency. With increased efficiency, it could also explore how connectivity in higher dimensions changes the critical temperature of a system or how systems of larger sizes change relative to systems of smaller sizes.

References:

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Erdős–Rényi model

https://en.wikipedia.org/wiki/Erd%C5%91s%E2%80%93R%C3%A9nyi_model

Adjacency matrix

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http://web.mit.edu/8.334/www/grades/projects/projects15/EltingeStephen.pdf

J. Oitmaa:

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