Examining Macroscopic Thermal Behaviors of Maximum Cut Mapped to the Ising Model

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1 An Introduction to Maximum Cut

1.1 Research Objectives

- Utilize Ising Machines to solve NP-Hard combinatorial problems, like Maximum Cut
- Use what we've learned in class to arrive at analytical expressions for thermodynamic quantities.
- Verify thermodynamic quantities with simulations.

1.1.1 The Max Cut Cost Function

The equation for the number of cuts in a lattice is

$$C(|\psi\rangle) = \sum_{<i,j>} \frac{1 - \sigma_i \sigma_j}{2} \tag{1}$$

where σ_i is a binary spin variable i.e. $\sigma_i \in \{-1, 1\} \forall i$.

As the name implies, the goal of max cut is to maximize the cost function $C(|\psi\rangle)$.

1.1.2 Mapping Max Cut to an Ising Hamiltonian

Maximizing $C(|\psi\rangle)$ is the same as minimizing

$$C'(|\psi\rangle) = -\sum_{<i,j>} \frac{1 - \sigma_i \sigma_j}{2} \tag{2}$$

Constants and multiplicative scalars can be omitted – This doesn't change our optimal eigenstate solution, but it does shift the eigenvalues.

$$\mathcal{H} = \sum_{<i,j>} \sigma_i \sigma_j \tag{3}$$

This is our *Ising Hamiltonian* whose ground state wave function and corresponding eigenenergy are given by $\mathcal{H}|\psi_0\rangle = \varepsilon_0|\psi_0\rangle$. When we eventually solve this Hamiltonian for $|\psi_0\rangle$ and ε_0, we can translate it back into its *cut* value via the following analysis.

$$\begin{aligned} C|\psi_0\rangle &= \sum_{<i,j>} (\frac{1-\sigma_i\sigma_j}{2})|\psi_0\rangle \\ &= [\sum_{<i,j>} (\frac{1}{2}) - \frac{1}{2}\sum_{<i,j>} \sigma_i\sigma_j]|\psi_0\rangle \\ &= [\sum_{<i,j>} (\frac{1}{2}) - \frac{1}{2}\mathcal{H}]|\psi_0\rangle \\ &= (\frac{1}{2})\sum_{<i,j>} (1)|\psi_0\rangle - \frac{1}{2}\varepsilon_0|\psi_0\rangle \end{aligned}$$

The expression $\sum_{<i,j>} 1$ is equal to the number of edges in the lattice n_e. n_e is specific to the geometry and number of interactions in a lattice

$$\begin{aligned} C|\psi_0\rangle &= (\frac{1}{2}n_e - \frac{1}{2}\varepsilon_0)|\psi_0\rangle \\ C|\psi_0\rangle &= \frac{n_e - \varepsilon_0}{2}|\psi_0\rangle \end{aligned}$$

The ground state eigenvalue of C is equal to the max cut eigenvalue. Thus

$$\text{max cut} = \frac{n_e - \varepsilon_0}{2} \tag{4}$$

1.2 Algorithms for Solving Max Cut

Since max cut is an optimization of *binary* variables, not continuous ones, continuous optimization methods such as gradient descent do not work on this class of problems. Instead, we will utilize the Random Guessing, Metropolis, and Simulating Annealing algorithms outlined in the subsections below.

1.2.1 The Random Guessing Algorithm

In an exponentially growing solution space, the random guessing algorithm usually succeeds with complexity $\mathcal{O}(2^n)$.

Although random guessing is not a sophisticated algorithm, we will show that it is not useless for the FIEW Lattice in the later section. The following algorithms can be considered as an upgrade from random guessing.

Algorithm 1: The Random Guessing Algorithm

Data: A Randomly Generated Statevector $|\psi\rangle$
Result: A "near"-optimal solution
Generate a random statevector $|\psi\rangle$;
while *not near-optimal* **do**
  Evaluate the cut value of $|\psi\rangle$;
  if $|\psi\rangle$ *is near-optimal* **then**
    end;
  end
  Generate a new random statevector $|\psi\rangle$;
end

Algorithm 2: Metropolis Algorithm

Data: Initial state $|\psi\rangle$, coupling constant J, temperature parameter $\beta \equiv 1/T$
Result: An optimized state $|\psi_0\rangle$ that yields an optimal/near-optimal max cut
while *not converged* **do**
  Randomly select a spin σ_i in $|\psi\rangle$;
  Calculate $dE = \sum_{i,j} J_{ij}\sigma_i\sigma_j$, where j are the nearest neighbors of i;
  if $dE < 0$ **then**
    Flip the selected spin σ_i with 100% probability;
  else
    Calculate the Boltzmann probability $P = e^{-\beta\, dE}$;
    With probability P, flip the selected spin σ_i;
  end
end

1.2.2 Ising Machines (Metropolis Algorithm)

We can perform the Metropolis Algorithm on the Ising model at a given temperature T to find the statevector $|\psi_0\rangle$ that yields the maximum cut value.

One may notice that lower temperatures do not encourage random spin-flips, which may cause the lattice to converge to a local minimum. However, too high of temperatures may allow stochastic noise to dominate, not allowing the algorithm to converge at all. It turns out that a process called *simulated annealing* performs the metropolis algorithm over a temperature range, adiabatically decreasing the temperature to encourage minima exploration while allowing convergence.

1.2.3 Simulated Annealing

Algorithm 3: Simulated Annealing Algorithm

Data: Randomly generated $|\psi\rangle$, coupling constant J, and temperature schedule $T \in (T_{\text{initial}}, T_{\text{final}})$ where $T_{\text{Initial}} < T_c$ and $T_{\text{Final}} < T_{\text{Initial}}$

Result: An optimized state $|\psi_0\rangle$

Randomly generate initial state $|\psi\rangle$;

Define a temperature schedule over $T \in (T_{\text{initial}}, T_{\text{final}})$ with k steps;

for *each temperature T in the schedule* **do**

  while *not converged at this temperature* **do**

    Do Metropolis Algorithm;

  end

  Update $|\psi\rangle$ for the next temperature;

end

We can see that to do simulated annealing effectively, we need to know T_c before we run the algorithm to properly define our temperature schedule. This limitation motivates the examination of macroscopic properties of a max cut problem mapped to an Ising lattice.

1.3 The Metropolis Algorithm and Code Implementation

In the code we use the *networkx* package to visualize our lattice and store interaction strength information. We implement the metropolis algorithm on the lattice to determine final state for a given T. We notice that below a critical temperature threshold, the metropolis algorithm converges to an optimal solution and diverges for temperatures greater than the critical temperatures. Therefore, we also do a temperature sweep to record magnetization and magnetic susceptibility as a function of temperature. We apply machine learning tools in the *scipy* package to detect abrupt changes in $\chi(T)$ which usually correspond to a critical temperature.

2 Special Lattices

2.1 The FIEW Lattice

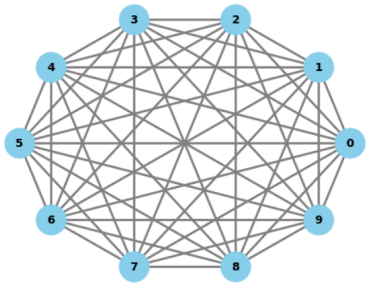

Figure 1: The FIEW Lattice for $n = 10$ nodes

The Fully-Interconnected Equally-Weighted (FIEW) Lattice. Is an n-node lattice where all nodes are neighbors with each other. Thus, each node has $n-1$ nearest neighbors since a node can't be a neighbor with itself. We also may note that if there are n number of nodes and $n-1$ interactions per node, then we will have $n(n-1)$ number of interactions in total. Thus, the total number of interactions will scale by $\mathcal{O}(n^2)$. Thus we expect the time complexity of the Metropolis Algorithm on Fully-Interconnected Lattices to be $\mathcal{O}(n^2)$ whereas other classical methods such as exact diagonalization are order $\mathcal{O}(2^n)$ due to an exponentially growing Hilbert space with each added node.

2.1.1 FIEW Ground State Solutions

Due to the symmetry of the FIEW lattice, it has trivial max cut solutions. To obtain a maximum partition between nodes, any half of the nodes must have spin $+1$ and the other half -1 in any order. This means, for a lattice of size N, that the total number of ground states is $\binom{N}{N/2}$. The ground state solution for even-n may be considered as an unordered antiferromagnetic state. Although a "half & half" configuration can be applied nicely to an even-n FIEW lattice, an odd n FIEW-lattice leads to *frustrated magnetism* where it is impossible for the model to converge to a single ground state. Frustrated magnetism occurs here since we cannot have a "half and half" configuration since there will be always one extra spin with magnetic moment ± 1 that will dictate the ferromagnetic nature of the entire lattice. In this case, the total number of ground states is $\binom{N-1}{N/2}$.

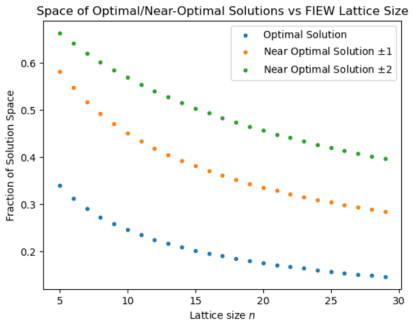

Figure 2: Near Optimal Solution Space of the FIEW Lattice

Due to the symmetry of a FIEW lattice, at node size $n = 15$, about 50% of the solution space are near-optimal solutions within 2 spin flips! This suggests that randomly guessing is a valid strategy for determining near-optimal solutions for smaller lattice size regimes. However, we can improve random guessing by utilizing the Metropolis Algorithm as a numerical optimizer.

2.1.2 FIEW Theory

Let's find the critical temperature, and behavior, of the FIEW lattice using MFT. We begin with the Hamiltonian.

$$\mathcal{H} = \sum_{\langle i,j \rangle} [J\sigma_i\sigma_j]$$

We can extract the j sum from the Hamiltonian, in order to retrieve the contribution per site.

$$\mathcal{H} = \sum_j \left[\sigma_j \sum_i [J\sigma_i] \right]$$

Then, with the mean field $h = \Sigma[J\sigma_i]$,

$$h = \sum_i [J\sigma_i] = \sum_i [Jm] \,.$$

For $n-1$ neighbors, the mean contribution is $(n-1)/2$.

$$h = Jm\frac{n-1}{2}$$

We can insert this into the self-consistent equation for m.

$$m = \arctan\left[\beta J \frac{n-1}{2} m\right]$$

Now, in order to discover the critical temperature, we can do an asymptotic expansion of order 1.

$$m = \beta J \frac{n-1}{2} m + \mathcal{O}\left(m^2\right)$$
$$\beta_c = \frac{2}{J(n-1)}$$

Then, to recover the behavior of m beyond the critical temperature, we can do an asymptotic expansion of order 2.

$$m = \beta J \frac{n-1}{2} m - \frac{\left[\beta J \frac{n-1}{2} m\right]^3}{3} + \mathcal{O}\left(m^4\right)$$
$$1 = \beta J \frac{n-1}{2} - \frac{\left[\beta J \frac{N-1}{2}\right]^3}{3} m^2$$
$$\frac{\left[\beta J \frac{n-1}{2}\right]^3}{3} m^2 = \beta J \frac{n-1}{2} - 1$$
$$m^2 = 3\left[\frac{2}{\beta J(n-1)}\right]^2 - 3\left[\frac{2}{\beta J(n-1)}\right]^3$$
$$m = \pm \frac{2}{\beta J(n-1)} \sqrt{3 - 3\frac{2}{\beta J(n-1)}}$$

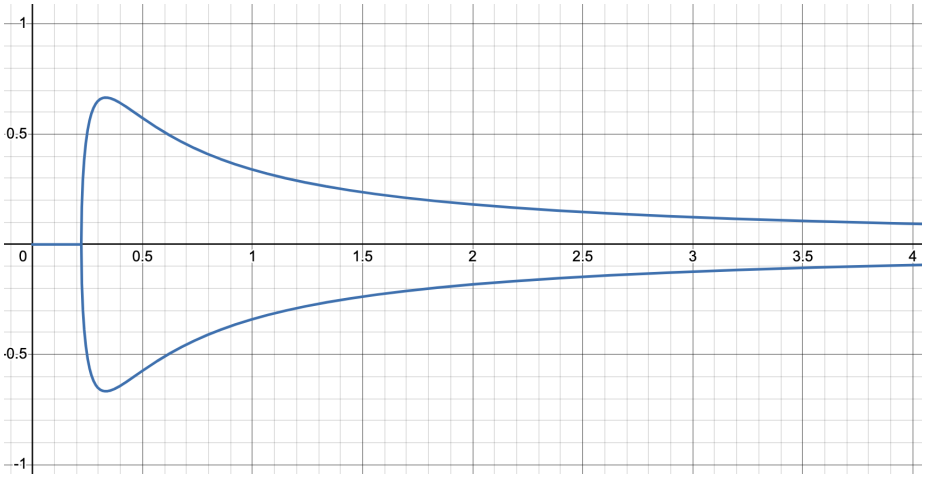

Figure 3: Plotting m vs β, for $n = 10$. Note the bifurcation happening at $\beta_c = 2/9$.

2.1.3 FIEW Numerics

We start by randomly generating an initial lattice

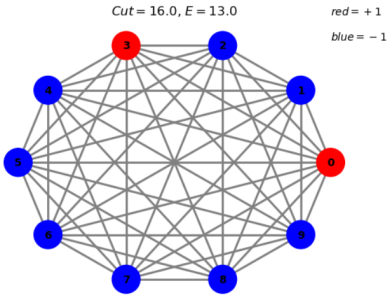

Figure 4: A Randomly Generated $n = 10$ FIEW Lattice

Then, we perform the metropolis algorithm on the lattice at a temperature $T = 0.1$ for 100 metropolis iterations and converge to the max cut solution:

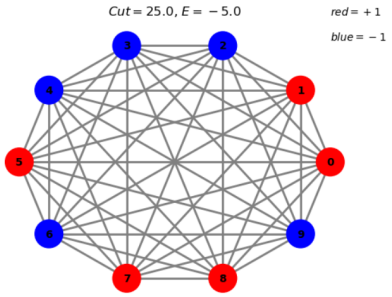

Figure 5: A Max Cut Solution to the $n = 10$ FIEW lattice

Although we are able to successfully solve the max cut problem at $T = 0.1$ for the $n = 10$ FIEW lattice specifically, we want to capture the thermal properties of the lattice as a function of temperature.

We compute the magnetization m as a function of temperature through the metropolis algorithm for 2000 metropolis interactions per temperature, but only saving data after the first 300 iterations to avoid averaging exploration behaviors into m,

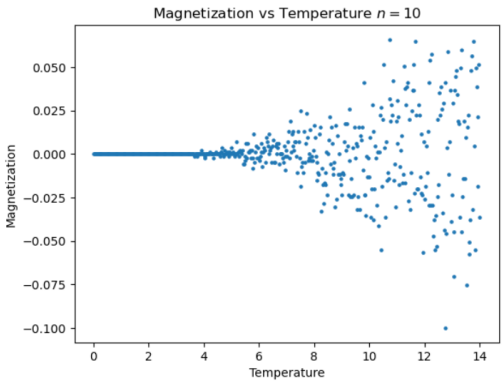

Figure 6: Magnetization vs Temperature

What's very interesting is that it although it seems we have symmetry breaking, we don't have *spontaneous* symmetry breaking. It seems that T_c could live somewhere between $4 < T_c < 6$, but it is not clear since the transition from AFM to FM seems smooth.

We can analyze a magnetic susceptibility χ vs T graph to try to detect a critical temperature.

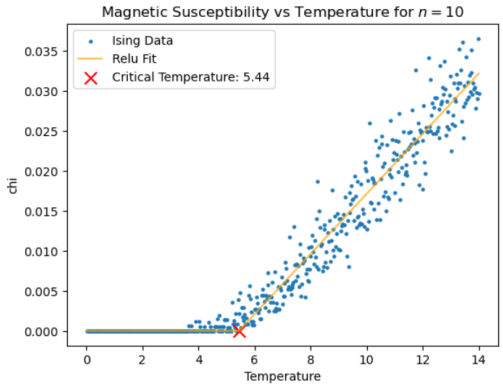

Figure 7: Magnetic Susceptibility vs Temperature

Here, the critical temperature is still "fuzzy," mostly due to the stochastic noise that happens near and after the critical temperature. We assume that a ReLU function can fit the curve and define the critical temperature to be where the ReLU is not differentiable in the fit. Here, that yields an experimental critical temperature value of $T_c^{exp} = 5.44$. Using the analytical solution for T_c from proof 4.1: $T_c = \frac{N-1}{2} = \frac{(10)-1}{2} = 4.5$. We can improve our T_c^{exp} value by choosing a smaller temperature domain centered around T_c, including more data points, and increasing the number of metropolis iterations per temperature.

3 The FIGW Lattice

The Fully Interconnected Gaussian Weighted (FIGW) Lattice is an extension of the FIEW Lattice except the interaction strength are sampled from some Normal Distribution $J_{ij} \sim \mathcal{N}(\mu = J_0, \sigma = s)$. The FIGW lattice is an extension of the FIEW lattice in the sense that in the limit as $s \to 0$. we recover the FIEW lattice. For small s, we expect the FIGW to represent a "fuzzy" max cut problem where all the interaction strengths are slightly randomly perturbed causing several cascading interaction effects. Despite the consequences of the FIGW, the numerics suggest that for different initial seeds of Gaussian-generated interactions, we can consistently shift the critical temperature T_c by adjusting s as a free parameter. Although a FIGW is structurally asymmetric due to its random nature, it is actually symmetric in the Mean Field Theory perspective.

3.0.1 FIGW Theory

Instead of $J_{ij} = 1$, we have $J_{i,j} = J_0 + \epsilon_{i,j}$ where $\epsilon_{i,j}$ is a normally distributed random variable with mean 0 and standard deviation s. Since each weight on the graph has a different value associated with it, this is a **weighted** max cut! This means certain cuts are more valuable to make than others! Here, the lattice is asymmetrical in physical space, but symmetrical in the Mean Field Theory perspective. If the weights between nodes are random, then the lattice is asymmetrical, which may lead to some nontrivial ground states.

$$\rho_J = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(J-J_0)^2}{2s^2}}.$$

What is the resultant critical temperature? One can try an analysis using MFT using the assumption that $J = J_0 \pm \epsilon$.

$$\mathcal{H} = \sum_{\langle i,j \rangle} [(J_0 \pm \epsilon)\sigma_i \sigma_j]$$

$$\mathcal{H} = \sum_j \left[\sigma_j \sum_i [(J_0 \pm \epsilon)\sigma_i] \right]$$

However, we reach a critical problem upon applying MFT to this expression of $\mathcal{H}$: $\langle J_0 + \epsilon \rangle = J_0$. This means that applying MFT to this weighted lattice will give us results that are the same as the regular lattice. Let's try a different approach.

Let's say we have some $\rho_x \in \mathbb{R}$ such that $\int_{\mathbb{R}} [\rho_x] dx = 1$, and we want to represent it in terms of another variable y such that $\int_{\mathbb{R}} [\rho_y] dy = 1$. In order to do a proper change in variables,

$$|\rho_x dx| = |\rho_y dy|$$

must hold true for all x and y. Rearranging, we get

$$\left|\frac{\rho_x}{\rho_y}\right| = \left|\frac{dy}{dx}\right|,$$

which allows us to write one probability density in terms of another probability density, given that we have a function that relates one variable x to the other y. In the context of this problem, we have the probability distribution of J, and we also have $\beta_c(J) = 2/J(n-1)$. Let's rewrite the probability law above to retrieve a more relevant form.

$$\left|\frac{\rho_J}{\rho_\beta}\right| = \left|\frac{d\beta}{dJ}\right|,$$

And, with $\frac{d}{dJ}\beta = -2/J^2(n-1)$,

$$\frac{1}{\rho_\beta}\frac{1}{\sqrt{2\pi}s}e^{-\frac{(J-J_0)^2}{2s^2}} = \frac{2}{J^2(n-1)},$$

Let's solve for ρ_β.

$$\rho_\beta = \frac{J^2(n-1)}{2}\frac{1}{\sqrt{2\pi}s}e^{-\frac{(J-J_0)^2}{2s^2}}$$

And then, substituting for $J = 2/\beta(n-1)$,

$$\rho_\beta = \frac{4}{\beta^2(n-1)^2}\frac{(n-1)}{2}\frac{1}{\sqrt{2\pi}s}e^{-\frac{(2/\beta(n-1)-J_0)^2}{2s^2}}$$
$$\rho_\beta = \frac{2}{\beta^2(n-1)}\frac{1}{\sqrt{2\pi}s}e^{-\frac{(2/\beta(n-1)-J_0)^2}{2s^2}}.$$

We can take the critical point of this function to find the maximum probable β, giving the critical temperature.

$$\frac{d}{d\beta}\rho_\beta = 0$$
$$\frac{d}{d\beta}\left[\frac{2}{\beta^2(n-1)}\frac{1}{\sqrt{2\pi}s}e^{-\frac{(2/\beta(n-1)-J_0)^2}{2s^2}}\right] = 0$$

$$-\frac{2}{\beta^3}e^{-\frac{(2/\beta(n-1)-J_0)^2}{2s^2}} + \frac{1}{\beta^2}e^{-\frac{(2/\beta(n-1)-J_0)^2}{2s^2}}\frac{2}{2s^2}\left(\frac{2}{\beta(n-1)} - J_0\right)\left(-\frac{2}{\beta^2(n-1)}\right) = 0$$

$$\beta + \frac{1}{s^2}\left(\frac{2}{\beta(n-1)} - J_0\right)\frac{1}{(n-1)} = 0$$
$$\beta^2 + \frac{1}{s^2}\left(\frac{2}{(n-1)} - \beta J_0\right)\frac{1}{(n-1)} = 0$$
$$\beta^2 + \frac{1}{s^2}\frac{1}{n-1}\beta J_0 - \frac{2}{s^2}\left(\frac{1}{n-1}\right)^2 = 0$$

$$\beta = \frac{-\frac{1}{s^2}\frac{1}{n-1}J_0 \pm \sqrt{\frac{1}{s^4}\frac{1}{(n-1)^2}J_0^2 + \frac{8}{s^2}\frac{1}{(n-1)^2}}}{2}$$
$$\beta = \frac{-\frac{1}{s^2}\frac{1}{n-1}J_0 \pm \frac{1}{s^2}\frac{1}{n-1}\sqrt{J_0^2 + 8s^2}}{2}$$
$$\beta = \frac{-J_0 \pm \sqrt{J_0^2 + 8s^2}}{2(n-1)s^2}$$

And the positive β is the solution.

$$\beta = \frac{-J_0 + \sqrt{J_0^2 + 8s^2}}{2(n-1)s^2}$$

We can verify that this expression reduces to the unweighted case by taking a limit as $\sigma \to 0$.

$$\begin{aligned}
\lim_{\sigma\to 0}\left[\frac{-J_0 + \sqrt{J_0^2 + 8s^2}}{2(n-1)s^2}\right] &= \lim_{\sigma\to 0}\left[\frac{+\frac{16s}{2\sqrt{J_0^2+8s^2}}}{4(n-1)s}\right] \\
&= \lim_{s\to 0}\left[\frac{+\frac{2}{\sqrt{J_0^2+8s^2}}}{n-1}\right] \\
&\to \frac{1}{n-1}\frac{2}{J_0} \\
&= \beta_{unweighted}
\end{aligned}$$

3.0.2 FIGW β_c Probability Distribution

Following the result for ρ_β, we find that the critical β probability distributions look like:

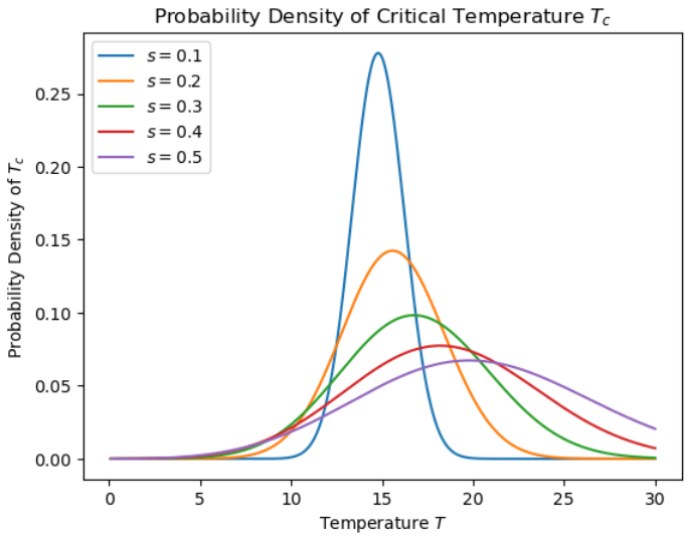

Figure 8: Critical Temperature Probability Distribution for $n = 30$, $J = 1$

where we assume the peaks of each distribution to be the expectation value of T_c. Each of the overlapping "Gaussian-like" probability distributions here are for progressively decreasing s-values. As expected, turns the probability distribution into a delta function that converges on the FIEW value of β.

3.0.3 FIGW Numerics

Like we did for the FIEW lattice, we compute χ vs T curves except now for an $n = 30$ lattice.

At a standard deviation of $s = 0$, we see

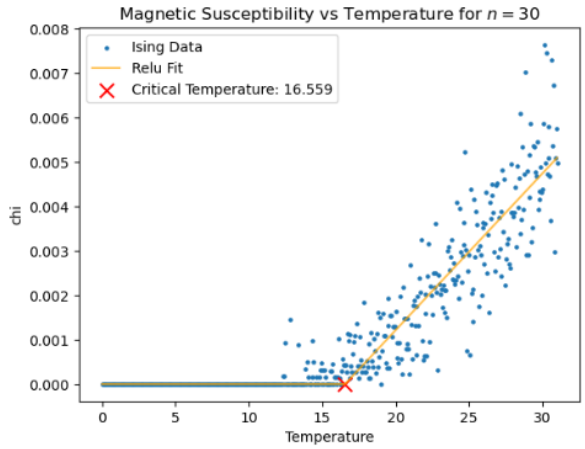

Figure 9: Magnetic Susceptibility vs Temperature. $n = 30$, $s = 0$

As we increase the standard deviation to 1,

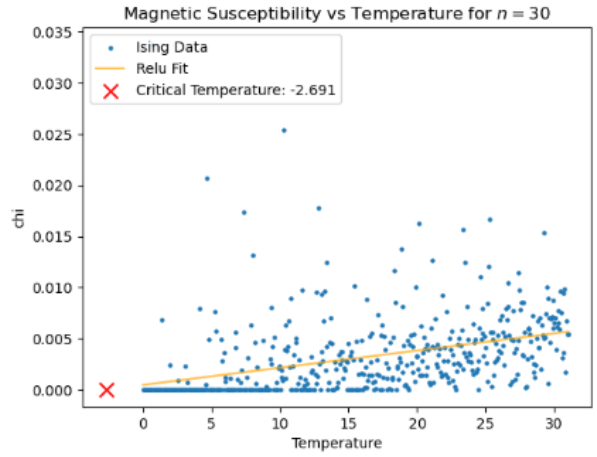

Figure 10: Magnetic Susceptibility vs Temperature. $n = 30$, $s = 1$

The ReLU fit fails here, incorrectly predicting a critical temperature. There is a critical temperature shift here as described by the ρ_{β_c} probability distribution, but that shift isn't so obvious here because of the stochastic noise.

4 Conclusion

Since we have found a solution to the fully interconnected Gaussian-weighted lattice, we believe that implies that there exist other solutions for different

weights, so long as the probability distribution of bond lengths is an analytic function.

We haven't been able to verify the second-order asymptotic behavior with the simulated behavior of m. The source of this error could have been anything from a convoluted execution of the code, to a convoluted execution of the theory. The second order asymptotic expansion - and discovery of behavior beyond T_c are both very involved processes.

One of our most important finds, with regards to both the FIEW and the FIGW lattices, were that T_c scales with $n-1$. Let's verify the physical meaning of this, taking into account that $n-1$ is the number of bonds per site. Imagine a 3-lattice. To "break out" of T_c, one has to flip a site, which requires the energy of 2 bonds. If the lattice was a 4-lattice instead, we would require the energy of 3 bonds. Of a 10-lattice, we would require the energy of 9 bonds. So on and so forth. Having any energy LESS than $n-1$ bonds present in the system does not result in spontaneous spin-flips. Having any energy MORE than $n-1$ bonds present in the system results in the system having spontaneous spin-flips. This means that the number of bonds per site determines the critical temperature of the system, and is why T_c scales as $n-1$.

5 Authors' Contributions

In this collaborative project, James worked on developing the *maxcut.ipynb* code to run the Metropolis Algorithm and numerically compute macroscopic properties of the max cut problem mapped to an Ising lattice. Furthermore, James accomplished mapping the max cut cost function to an Ising Hamiltonian and demonstrated that max cut can be solved on an Ising-inspired optimizer. James also contributed to the major portions of this midterm document as a submission item. Kyle was in charge of using the ideas taught in class to develop theories, simulation targets/unit verification, and analytical solutions to the various questions posed. This included using MFT to grab an theoretical β for James to interface with, and then further developing other behaviors such as m beyond T_c, and probability density functions for FIGW. Kyle was also responsible for developing the powerpoint for the class presentation.

6 Future Work

- Examine the frustrated magnetism in odd-n FIEW lattice structures
- Perform Simulated Annealing leveraging the metropolis algorithm
- Find other alternative methods to numerically extract a value for the critical temperature