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Unsupervised Machine Learning applied to the Dilute Ising Model

Author
William KNOTTENBELT

Supervisor
Dr. Evgeny KOZIK

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1 Abstract

In this report we investigate the extent to which unsupervised machine learning methods can decipher the underlying physics of the 2D dilute Ising model above the percolation threshold. We first reproduce results of applying principal component analysis (PCA) to the 2D pure Ising model, then present a method for finding the critical temperature using KMeans clustering, and finally we extend the same methodology to the 2D dilute Ising model with site concentration $p = 0.8$. We find that the clustering method is an accurate method for finding an estimate of the critical temperature when dealing with small datasets. This study determines that PCA and KMeans clustering can successfully distinguish between the ordered ferromagnetic phase and disordered paramagnetic phase of the dilute Ising model, and is capable of finding it's critical temperature, but is less accurate at doing so than for the pure Ising model.

2 Introduction

The study of statistical models of ferromagnetic materials is of great importance in condensed matter physics. A ferromagnetic material is one that experiences spontaneous magnetisation in the absence of a magnetic field, typically as a result of it being energetically favourable for unpaired electron spins in the material to align in the same direction [1]. The Ising model is a very simple mathematical model of a ferromagnet [2], which consists of a lattice of sites that can take a spin of +1 (up) or -1 (down). At a certain critical temperature, the Ising model exhibits a phase transition from a ferromagnetic phase, where all spins align, to a disordered paramagnetic phase, where the spins orient up or down randomly [2]. The dilute Ising model is a variant of the Ising model, where some proportion of the lattice sites are vacant/non-magnetic [3]. This is a very important model as it simulates the presence of imperfections in real-world materials.

In recent years, machine learning approaches have frequently been used to study various statistical models of ferromagnets, by using training data of raw spin configurations obtained with Monte Carlo simulations. This research has included the use of a variational autoencoder to find the crossover region of the 2D Ising model [4], the use of neural networks to identify the body-localization transition in a disordered quantum spin chain [5], and a convolutional neural network to investigate the phase transition of 2D complex plasmas [6]. This type of analysis is particularly important for unconventional models which give rise to exotic and complex phases of matter. The dimensionality-reduction technique 'principal component analysis' (PCA) has been used extensively to study phases and critical behaviour of various models of ferromagnets, including but not limited to; the 2D ising model [7], 3D ising model [8], 2D potts model [9], 3D Fermi-Hubbard model [10] and the Blume-Capel model [7]. By performing PCA on raw configurations of these models, one can extract macroscopic quantities that describe the system's behaviour, as well as find the critical point of phase transitions. For example, using raw configurations of the 2D Ising model, PCA is able to recover the magnetisation and the magnetic susceptibility [7].

The focus of this report is to extend this methodology to the dilute Ising model, which, to date, has not been explored. As a benchmark, we first reproduce results of using PCA to study the 2D pure Ising model, original results of which can be found in [7]. We then present

a new method to find the critical temperature by combining PCA and clustering analysis, without relying on any knowledge of the physics of the system. Finally we perform both of these methods on the 2D dilute Ising model, and assess their capability for understanding the model.

3 Theory

3.1 Pure Ising Model

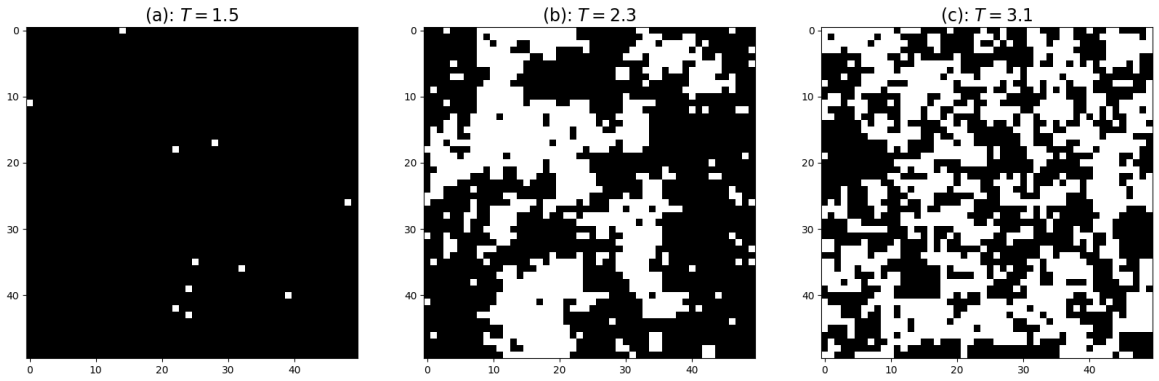

Figure 1: Visualization of the 2D pure Ising model, L=50, for temperatures (a) $T << T_c$ (b) $T \approx T_c$ (c) $T >> T_c$. White/Black sites are spin up/down respectively.

In this report we consider the case of the 2D square Ising model, with zero external magnetic field applied to it. The Hamiltonian (energy) for the Ising model in this case is [2]:

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \,, \tag{1}$$

where $\sigma_i = \pm 1$ is the spin at site i, J is the interaction coupling constant between neighbouring spins, and the sum over <i,j> is a sum over all nearest-neighbour pairs on the lattice.

If the coupling constant, J, is positive then the system favours the alignment of spins (ferromagnet) and if J is negative then the system favours the anti-alignment of spins (antiferromagnet). In this report we take $J = +1$ necessarily. The Ising model has two phases: the ordered ferromagnetic phase that occurs below a critical temperature, and the disordered paramagnetic phase above the critical temperature. In the ferromagnetic phase, the system tends to the ground energy state where all spins are aligned in the same direction and the system experiences spontaneous magnetisation. Above the critical temperature, random thermal fluctuations overcome this tendancy for order and the spins take random values, making the system paramagnetic [1]. The critical temperature, T_c, at which this phase transition occurs depends on the value of J and the size and shape of the lattice [2]. The critical temperature for the Ising model on a infinite 2D square lattice, with $J = +1$, as obtained by Onsager [11] is:

$$T_c = \frac{2}{ln(1+\sqrt{2})} \approx 2.269\,, \tag{2}$$

where we have set the Boltzmann constant, $k_B = 1$, as a convention.

Fig. 1 displays a visualization of the 2D pure Ising model configurations at temperatures below T_c, at T_c, and above T_c. We see that below the critical temperature, the spins are (mostly) all aligned in the same direction, representing long-range magnetic order. Above the critical temperature, the spins appear completely random and uncorrelated. There are many macroscopic variables that can characterise the behaviour of the system, two of which are used this report. The magnetisation is calculated [2]:

$$m = \frac{1}{N}\sum_i \sigma_i\,, \tag{3}$$

where N is the number of spin sites in the lattice, $\sum_i$ is a sum over all lattice sites.
The magnetic susceptibility is calculated [2]:

$$\chi = \frac{1}{k_B T}\left(\langle m^2\rangle - \langle|m|\rangle^2\right)\,, \tag{4}$$

where $\langle\cdot\rangle$ is the statistical mean operator.

The phase transition of the Ising model is associated with a sharp drop in the magnetisation from 1 to 0 and a sharp peak in the magnetic susceptibility [2].

When studying the Ising Model computationally, it is important to consider the effect of using finite system sizes on the behaviour of the model. One of the main consequences of finite system sizes is that when an estimate of the critical temperature is calculated, there tends to be a deviation from the ideal infinite-lattice value [12]. Thus, when attempting to calculate the critical temperature, one must use methods which account for these effects. One such method is called finite size scaling [13], which (assuming we are studying the 2D square Ising model) works by finding the critical temperature at a range of different system sizes then plotting the critical temperature against $1/L$, where L is side length of the lattice. Then, the y-intercept of the line of best fit is the infinite-lattice critical temperature since $1/L = 0$ implies $L \to \infty$.

Another method for finding the infinite-lattice critical temperature of the Ising model is the Binder ratio method, as introduced by Kurt Binder [14]. The Binder ratio, Q, is defined as [12]:

$$Q = \frac{\langle m^2\rangle}{\langle|m|\rangle^2}\,, \tag{5}$$

where m is the magnetisation, $\langle\cdot\rangle$ is the statistical mean operator.

At the critical temperature, the Binder ratio is independent of the lattice size. This is because the ratio of two quantities that have the same finite-size scaling exponents at T_c is independent of lattice size at T_c [12]. $\langle m^2\rangle$ and $\langle|m|\rangle^2$ are the same power of magnetisation, thus they satisfy this condition. Therefore, by plotting the Binder ratio as a function of

temperature for different lattice sizes, the point at which the curves intersect will be the critical temperature [12]. This method is a very effective method for finding the infinite-lattice critical temperature, but can be computationally expensive to implement properly.

3.2 Dilute Ising Model

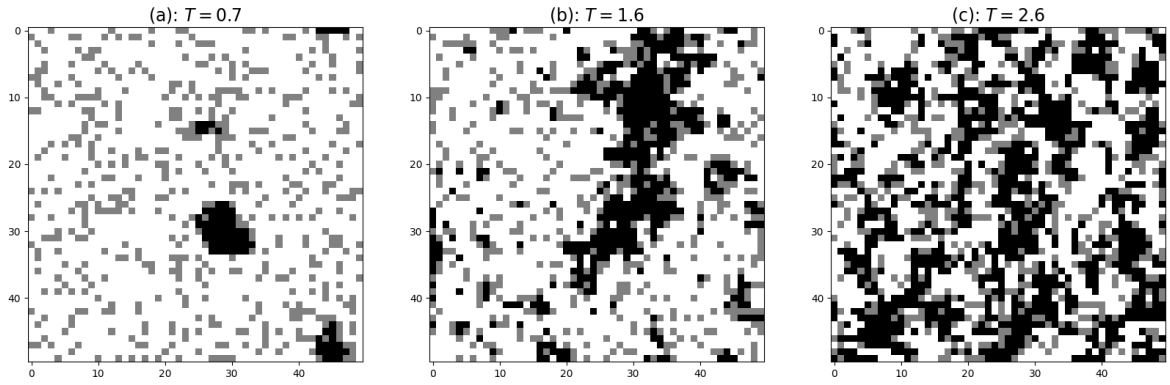

Figure 2: Visualization of the 2D square dilute Ising model with L=50, $p = 0.8$ for temperatures (a) $T << T_c$ (b) $T \approx T_c$ (c) $T >> T_c$. The grey sites are empty sites. White/Black sites are spin up/down respectively.

The dilute Ising model [3] is a special case of the Ising model, where only a proportion, p, of the sites in the lattice are occupied with a spin, and the rest are empty/non-magnetic. As the concentration of magnetic sites, p, decreases from 1 (pure case), the critical temperature of the system decreases [3] (see Fig. 3). This is because a smaller site concentration means there are fewer connections between spins, so it is easier for thermal fluctuations to overcome the tendency for spins to align and form ferromagnetic order. In the context of the dilute Ising model, the percolation threshold, p_c, is the critical concentration of magnetic sites above which an infinite cluster of connected magnetic sites is formed [3]. Below the percolation threshold, an infinite cluster is not formed and the lattice consists of isolated finite-sized clusters of spins. This means that long-range correlation between spins is impossible, and thus there is no 'critical temperature' at which the system undergoes a phase transition between a paramagnetic state and a ferromagnetic state with long-range magnetic order [3]. In this regime, the system can still exhibit local magnetic order, but this would not produce spontaneous magnetisation of the infinite system. Above the percolation threshold, there is an infinite cluster of connected spins, so the system can exhibit long-range magnetic order and spontaneous magnetization below the critical temperature [3]. In Fig. 3 we have displayed a schematic of the critical temperature vs the site concentration for the 3D cubic dilute Ising model.

The percolation threshold for the 2D square dilute Ising model is $p_c \approx 0.59274$ as found first in [15]. In this report we will investigate the 2D square dilute Ising model above the percolation threshold, with site concentration $p = 0.8$ (so 20% of sites are vacant/non-magnetic).

In Fig. 2 we show a visualization of configurations of the dilute Ising model at different temperatures, which we obtained using Monte-Carlo Metropolis simulations. We can see in Fig. 2(a) that there are some clusters of oppositely aligned spins (black patches) surrounded by mostly vacant sites. This shows how the presence of vacant sites can create partially disconnected clusters of spins which are harder to align with the rest of the system.

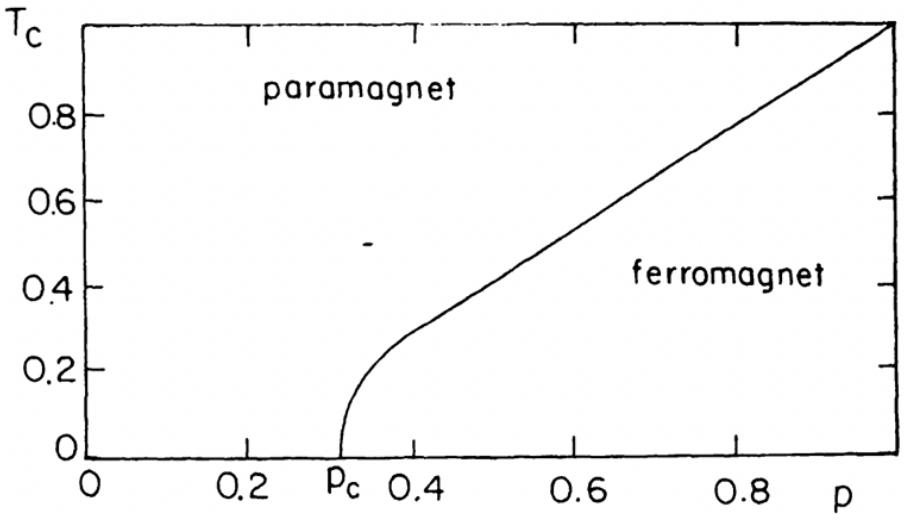

Figure 3: Schematic of critical temperature vs site concentration, p, for 3D cubic dilute Ising model as found in [3] "Introduction to Percolation Theory" chapter 7: "Application to Thermal Phase Transitions". p_c is the percolation threshold

4 Methodology

4.1 Monte Carlo simulation: Metropolis

Metropolis is a type of Monte Carlo simulation algorithm, which involves iteratively proposing a spin flip at a random site in the lattice, and accepting the flip with a probability related to the change in energy of the system [2]. Specifically, the probability of accepting the spin flip is given by the Boltzmann distribution [16], which dictates the ratio of probabilities of finding the system in the states prior to and after the spin flip. The Metropolis algorithm satisfies the condition of detailed balance, which states that for any given pair of states A and B, the probability of transitioning from A to B must be related to the probability of transitioning from B to A according to the equation [16]:

$$P_A \cdot W(A \to B) = P_B \cdot W(B \to A)\,, \tag{6}$$

where W is the transition rate, and P_A and P_B are the probabilities of finding the system in states A and B, respectively.

In statistical mechanics, the probability of finding a system in a state A is given by [16]:

$$P_A = \frac{e^{-\beta E_A}}{Z}, \tag{7}$$

where E_A is the energy of state A, Z is the partition function and $\beta^{-1} = k_B T$.

By substituting equation (7) into the detailed balance condition (6), we obtain

$$\frac{W(A \to B)}{W(B \to A)} = \frac{P_B}{P_A} = e^{-\beta(E_B - E_A)}. \tag{8}$$

The metropolis algorithm works as follows [16]:

1. Initialize all spins randomly.
2. Perform N trial moves of the following:
   (a) Current configuration is denoted A.
   (b) Pick a random site and flip the spin, denote this configuration B.
   (c) Calculate the change in energy $\Delta E = E_B - E_A$ of the system before and after the flip.
   (d) If $\Delta E > 0$ then set $W(B \to A) = 1$, then from equation (8): $W(A \to B) = e^{-\beta \Delta E}$.
   (e) If $\Delta E < 0$ then set $W(A \to B) = 1$.
   (f) Keep the new spin with a probability $W(A \to B)$, otherwise, flip back to the original spin.

If the number of trials is $N = L^2$, this is called a sweep of the lattice.

4.2 Principal Component Analysis (PCA)

Principal Component Analysis (PCA) is an unsupervised learning technique that was first introduced in 1901 by Karl Pearson and later developed in 1933 by Harold Hotelling [17]. PCA is primarily used for dimensionality-reduction of datasets, by converting the features of each sample to a shorter set of features, called principal components, which contain most of the original information. PCA is a powerful and extremely fast technique, and has been widely employed in numerous fields. For example, in finance, PCA has been employed for reducing the dimensionality of large datasets, helping to identify significant factors affecting asset returns and market trends [18].

Let $\mathbf{X}$ be a dataset with n rows (samples) and m columns (features), and X_i be the i-th column (feature) of $\mathbf{X}$. PCA works as follows [9], [10]:

1. First, each column is standardized to ensure all features have an equal contribution:

$$X_i^{std} = \frac{X_i - \mu_i}{\sigma_i}, \tag{9}$$

where μ_i and σ_i represent the mean and standard deviation of X_i, respectively.

2. The covariance matrix, $Cov(\mathbf{X})$, is calculated via:

$$Cov(X)_{i,j} = cov(X_i, X_j) = E((X_i - E(X_i))(X_j - E(X_j)))\,, \tag{10}$$

where E denotes the expected value (mean) operation.

3. The eigenvectors, v_j and eigenvalues, λ_j, of the covariance matrix are computed. These are ordered in descending order of eigenvalue magnitude, $|\lambda_j|$. The eigenvalues represent the amount of variance in the data in the direction of the corresponding eigenvector, so v_1 is the direction of maximum variance, v_2 is the direction of maximum variance that is orthogonal to v_1, and so on.

4. The principal components are then obtained via:

$$p_j = \mathbf{X} \cdot v_j\,, \tag{11}$$

where $\cdot$ represents the matrix action of $\mathbf{X}$ on v_j.

Typically, the first principal components, with the largest eigenvalue magnitudes, contain the most information of the original dataset. Thus, by choosing only the top k principal components, we can reduce the dimensionality of the data from m features to k features. Ie. the $n \times k$ dataset $\tilde{X}$ where the i-th column is $\tilde{X}_i = p_i$, is the dimensionality-reduced version of the $n \times m$ dataset X, where $k \leq m$.

4.3 KMeans Clustering

KMeans is an algorithm that partitions a dataset into a predefined number of clusters of similar data points. For an $n \times m$ dataset, $\mathbf{X}$, each row is a data-point (sample), so one can imagine plotting the n data-points in m-dimensional space. The algorithm works as follows [9]:

1. Choose k random points in the space that the data-points are embedded in. These are called centroids.

2. The i-th cluster, C_i, is the set of data-points that are closer (in euclidean distance) to the i-th centroid than any other centroid

3. The i-th centroid is updated to be the mean of cluster C_i

4. Repeat step 2 and 3 until the positions of the centroids stop changing, or the predefined maximum number of steps is reached.

The algorithm aims the minimize the sum of squares (variance) within each cluster. That is, it aims to minimize the following expression [9]:

$$\sum_{i=1}^{k} \sum_{\vec{x} \in C_i} ||\vec{x} - \vec{\mu}_i||^2\,, \tag{12}$$

where k is the predefined number of clusters, C_i is the i-th cluster, $\vec{x}$ is a data-point, $\vec{\mu}_i$ is the mean of the i-th cluster, $||\cdot||$ computes euclidean distance.

5 Results and Analysis

5.1 Pure Ising Model

We first use these methods to investigate the pure Ising model on $L \times L$ square lattices with periodic boundary conditions. We generate independent snapshots of the lattice configurations using Monte Carlo Metropolis simulations. For each snapshot, we initialise a lattice randomly with 75% of one spin state (+1 or -1) and perform 100 Metropolis sweeps of the lattice to converge to equilibrium, then record the final configuration, stored as an L^2 dimensional vector. Imposing 75% of one spin type at the initialisation was found to greatly speed up convergence. Using this method, we generate $a \approx 100$ configurations for $n_T = 17$ temperatures around the expected critical temperature and obtain a dataset, X, with dimensions $n_T a \times L^2$

Using the raw configurations, we calculate the magnetisation and magnetic susceptibility, and plot them in Fig.4. From Fig.4(a) we see that the magnetisation exhibits the expected behaviour of an order parameter, that is, it drops steeply from ≈ 1 to ≈ 0 around the expected critical temperature. The errorbars in the magnetisation plot, calculated as the standard error of the mean, were of order 10^{-2} or below, and are barely visible as a result. We see from Fig.4(b) that the magnetic susceptibility also exhibits the expected behaviour; a sharp peak close to the expected critical temperature. The errorbars were calculated as the standard error on the mean from taking multiple independent measurements of the magnetic susceptibility. They tell us that the most variance occurs around the critical temperature.

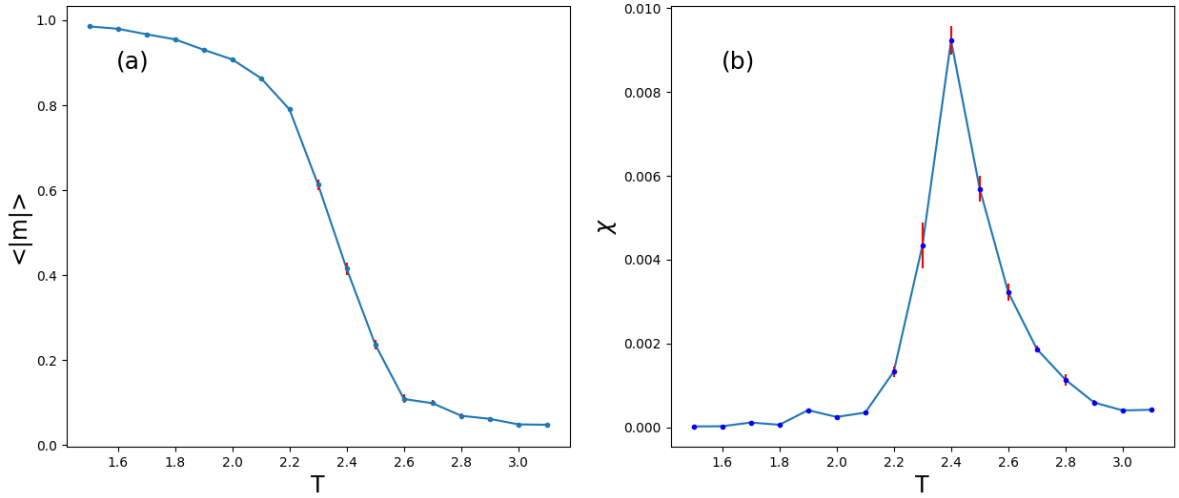

Figure 4: Macroscopic Variables of 2D square pure Ising model with L=50. (a) Mean of absolute value of Magnetisation vs Temperature. (b) Magnetic Susceptibility vs Temperature

Fig.5 shows the results of performing PCA on the dataset of spin confiurations, X. The size of the covariance matrix, and hence the number of principal components we obtain is $N = 1500$. Fig.5(a) displays (the mean of the absolute value of) the first principle component

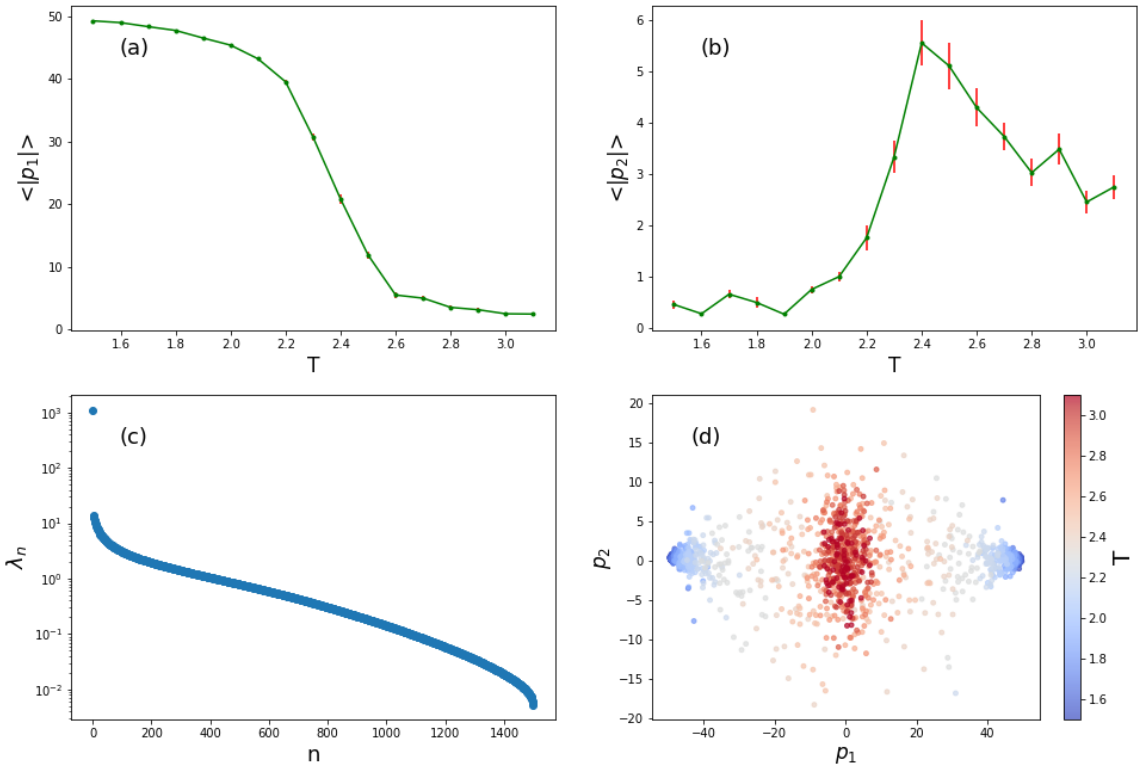

Figure 5: PCA results for 2D square pure Ising model with L=50. (a) Mean of absolute value of the first principal component vs temperature. (b) Mean of absolute value of the second principal component, p_2, vs temperature. (c) Eigenvalues corresponding to each principal component (d) Projection of raw Ising configurations onto the 2D plane spanned by p_1 and p_2. Each point is a 2D representation of a Ising configuration. Colourbar corresponds to temperature of the configuration.

against temperature, which we see is a perfect analogue of the magnetisation of the system by comparing it to Fig.4(a). In Fig.5(b) we plot the second principle component vs temperature, and we see by comparing it to Fig.4(b) that it is loosely analogous to the magnetic susceptibility. Both plots are ≈ 0 at low temperature and peak at the same temperature, except the real magnetic suceptibility decays much quicker after the peak. From Fig.5(c) we see the first eigenvalue (corresponding to p_1) is more than one order of magnitude greater than the next largest eigenvalue. Since p_1 is an analogue of the magnetisation, the implication from this is that the magnetisation is the most important variable to characterise the phase transition since it contains the most information from the original dataset. This is a reasonable suggestion as the magnetisation alone can distinguish whether the system is the ordered ferromagnetic phase or disordered paramagnetic phase. The first two principal components provide 2D representations of each of the raw spin configurations. We plot these in Fig.5(d) and add a colourbar corresponding to the temperature of each configuration. We see that above the critical temperature, the points form a cluster at the origin, and below the critical temperature there are 2 distinct clusters either side of the central high temperature cluster. These two low temperature clusters correspond to spins aligned 'up' and 'down' re-

spectively. This clearly demonstrates the ability of PCA to distinguish between the ordered states below the critical temperature and the disordered states above the critical temperature.

Finding the critical temperature when dealing with relatively small amounts of data can be difficult. The binder ratio method is a well-tested and very effective method to find the critical temperature of the Ising model, provided that enough measurements are made. In this case however, we only have ≈ 100 independent configurations per temperature, which may not be sufficient for the binder method to produce an accurate result. To show this, in Fig.6 we display the results of the binder ratio method, which finds the critical temperature $T_c = 2.52 \pm 0.04$. The true critical temperature, $T_c \approx 2.269$, does not lie within the uncertainty of our obtained result, and we have a percentage error of 11%.

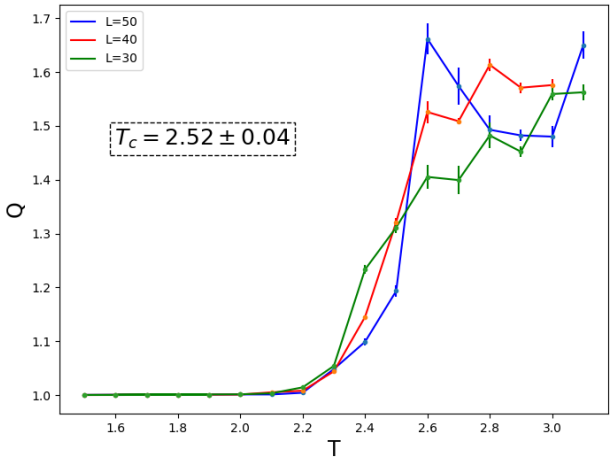

Figure 6: Binder Ratio vs Temperature for L=30,40,50 of 2D square pure Ising Model

We propose here a new method to find an estimate of the critical temperature, by combining PCA and KMeans clustering. We saw in Fig.5(d) that PCA can successfully separate high temperature disordered states from low temperature ordered states. We perform KMeans clustering on this 2D data and obtain three distinct clusters as can be seen in Fig.7. Cluster 0 and 1 are the clusters of low temperature ordered configurations and cluster 2 consists of high temperature, disordered configurations. We can then obtain an estimate for the critical temperature by finding the temperature at which a configuration will change from being in cluster 0 or 1, to being a member of cluster 2 (ie. the temperature at which a configuration transitions from order to disorder). To find the critical temperature using the KMeans cluster labels, we calculate the proportion of each cluster at each temperature, and use this to assign a weight to the temperature related to the likelihood of being the critical temperature. The critical temperature and error is given by the weighted mean and standard error on the mean. See appendix A for a full description of this algorithm to find T_c using the cluster labels.

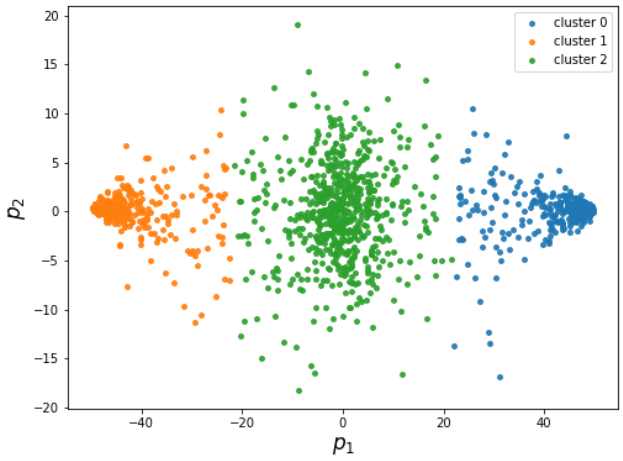

Figure 7: KMeans clustering performed on the 2D Ising configurations

Using this method, we calculate the critical temperature for L=50, 40, 30 and use finite size scaling, displayed in Fig.8, to find the critical temperature for the infinite 2D square Ising model as $T_c = 2.33 \pm 0.08$. The error in this value is found by projecting the steepest and shallowest gradients permitted by the error bars in Fig.8 and calculating half the range between the two limits.

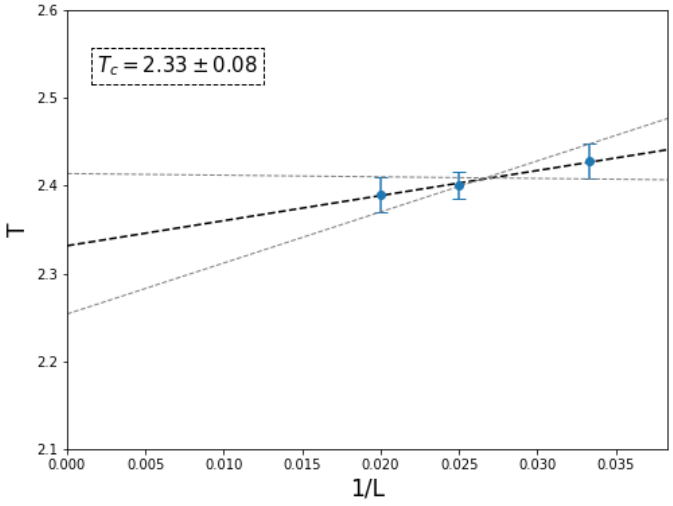

Figure 8: Finite Size Scaling of the pure 2D Ising model. The critical temperature is found from the y-intercept

The true value for the critical temperature is $T_c \approx 2.269$, thus the percentage error is 2.6%. The true value is within the uncertainty of our obtained value and the obtained value is correct to one decimal place. This is a considerably more accurate result than what we obtained using the binder ratio method. This tells us that combining PCA + KMeans clustering is a more accurate method to find the critical temperature when dealing with small datasets.

It is somewhat unsurprising that our unsupervised method slightly overestimated the critical temperature. The random fluctuations of the Ising model above the critical temper-

ature will cause some high temperature configurations to appear ordered and be placed in the wrong cluster, which will cause the 'change point' to be found at a higher temperature than the true critical temperature. Nevertheless, this is still an effective method to find an estimate of the critical temperature when dealing with small datasets. In what follows, this is the method we will use to estimate the critical temperature of the dilute Ising model.

5.2 Dilute Ising Model

We now repeat the same procedure on the 2D square dilute Ising model with site concentration $p = 0.8$. To generate the configurations, the same Metropolis method was used, except that during initialisation of the lattices 20% of the sites were made randomly vacant such that each configuration had a new random arrangement of vacant sites. The vacant sites were not allowed to move as the system converged to equilibrium (quenched dilution). Each configuration was initialised separately to ensure independence with respect to the spins and the vacancies. We generate $a \approx 100$ independent configurations for $n_T = 20$ temperatures around the expected critical temperature.

In Fig. 9 we plot the magnetisation and the magnetic susceptibility, and retrieve similar results to the pure case, except the magnetic susceptibility has a wider peak. The reason for this is unclear.

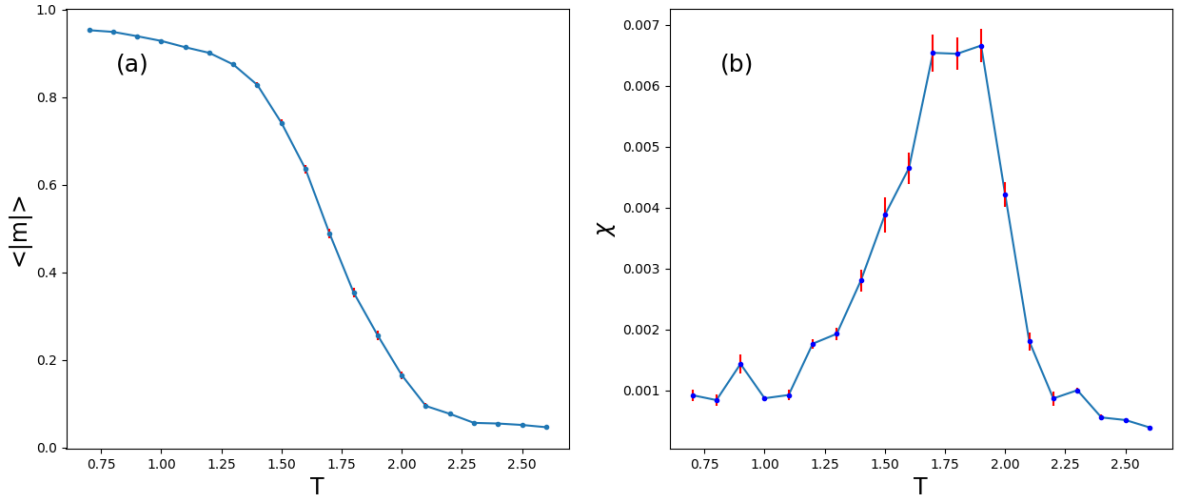

Figure 9: Macroscopic Variables of 2D square dilute Ising model for L=50. (a) Mean of absolute value of Magnetisation vs Temperature. (b) Magnetic Susceptibility vs Temperature

The PCA results of the dilute Ising model are shown in Fig. 10. We see that, once again, the first principal component becomes analogous to the magnetisation, and has the largest eigenvalue by more than one order of magnitude. However, we see in Fig. 10(b) that the connection between the second principal component and the magnetic susceptibility is lost for the dilute Ising model. This likely arises due to the randomly empty sites in the lattice complicating the data.

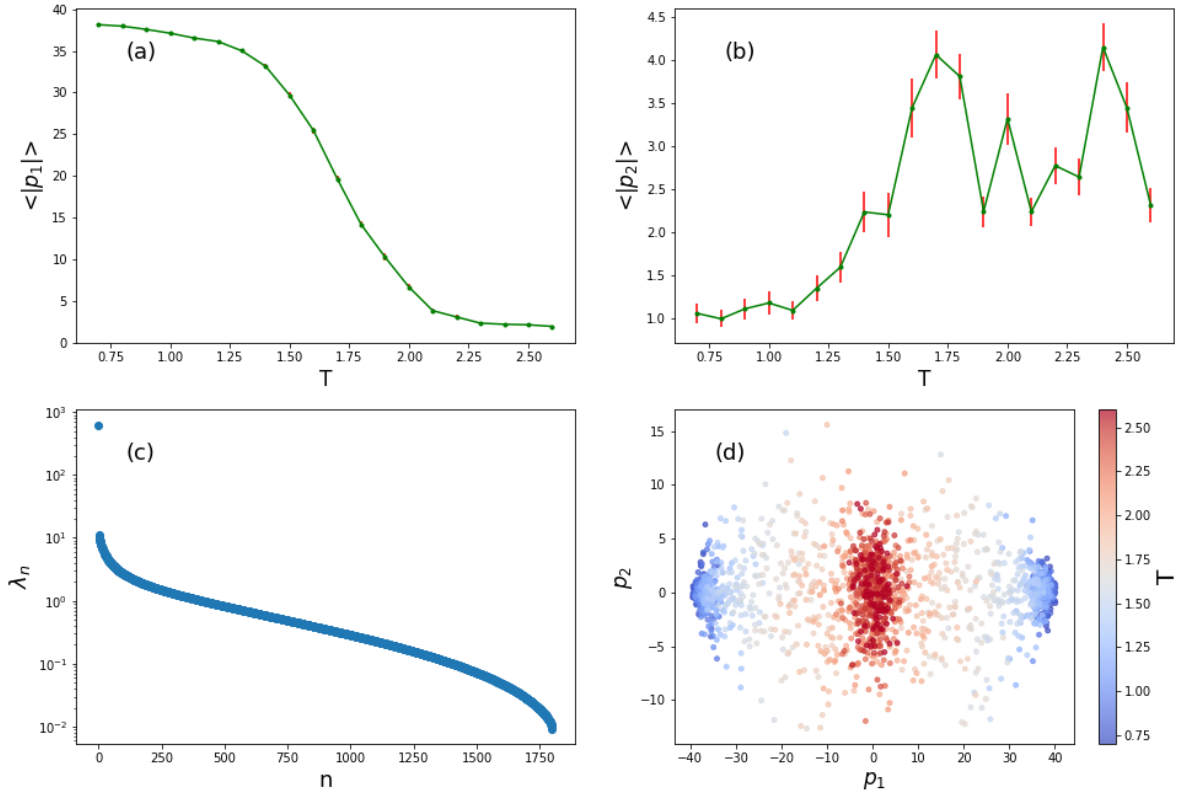

Figure 10: PCA results for 2D square dilute Ising model with L=50. (a) Mean of absolute value of the first principal component vs temperature (b) Nean of absolute value of the second principal component vs temperature. (c) Eigenvalues corresponding to each principal component in order (d) 2D Projection of raw configurations

The 2D representations of the dilute Ising configurations are plotted in Fig. 10(d), and we see that the behaviour is very similar to that of the pure case in Fig. 5(d). The only minor difference is the data points are somewhat more spread out along the axis of the second principal component, and the clusters appear less dense and distinct. This may suggest that PCA is slightly less effective at separating ordered and disordered states in the dilute Ising case, compared to the pure case. This is unsurprising, as there is additional disorder with the presence of vacant sites.

Using the same method as before to find the critical temperature using PCA + KMeans, we find T_c for L=50,40,30 and produce the finite size scaling plot in Fig. 11. This finds the critical temperature to be $T_c = 1.76 \pm 0.08$.

The reference value of the critical temperature of the dilute Ising model with site concentration $p = 0.8$ as found in [19] is $T_c = 1.50 \pm 0.06$. This does not lie within the uncertainty of our obtained value and we have a percentage error of 17%. We successfully identified that the critical temperature is smaller than in the pure case, but despite this, our result shows a significant deviation from the reference value. However, the reliability of the reference value must be questioned, as it was obtained from source [19], which is an unpublished Master's thesis and has not been peer-reviewed. No other published data with which to compare our

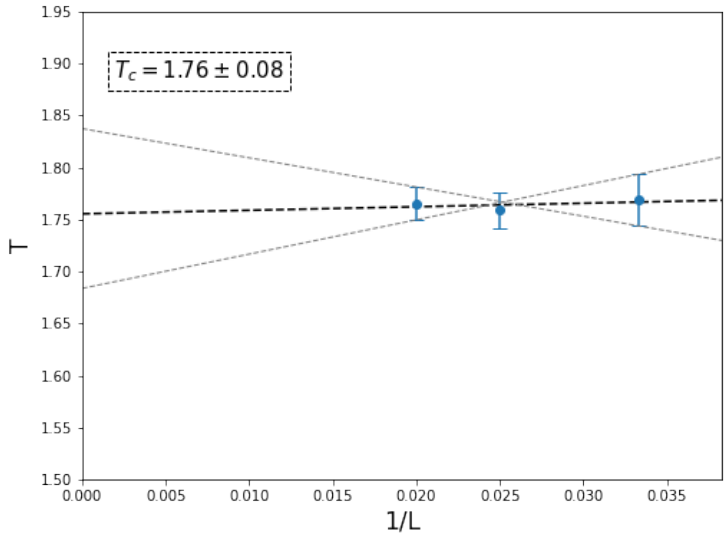

Figure 11: Finite Size Scaling of the 2D square dilute Ising model

results was found. Assuming that [19] is reliable, we now discuss the possible sources of error in our result. It is possible that unusual behaviour caused by the presence of empty sites may have confused the unsupervised learning process. For instance, the vacant sites can give rise to islands of spins which are disconnected or partially disconnected from the rest of the lattice, which means that when the system is in its ferromagnetic phase close to its ground state, there can exist isolated clusters of oppositely aligned spins, as can be seen in Fig. 2(a). This behaviour complicates the training data and may have contributed to the error in the result. Additionally, the dilution causes fewer connections between spins, which makes thermal fluctuations easier. This may have caused higher variance in the training data, contributing to the error of any measurements. It is also possible that ≈ 100 configurations per temperature is not sufficient to produce an accurate result, even though it was sufficient for the pure Ising model. In the dilute Ising model, different arrangements of vacant sites in the lattice can yield different critical temperatures, and the value we search for is the **dilution-averaged** critical temperature. Hence it is possible that the random arrangements of vacant sites in the training data on average biased the system to make it harder to overcome the tendency for order, thus raising the critical temperature. Any biases like this can be eliminated by simply generating a higher quantity of training data.

6 Conclusion

In this report, the application of principal component analysis and KMeans clustering to the pure and dilute 2D square Ising model was explored. For the pure Ising model, it was found that PCA successfully distinguishes the ordered ferromagnetic phase from disordered paramagnetic phase. The first principal component was shown to be exactly analagous to the magnetisation, and the second principal component loosely mimiced the behaviour of the magnetic susceptibility. By searching for the critical temperature using the classical Binder ratio method and then again using the combination of PCA, KMeans and change point detection, the results indicate that our original clustering-based method is more accurate for finding an estimate of the critical temperature than the binder method when dealing with small datasets. Using the binder method, we had a percentage error of 11%, and using clustering we had a percentage error 2.6%. Since this method uses purely unsupervised learning and does not require any knowledge of the physics of the system, it provides a generic tool to aid with future work in analysing unexplored phase transitions. For the dilute Ising model, this study reveals that PCA has a similar effect to that of the pure case, with a few differences. Firstly, while the first principal component is still exactly analagous to the magnetisation, the relation between the second principal component and magnetic susceptibility is completely lost for the dilute Ising model. Additionally, similarly to the pure case there were 3 main clusters of states, 2 low temperature and 1 high temperature, but they appeared slightly less distinct for the dilute Ising model, suggesting that PCA is capable but slightly less effective at distinguishing between different phases of the dilute Ising model. This is likely due to unusual behaviour caused by the vacant sites, which complicates the training data and increases the variance. Using our clustering-method, we find the critical temperature of the 2D square dilute Ising model with site concentration $p = 0.8$ is $T_c = 1.76 \pm 0.08$, which has a percentage error of 17% compared to the reference value, although the reliability of our reference value is questionable. The main source of error in this reading is likely that the size of our dataset was not sufficient to produce an accurate dilution-averaged result. In summary, the use of PCA and KMeans clustering to study phases and critical behaviour works very well for the pure Ising model, and is useful to some extent for the dilute Ising model, but is somewhat less accurate. This work could be expanded upon by generating considerably more training data, and investigating the relationship between the number of configurations per temperature, and the accuracy of the measurement of the dilution-averaged critical temperature. Additionally, in future work, it would be interesting to test other unsupervised learning techniques on the dilute Ising model, such as variational autoencoders [20], UMAP [21], or t-SNE [22], to see if they can yield more accurate results.

References

[1] S. Simon, The Oxford Solid State Basics. Oxford University Press, 2013.

[2] J. Kotze, "Introduction to Monte Carlo methods for an Ising Model of a Ferromagnet", arXiv:0803.0217 (2008).

[3] D. Stauffer and A. Aharony, Introduction to Percolation Theory, 2nd ed. Taylor & Francis, 1994.

[4] N. Walker, K. M. Tam, and M. Jarrell, "Deep learning on the 2-dimensional Ising model to extract the crossover region with a variational autoencoder", Sci. Rep. **10**, 13047 (2020).

[5] E. van Nieuwenburg, Y. H. Liu, and S. Huber, "Learning phase transitions by confusion", Nat. Phys. **13**, 435-439 (2017).

[6] H. Huang, V. Nosenko, H.-X. Huang-Fu, H. M. Thomas, and C.-R. Du, "Machine learning in the study of phase transition of two-dimensional complex plasmas", Phys. Plasmas **29**, 073702 (2022).

[7] W. Hu, R. R. P. Singh, and R. T. Scalettar, "Discovering phases, phase transitions, and crossovers through unsupervised machine learning: A critical examination", Phys. Rev. E **95**(6), 062122 (2017)

[8] R. Zhang, B. Wei, D. Zhang, J.-J. Zhu, and K. Chang, "Few-shot machine learning in the three-dimensional Ising model", arXiv:1903.08061 (2019).

[9] A. Tirelli, D. O. Carvalho, L. A. Oliveira, J. P. Lima, N. C. Costa, and R. R. dos Santos, "Unsupervised machine learning approaches to the q-state Potts model", arXiv:2112.06735 (2021).

[10] E. Khatami, "Principal component analysis of the magnetic transition in the three-dimensional Fermi-Hubbard model", J. Phys.: Conf. Ser. **1290**, 012006 (2019)

[11] L. Onsager, "Crystal statistics. I. A two-dimensional model with an order-disorder transition", Phys. Rev. **65**, 117 (1944).

[12] A. Sandvik, "Monte Carlo simulations in classical statistical physics," in Computational Physics, Fall 2018 Department of Physics, Boston University.

[13] N. Crokidakis, D. O. Soares-Pinto, M. S. Reis, A. M. Souza, R. S. Sarthour, and I. S. Oliveira, "Finite size analysis of a two-dimensional Ising model within a nonextensive approach," arXiv:0910.2218 (2009)

[14] K. Binder, "Finite size scaling analysis of Ising model block distribution functions", Z. Phys. B Condens. Matter **43**(2), 119-140 (1981).

[15] B. Derrida and D. Stauffer, "Corrections to scaling and phenomenological renormalization for 2-dimensional percolation and lattice animal problems", J. de Phys. **46**, 1623 (1985).

[16] J.-C. Walter and G. T. Barkema, "An introduction to Monte Carlo methods", arXiv:1404.0209v1 (2014).

[17] I. Jolliffe, Principal Component Analysis, 2nd ed. (Wiley, Hoboken, New Jersey, 2002)

[18] G. Connor and R. A. Korajczyk, "Risk and return in an equilibrium APT: Application of a new test methodology", J. Financial Econ. **21**, 255 (1988).

[19] P. J. Meyer, "Computational Studies of Pure and Dilute Spin Models", (Unpublished master's thesis), University of Derby, UK. Retrieved from: https://www.hermetic-systems.com/compsci/thesis/index.html

[20] D. P. Kingma and M. Welling, "An Introduction to Variational Autoencoders", arXiv:1906.02691v3 (2019).

[21] L. McInnes, J. Healy, and J. Melville, "UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction", arXiv:1802.03426 (2018).

[22] L. van der Maaten and G. Hinton, "Visualizing Data using t-SNE", Journal of Machine Learning Research **9**, 2579-2605 (2008).

Appendix

A Change Point Detection

We estimate the critical temperature using the cluster labels as follows;

The total number of data-points in the central (high temperature) cluster and the collective side (low temperature) clusters are n_h, n_l respectively. For each temperature, T_i, count the number of data-points in the high temperature cluster, $n_{h,i}$ and in low temperature clusters, $n_{l,i}$

Then the probability of temperature, T_i, being higher than the critical temperature is:

$$P(T_i > T_c) = \frac{(n_{h,i}/n_h)}{(n_{l,i}/n_l) + (n_{h,i}/n_h)}$$

We then convert this to the weight of temperature, T, via:

$$Weight(T) = 1 - 2|0.5 - P(T > T_c)|$$

This weight was chosen such that the closer $P(T > T_c)$ is to 0.5, the more likely it is to be the critical temperature so the higher the weight.

Then we find the critical temperature by taking the weighted mean of the temperatures, and we use the standard error of the weighted mean as the error for T_c