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Original Article

Machine Learning of the Two-dimensional Diluted Bond Ising Model

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Abstract. Bond-diluted 2D Ising model is essential for understanding the effects of disorder on magnetic systems. Although the *T-p* phase diagram of this model has been developed through analytical methods and Monte Carlo simulations, the region near the percolation threshold p_c remains insufficiently explored. In this work, we investigated the impact of bond dilution on phase transitions in the bond-diluted 2D Ising model using a machine learning approach. A convolutional neural network, initially trained on data from the pure (undiluted) 2D Ising model, is employed through transfer learning to analyze bond-diluted systems. The numerical results show that as bond concentration decreases, the critical temperature also decreases, in agreement with previous Monte Carlo simulation results. Moreover, these findings are instrumental in estimating the critical bond dilution near the percolation threshold p_c. As a result, a comprehensive phase diagram for the bond-diluted 2D Ising model has been constructed.

Keywords: Monte Carlo simulations, phase transitions, magnetic materials.

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1. Introduction

The Ising model is a fundamental concept in statistical physics, renowned for its simplicity and sufficiently complex to exhibit interesting phenomena such as phase transitions and criticality. Originally conceived to understand ferromagnetism, it has become a staple for studying a wide range of phenomena. The pure Ising model considers a lattice of spins that interact with their nearest neighbors.

In real materials, perfect purity is rare and impurities are often inevitable. To investigate the effects of such imperfections, variants of the Ising model have been proposed, common ways to model impurities include randomly removing spins (site dilution) [1-3] or bonds (bond dilution) [4-6], or by randomly modifying the interaction strengths. Bond dilution involves randomly removing bonds between neighboring spins with a probability (1 - p), where p is the bond concentration. This introduces disorder, affecting properties like the critical temperature for phase transitions. In a two-dimensional bonddiluted Ising model, the critical temperature decreases as the bond concentration p decreases, reaching zero at the percolation threshold (p_c = 0.5) [7, 8]. Studying the phase transitions and critical behavior of the diluted Ising model presents challenges for analytical and numerical techniques [6, 9,10]. However, increasing availability of data and computational power has led to the successful application of machine learning (ML) methods and neural networks (NN) in various fields, including physics, for discovering knowledge in complex systems. In the field of physics, machine learning has been successfully employed to study phase transitions in Ising models [11-13] and the site-dilution Ising model [14].

This work examines the use of machine learning, specifically convolutional neural networks (CNNs), to analyze the two-dimensional bond-diluted Ising model. By training a CNN on configurations from the pure Ising model, the research aims to assess its effectiveness in identifying and characterizing different phases, determining critical temperatures for various bond concentrations, and exploring the percolation transition. This method leverages the pattern recognition strengths of neural networks to address challenges in studying this complex model with traditional techniques. The focus is on how machine learning can enhance our understanding of the interaction between disorder and thermal fluctuations in magnetic systems

2. Model and Method

We consider the bond diluted Ising model on a two-dimensional square lattice of size $L \times L$. This model is a variant of the regular Ising model, in which interactions between nearest-neighbor spins are randomly removed with a probability (1 - p), where p represents the bond concentration. The Hamiltonian of the bond-diluted Ising model can be written as:

$$H = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j \qquad (1)$$

where σ_i and σ_j are Ising spins taking values +1 or -1 at lattice sites i and j, and the summation is over nearest neighbor pairs <ij>. The exchange coupling constant J_{ij} is non-zero (typically set to $J > 0$ for ferromagnetic interactions) only if a bond exists between sites i and j; otherwise, J_{ij} = 0. The bond configuration is typically generated randomly at the beginning of each simulation based on the bond concentration p.

$$P(J_{ij}) = p\delta(J_{ij} - 1) + (1 - p)\delta(J_{ij}) \qquad (2)$$

Here we use $\delta(J_{ij})$ is an indicator function that yields one if J_{ij} = 0 and zero otherwise. where p corresponds to the probability of drawing a ferromagnetic bond with J_{ij} = 1, while 1 - p is the probability of missing bonds with J_{ij} = 0.

To train and evaluate our machine learning model, we generate spin configurations of the two-dimensional bond diluted Ising model using Monte Carlo simulations (5,000 spin configuration for p = 1 and 1,000 spin configurations for another p). Specifically, we employ the Metropolis algorithm to efficiently sample equilibrium configurations at various temperatures T (34 temperatures) and bond concentrations p (p = 0.45, 0.49, 0.5, 0.51, 0.55, 0.6, 0.7, 0.8,0.9, and 1.0). For each chosen value of p, we perform simulations at a range of temperatures around the expected critical temperature $T_c(p)$. The simulations are run for a sufficient number of Monte Carlo steps (e.g., Metropolis sweeps per lattice site) to ensure that the system reaches thermal equilibrium. This typically involves a thermalization period followed by a production run where spin configurations are stored. We generate datasets of spin configurations for different lattice sizes L = 8, 16, 32 to study finite-size scaling effects. To validate the convolutional neural network, independent sets of 500 simulated configurations are generated for p = 1 that are not used during the training phase.

We utilize a convolutional neural network with two hidden layers, to classify the phases of the bond-diluted Ising model. The input to the convolutional neural network is typically a flattened representation of the spin configuration on the $L\times L$ lattice. We construct a CNN architecture similar to that of Efthymiou et al., [13]. There are two convolutional layers: a max-pooling layer connected to a fully connected neuron network (NN) layer and a softmax output layer for classifying phases. We employ the Keras interface as implemented in the Tensorflow package. The cross-entropy loss function (categorical cross entropy) is used with the Adam optimizer. We employ the softmax function to convert raw output values into probabilities. The output layer consists of neurons representing the different phases of the system, such as ferromagnetic and paramagnetic phases. The convolutional neural network is trained on a dataset of labeled spin configurations generated from Monte Carlo simulations at various temperatures and bond concentrations p = 1. The labels correspond to 0 for spin configuration of $T > T_c$ and 1 for spin configuration at $T < T_c$. The convolutional neural network is trained using a supervised learning approach, where the network learns to map input spin configurations to their corresponding phase labels by adjusting its internal weights and biases to minimize a chosen loss function. Training is performed using an optimization algorithm such as stochastic gradient descent. The training process involves iterating over the training data for a certain number of epochs = 250, batch size = 32, and the performance on a separate validation set is monitored to prevent overfitting.

After training, the convolutional neural network's ability to identify and characterize the phases of the bond-diluted Ising model is evaluated on a separate test dataset of spin configurations for each p. The trained network's classification accuracy is assessed by comparing its phase predictions with the known phases of the test configurations. The network's output probabilities for different phases can be analyzed as a function of the temperature for various bond concentrations to identify the phase transition. The critical temperature $T_c(p)$ can be estimated by finding the temperature at which the probabilities of the ordered and disordered phases are equal.

3. Results and Discussion

This section discusses the learning performance outcomes of the 2D diluted bond Ising model. By analyzing the average output of the three softmax neurons in the output layer, we estimate the critical temperature for each case. The phase diagram will illustrate the critical temperatures and the nature of the phase transitions.

First, we train and test the model at bond concentration p = 1. Fig. 1 presents the estimated probabilities from our convolutional neural network for the ferromagnetic (blue curves) and paramagnetic (red curves) phases of the 2D diluted bond Ising model on a square lattice with size L =

8, 16, 32 as a function of temperature T (in units of *J/kB*). These probabilities are computed by averaging the network's predictions over 1,000 independent spin configurations at each temperature.

As seen in Fig. 1, for *p* = 1 (corresponding the pure Ising model), the probability of the paramagnetic phase is close to 1 at high temperatures, indicating a disordered state. Conversely, the probability of the ferromagnetic phase approaches 1 at low temperatures, signifying an ordered state. The transition temperature T_c is estimated as the temperature at which the ferromagnetic and paramagnetic probability curves intersect, with each phase having a probability of 0.5. For *p* = 1, this intersection occurs at T = 2.269, consistent with the known analytical T_c = 2.269 from exact solutions, Monte Carlo simulations, and previous machine learning studies [12]. These results validate the accuracy of our model in identifying the phase transition in the 2D Ising model.

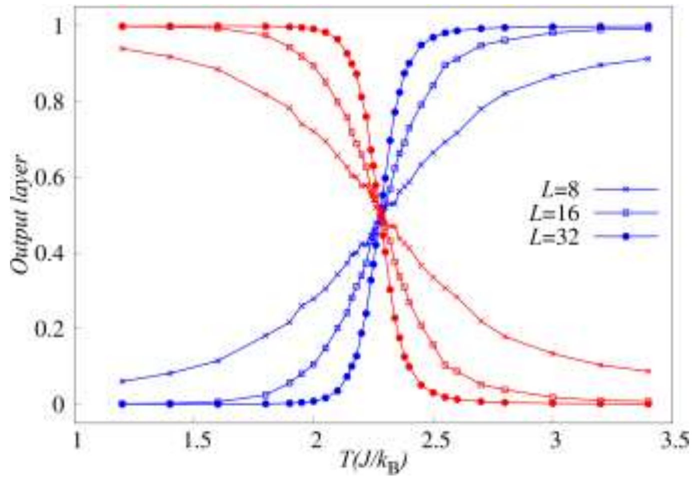

Figure 1. The output layer averaged (y-axis) over a test set as a function of temperature *T*/*J (x-axis)* for *p* = 1.

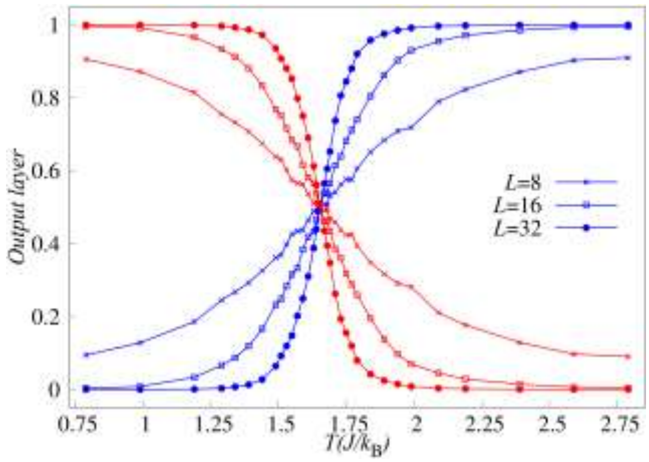

Figure 2. The output layer averaged (y-axis) over a test set as a function of temperature T/J (x-axis) for p = 0.8.

Next, we train at *p* = 1 and test the model across a range of bond concentrations $0.55 \leq p \leq 1$, including *p* = 0.9, 0.8, 0.7, 0.6, and 0.55. Fig. 2 shows the temperature dependent of output layer probability for *p* = 0.8. As the system size increases, the probability curves become sharper near the transition point, suggesting that larger system sizes yield more precise estimates of the critical behavior.

From the crossing points of the curves, we determine critical temperatures of T_c = 1.652 for p = 0.8. Similarly, we also obtain T_c = 1.968 for p = 0.9, T_c = 1.329 for p = 0.7, and T_c = 0.970 for p = 0.6, and T_c = 0.748 for p = 0.55, respectively. A clear trend emerges: as the bond concentration p decreases, the critical temperature $T_c(p)$ also decreases. This is consistent with physical intuition, as fewer bonds weaken ferromagnetic interactions, lowering the temperature necessary for the onset of long-range order. These results are in strong agreement with previously published works, particularly Ref. [8, 15].

Next, we train at p = 1 and test the model at p < 0.55. Fig. 3 shows the temperature dependent of output layer probability for p = 0.51. As the system size increases, the paramagnetic probability approaches 1 at high temperatures but increases more gradually at low temperatures. Identifying the crossing point yields an estimated critical temperature T_c = 0.531 for p = 0.51. Similarly, T_c = 0.595 is obtained for p = 0.52. These are the first estimates of critical temperatures for p < 0.55, a regime where conventional Monte Carlo simulation methods analysis fail due to the lack of intersection points of Binder parameter [8, 15].

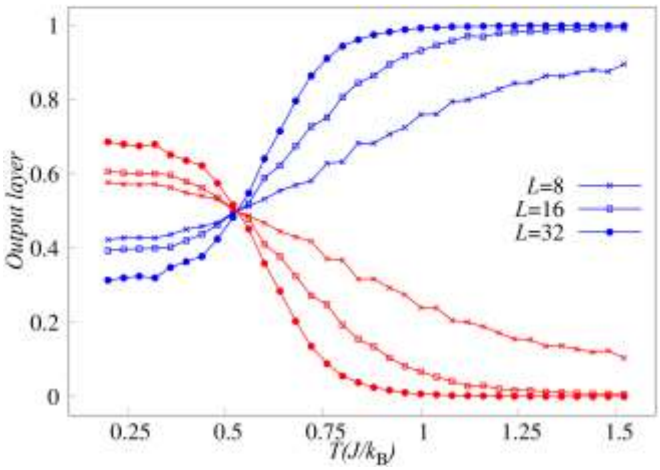

Figure 3. The output layer averaged (y-axis) over a test set as a function of temperature T/J (x-axis) for p = 0.51.

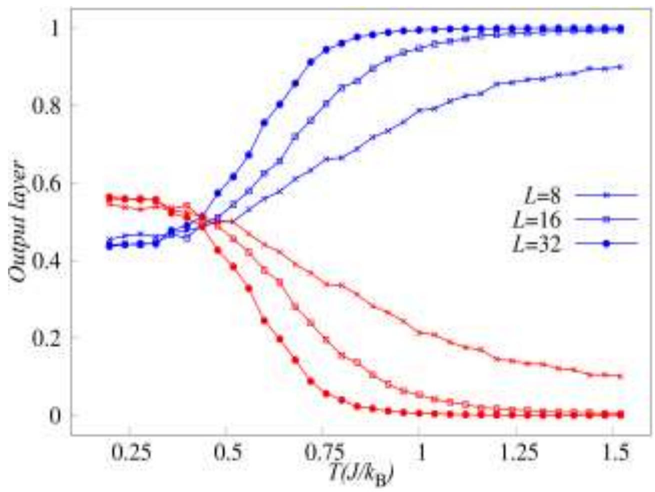

Figure 4. The output layer averaged (y-axis) over a test set as a function of temperature T/J (x-axis) for p = 0.5.

Fig. 4 shows the temperature dependent of output layer probability for $p = 0.5$. Here, the probability curves for different system sizes tend to collapse at low temperatures, suggesting a lack of clear phase transition. Although the curves still cross at $T_c = 0.407$, the absence of sharp phase separation indicates that the nature of the system at $p = 0.5$ requires further investigation.

Next, we train at $p = 1$ and test the model at $p < 0.5$, including $p = 0.49$ and $p = 0.45$ as shown in Fig. 5 and Fig. 6. We observe that the ferromagnetic and paramagnetic probability curves may no longer intersect at any finite temperature. This behavior indicates the absence of a phase transition and implies that the system remains in the disordered paramagnetic phase down to zero temperature. This finding suggests that the bond concentration is below the percolation threshold $p_c = 0.5$ for the square lattice.

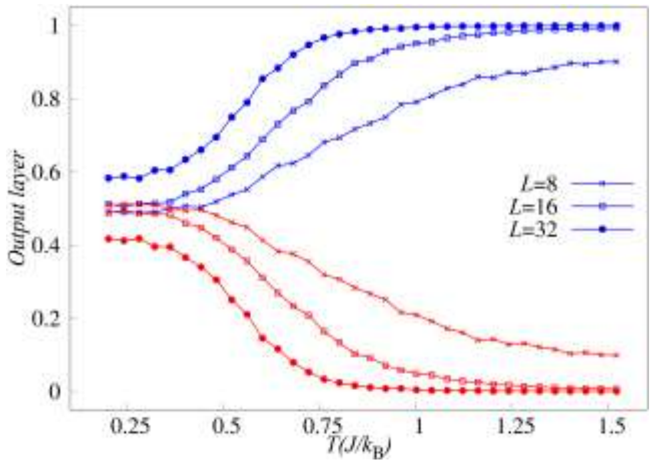

Figure 5. The output layer averaged (y-axis) over a test set as a function of temperature T/J (x-axis) for $p = 0.49$.

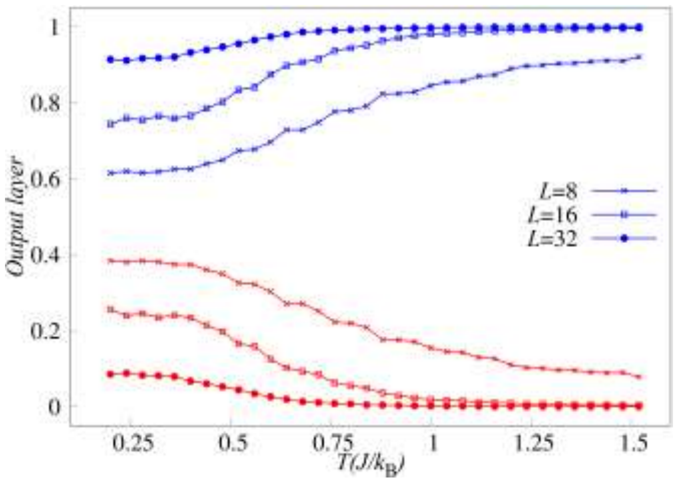

Figure 6. The output layer averaged (y-axis) over a test set as a function of temperature T/J (x-axis) for $p = 0.45$.

Remarkably, our model, trained solely on ordered and disordered configurations at $p = 1$ without explicit exposure to dilution or temperature dependence, accurately classifies phases and estimates critical properties for $p < 1$. This demonstrates its strong generalization ability. It suggests that the network's learned representations of the pure 2D Ising model are sufficiently robust to extrapolate to the diluted model. Moreover, compared to Monte Carlo simulation methods which require a large number of samples for accurate estimates the model achieves comparable accuracy using significantly fewer samples, as summarized in Table 1.

Table 1. Comparison of the number of Monte Carlo samples (N_{MC}) and the number of machine learning samples (N_{ML}) used to measure $T_c(p)$ across various bond concentrations

p	1	0.8	0.6	0.55	0.51	0.5	0.49	0.45
N_{MC}	500	20000	200000	400000				
N_{ML}	1000	1000	1000	1000	1000	1000	1000	1000

Finally, we plot the critical temperature $T_c(p)$ versus bond concentration in Fig. 7. The phase transition curve separates the ordered phase (below the curve) from the disordered phase (above the curve). Our estimated T_c *(p)* agree with those reported in [6, 8].

4. Conclusion

This paper employed machine learning to investigate phase transitions in the diluted bond 2D Ising model. A convolutional neural network is trained to predict phase transitions directly from spin configurations, successfully classifying the high-temperature (paramagnetic) and low-temperature (ferromagnetic) phases. The model demonstrates high efficiency, requiring only 1,000 configurations to accurately determine the critical temperature for $0.55 \leq p \leq 0.8$, representing a significant reduction compared to the 20,000 - 400,000 samples needed in previous studies for $0.55 \leq p \leq 0.8$. Furthermore, the critical temperature for the range $0.5 \leq p < 0.55$ is determined for the first time in this study. However, for $p = 0.5$, the nature of the phase transition remains unclear and requires further investigation.

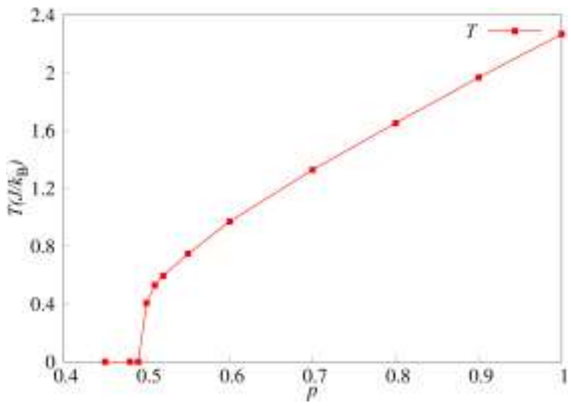

Figure 7. *T* - *p* Phase diagram of critical temperature *T*c versus bond concentration *p* in the diluted bond 2D Ising model.

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