Neural network evidence of a weakly first-order phase transition for the two-dimensional 5-state Potts model

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Abstract A universal (supervised) neural network (NN), which is trained only once on a one-dimensional lattice of 200 sites, is employed to study the phase transition of the two-dimensional (2D) 5-state ferromagnetic Potts model on the square lattice. In particular, the NN is obtained by using two artificially made configurations as the training set. Due to the unique features of the employed NN, results associated with systems consisting of over 4,000,000 spins can be obtained with ease, and convincing NN evidence showing that the investigated phase transition is weakly first order is reached.

1 Introduction

Phase transitions can typically be classified into two categories, namely the first-order and the second-order phase transitions. (Here we will not discuss more sophisticated division of phase transitions.) Intuitively speaking, if the order parameter continuously goes to zero when one approaches the critical point (CP), then the related phase transition is of second order. On the other hand, if the value of the order parameter drops to zero suddenly as one reaches the CP, then the corresponding phase transition is of first order. The correlation length diverges at CP for a system which undergoes a second-order phase transition, while it remains finite for a first-order phase transition. The identification of a weakly first-order phase transition is a challenge. This is because such a transition has a very large correlation length, and the (linear) system size must be much bigger than the correlation length in order to capture the true physics.

Recently, the techniques of machine learning (ML) are applied to study many-body systems [1–48]. In particular, the neural network (NN) methods have been demonstrated to be able to identify various phases of many physical models including the Ising model, the Potts models, the \( O(N) \) models, and the Hubbard type models [7, 9, 10, 22, 36, 39].

While satisfactory outcomes are obtained, some bottlenecks of employing the NN approach to investigate many-body systems remain. One noticeable example is to determine the nature of weakly first-order phase transitions definitely. Indeed, the standard NN calculations, particularly in the training stages, require huge amount of computing resources. As a result, with moderate computing power, most of the associated NN calculations are limited to small to intermediate system sizes. Apart from this, a separate training is required whenever a different system size or model is considered. Such a feature of the conventional NN training approach is not desirable since extra computing resources are needed if one wants to conduct a systematic NN calculations. Finally, real configurations over a wide range of parameter are used as the training set. This is time consuming as well.

To overcome the issues typically encountered in NN calculations, a one-dimensional (1D) NN was constructed in Ref. [49]. It is shown that the needed computing power for carrying the related investigation with the built 1D NN of Ref. [49] is much less than that of the standard NN approaches. In particular, when compared with the standard NN schemes, several hundred to few thousand factors in both the efficiency and the storage capacity is gained for the 1D NN. Moreover, the mentioned 1D NN is universal as well because it has successfully determined the CPs of many three-dimensional (3D) and two-dimensional (2D) models.

In order to further demonstrate the power and the advantage of the 1D NN of Ref. [49], in this study we employed that 1D NN to investigate the phase transition of the two-dimensional (2D) 5-state ferromagnetic Potts model on the square lattice. Apart from showing the high efficiency of the mentioned 1D NN, another motivation for carrying out such an investigation is that a NN guideline associated with a weakly first-order phase transition has not been established yet.

Due to the unique features of the constructed 1D NN, here we are able to study systems with more than 4,000,000 spins. In addition, by a comparison between the NN outcomes of the 2-state and the 5-state Potts models, a criterion of distinguishing a (weakly) first-order phase transition from a second-order one is established. With the obtained criterion, convincing (NN) evidence...
showing that the studied phase transition associated with the 5-state Potts model is (weakly) first order is reached. Our results also indicate that under some circumstances, the employed 1D NN may outperform the traditional methods.

With moderate computing resources, the calculations carried out here can hardly be achieved by the standard NN approaches of studying phase transitions available in the literature.

2 The constructed universal supervised neural network

Using the publically available libraries keras and tensorflow [50, 51], the 1D (supervised) NN employed here is a multilayer perceptron (MLP) which consists of one input layer, one hidden layer of 512 independent nodes, and one output layer. The training sets are two artificially made one-dimensional (1D) lattice of 200 sites. Specifically, all the sites of one configuration take 1 as their values, and each element of the other (configuration) is 0. The used labels are (1, 0) and (0, 1). The algorithm and optimizer employed are minibatch and adam, respectively. In addition, the used activation functions are ReLU and softmax which are defined by

\[ \text{ReLU}(x) = \max(0, x), \]
\[ (\text{softmax}(x))_i = \frac{e^{x_i}}{\sum_j e^{x_j}}. \]

The processes of one-hot encoding and flattening are implemented as well. The loss function utilized is the categorical cross-entropy which is given by

\[ -\frac{1}{n} \sum_x \sum_{j=1}^2 y_j \ln a_j, \]

where \( n \) is the total number of objects contained in the input set (for the training stage, \( n \) is the number of objects included in each batch). \( a_j \) are the outcomes obtained after applying all the layers. Moreover, \( x \) and \( y \) appearing above are the training inputs and the corresponding designed outputs (labels), respectively. A thorough introduction to the infrastructure of the considered 1D NN and the training as well as the testing (prediction) procedures are available in Ref. [49]. Figure 1 is the associated cartoon representation of the described 1D NN [49]. 800 epochs are conducted and the used batch size is 40. Here one cycle of training all batches is called one epoch. A short explanation of the NN terminologies mentioned here is available in Ref. [39]. Here we would like to emphasize the fact that no NN is trained in this investigation. In other words, the employed NN in this study is adopted directly from Ref. [49].

![Diagram of the NN](Fig. 1 The NN (MLP) used here and in Refs. [36, 39, 49]. The training set are made up of 200 copies of only two artificially made configurations. The steps of one-hot encoding and flattening are applied. ReLU and softmax are the employed activation functions. The output layer consists of two-component vector(s). The figure is reproduced from Refs. [36, 39, 49])
Readers who are interested in the fundamental details of applying NN to investigate physical systems are referred to Refs. [33, 34], and detailed definitions of the technical terms associated with NN (ML), such as one-hot encoding, activation functions ReLU and softmax, and categorical cross-entropy, can be found in Refs. [52, 53]. Finally, all the NN tunable parameters are the default ones unless specifically mentioned.

The loss for each epoch is shown in Fig. 2. Due to the used training set, the loss already reaches a small number after several epochs. The weight corresponding to the epoch with the smallest value of loss is saved for later calculations.

3 The microscopic model and the observable

The Hamiltonian of the studied 2D 5-state (q-state) ferromagnetic Potts model on the square lattice is given by Wu and Swendsen [54, 55]

$$\beta H_{\text{Potts}} = -\beta \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j},$$

where $\beta$ is the inverse temperature and $\langle ij \rangle$ stands for the nearest neighbor sites $i$ and $j$. In addition, $\delta$ refers to the Kronecker function and the Potts variable $\sigma_i$ at each site $i$ takes an integer value from $\{1, 2, 3, 4, 5\}$ ($\{1, 2, ..., q\}$). The observable considered here is the energy density $E$.

As the temperature ($T$) changes from low temperatures to high temperatures, a phase transition will take place for the studied model(s). It is well established theoretically that the related critical point $T_c$ for the 5-state Potts model is given by $T_c \approx 0.85153$ and that the nature of this phase transition is weakly first order [54].

4 Preparation of 1D configurations for the NN prediction

For each of the (5-state) Potts configurations generated by the Monte Carlo simulations, 200 sites are chosen randomly (and uniformly). For every one of these 200 sites, if the corresponding Potts variable is 1 or 3 (2 or 4), then integer 1 (0) is assigned to the associated spot of a 200 sites artificial configuration. If the Potts variable is 5, then 0 and 1 are picked with equal probabilities. The configurations built with such rules will be employed for the NN prediction. Similar rules are applied to the produced Monte Carlo configurations of the 2-state and the 20-state Potts models.

5 Numerical results

In this section the outcomes of applying the 1D NN to study the nature of the phase transition(s) of the considered model(s) are presented. In particular, we will provide convincing NN evidence to show that the studied phase transition of the 5-state Potts model is indeed (weakly) first order. The associated Monte Carlo simulations are done using the Wolff algorithm [56]. In addition, for every generated configuration (a configuration is generated after every 10 Monte Carlo sweeps), the spins of 2000 randomly chosen sites are stored and will be used to build the needed configurations for the NN testing. Finally, each of the histograms shown below consists of few million data points and is produced using the histogram function of pylab with 100 bins.
Theoretically, it is predicted that the phase transition of the 2D 5-state ferromagnetic Potts model on the square lattice is weakly first order. In other words, the associated correlation length is very large. As a result, data points on gigantic lattices as well as long simulations are needed in order to observe a clear signal of the predicted first-order phase transition.

Conventionally, studies related to first-order phase transitions would focus on investigating the histograms and the running histories of certain quantities. Here we will follow this guideline.

Before presenting our numerical results, we would like to point out that conventionally the histograms (probability distributions) $P_E(L)$ of energy density $E$ with various system sizes $L$ are studied when a first-order phase transition is considered. Moreover, a two-peak structure in $P_E(L)$ should appear. If one defines $\Delta F(L)$ to be the difference between the peak and the valley of $P_E(L)$, then it is argued theoretically that $\log(\Delta F(L))$ is proportional to $L^{d-1}$ for a first-order phase transition, where $d$ is the dimensionality of the investigated system. For a second-order phase transition, $\log(\Delta F(L))$ will saturate to a constant with $L$. As summarized in Ref. [57], the scenario $\log(\Delta F(L)) \propto L^{d-1}$ only shows up for extremely strong first-order phase transitions (such as the 20-state Potts model in [57, 58] or the 10-state Potts model in [59]). Hence in practice, a phase transition is considered to be first (second) order if $\log(\Delta F(L))$ grows (approaches a constant) with $L$. We will employ this criterion in our analysis.

Finally, the quantity employed here for studying the phase transitions of the considered models is the magnitude $R$ of the NN outputs. Since the NN outputs are two component vectors, one arrives at $\frac{1}{\sqrt{2}} \leq R \leq 1$.

5.1 Comparison between the NN and the traditional methods for estimating the critical point

Before conducting the proposed investigation, it is useful to carry out a comparison between the critical points estimated by the NN and the traditional approaches. When a relevant bulk quantity $O$ is considered as a function of $T$, a sudden jump in the magnitude of $O$ should appear at the critical point of a first-order phase transition. As a result, it is reasonable to take the temperature at which the employed $O$ begins to drop significantly as the critical temperature.

The magnetization density $m$ of the 5-state Potts model on the square lattice as functions of $T$ for three lattices ($L = 24, 48, \text{ and } 64$) are shown in the left panel of Fig. 3. Similarly, $R$ as functions of $T$ for $L = 24, 48, \text{ and } 64$ are demonstrated in the right panel of Fig 3. The vertical solid lines in both panels of Fig. 3 represent the expected critical point. As can be seen from Fig. 3, the precision of the estimated critical points from the NN and the traditional methods are of similar quality (Although it seems easier to employ this criterion for the traditional approach due to the less fluctuation in $m$). These results indicate that both the NN and the traditional methods lead to acceptable estimations of the critical point. In other words, the NN technique is a valid method for studying the phase transitions.

We will not go into the details of calculating the critical point accurately using finite-size scaling. Since we are interested in understanding which of the NN and the traditional approaches has a stronger signal for a first-order phase transition, the running history and the histogram of the energy density $E$ will be examined instead.

5.2 Validation of the NN approach for a first-order phase transition

The validity of our unconventional NN approach for studying the first-order phase transitions is verified by investigating the 20-state Potts model on the square lattice. Theoretically this model has a strong first-order phase transition. Figures 4 and 5 show the histogram and the running history of $R$ for the 20-state Potts model on a 20 by 20 square lattice, respectively. The extremely sharp two-peak structure appearing in Fig. 4 and the tunneling phenomenon showing up in Fig. 5 are consistent with the scenario that the considered phase transition is first order.
After validating the effectiveness of applying the 1D NN of Fig. 1 to study first-order phase transition(s), now we turn to present the main results of our investigation.

5.3 NN results of the 2D 5-state ferromagnetic Potts model

The left, middle and right panels of Fig. 6 show the histograms of the magnitude $R$ of the NN outputs for (linear) system sizes $L = 128, 512,$ and $2048$ of the 5-state Potts model, respectively. As can be seen from these results, the two-peak structures become more and more obvious with $L$. In other words, as $L$ increases, the ratio between the height of the peak and the height of the valley increases. Since the heights of the peaks in all the panels of Fig. 6 are about the same, such a scenario is transparent if one focuses on the data in the middle parts of these histograms. This is demonstrated in Fig. 7. Similarly, when the running history of $R$ is investigated, one finds that there are more and more empty spaces between the upper and the lower bounds of $R$ when $L$ increases from 128 to 2048, see Fig. 8. This implies that as the box size $L$ becomes larger, data accumulate at two particular values of $R$. This is without doubt a feature of a first-order phase transition. As we will demonstrate shortly, in comparison with the associated
outcomes from the 2D two-state Potts model, both results of the histograms and the running histories shown in Figs. 6 and 8 suggest strongly that the considered phase transition of the 5-state Potts model on the square lattice is first order.

5.4 NN results of the 2D two-state ferromagnetic Potts model

To compare the difference of the histograms of $R$ as well as the associated running histories between a weakly first-order and a second-order phase transitions, we have also simulated the 2D two-state ferromagnetic Potts model on the square lattice.

The histograms of $R$ for $L = 128$, 512, and 2048 of the 2-state Potts model are shown in Fig. 9. The two-peak structures shown in Fig. 9 are much milder than that found in Fig. 6. In particular, the two-peak structures do not get deepened with increasing system sizes $L$ (see also Fig. 10 which shows the middle parts of the associated histograms). Besides, from Fig. 11, which is the related running histories of $R$, one sees that the patterns stay more or less the same as the system size increases from $L = 128$ to $L = 2048$. This result differs significantly from that shown in Fig. 8. The outcomes related to the 2-state Potts model confirm that the two-peak structures as well as the corresponding running histories found in Figs. 6 and 8 are indeed evidence of (weakly) first-order phase transition for the 2D 5-state Potts model.
5.5 Monte Carlo results and the comparison with NN outcomes

The histograms of the quantity (minus) energy $-E$ for the 5-state Potts model are shown in Fig. 12. A comparison between the outcomes of Figs. 6 and 12 indicates that while the histograms of $-E$ resemble more closely the scenario of a first-order phase transition (see Fig. 13 as well), the two-peak structures are more obvious for $R$. Indeed, even for $L = 128$ the two-peak structure of $R$ is more noticeable than those shown in Fig. 12 (For the NN outcomes shown in Fig. 6, the distance between the peak and the valley is very large even for $L = 128$. Such a result can hardly be a property of a second-order phase transition). This implies that larger lattice (than $L = 2048$) data of $-E$ are required in order to obtain stronger evidence to show that the phase transition is first order. Such a task will take much more computing time.

It should be pointed out that the NN approach is an alternative and new method for studying phase transitions. Hence the resulting NN results presented here do not necessarily follow the criterion(s) established by the traditional techniques for a first-order phase transition. From comparisons among the outcomes of Figs. 6, 7, 8, 9, 10 and 11, one clearly reaches the conclusion that the phase transitions of the 5-state and the 2-state Potts models are different. Since it is well-known that the phase transition of 2-state Potts model is second order, it is beyond doubt that the phase transition of 5-state Potts model is likely first order using the NN outcomes shown here in conjunction with the conventional criterion for a first-order phase transition.
This running histories of $-E$ for $L = 128, 512, \text{and} 2048$ are shown in Fig. 14. Moreover, one finds that for $L = 2048$ the tunneling phenomenon of $R$ happens much more frequently than that of $-E$ (This statement is true for both the results shown in Figs. 8 and 11). Since tunneling phenomenon is a feature of a first-order phase transition, this finding implies that one needs to wait longer to observe a clear signal of first-order phase transition if the quantity $-E$ is considered. Under the circumstance that only small to intermediate system sizes (say, $L \leq 512$) can be accessible, then the NN outcomes seem to provide stronger evidence that the considered phase transition is of the weakly first order.

In summary, the outcomes shown in Figs. 6, 8, 12 and 14, in particular the observed tunneling frequencies, may lead to the conclusion that when weakly first-order phase transition is concerned, the performance of NN is better than that of the traditional approaches.

6 Discussions and conclusions

In this study, we use the 1D NN of 200 sites that was trained only once in Ref. [49] to investigate the nature of the phase transition of the 2D 5-state ferromagnetic Potts model on the square lattice. Due to the unique features of the employed NN, we are able to access systems of over 4,000,000 spins with no difficulty. Such huge system sizes cannot be easily handled using the conventional NN approaches available in the literature with moderate computing resources.

Each of the figures demonstrated here uses few million data points. With the conventional NN procedures, the storage space needed for such a huge amount of data is more than $10^{13}$ bytes and hence cannot be easily managed as well. Only with the idea used in Ref. [49] and here can one reach the outcomes presented in this study with moderate effort.

We would like to point out that typically the two-peak structure of a first-order phase transition should become more deepened when system size $L$ increases. In addition, a second-order phase transition may show a two-peak structure as well. However, such a phenomenon will cease to become more obvious with increasing system sizes. Our results are consistent with these expected scenarios.

Many of the NN studies in the literature have focused on repeating the results obtained by the traditional methods. Those NN investigations often do not demonstrate which of the NN and the traditional approaches is more efficient. In this study, by considering the histograms and the running histories of certain relevant quantities, we find that for the case that only small to intermediate system sizes are accessible, NN may outperform the traditional method(s) when first-order phase transition is concerned.
In conclusion, our NN outcomes provide convincing evidence that the targeted phase transition is weakly first order. This is in agreement with the associated theoretical prediction. It is remarkable that the simple 1D NN of Ref. [49] can be applied to study the phase transitions of many higher-dimensional systems. Finally, the use of only 200 spins out of more than 4,000,000 spins can determine the true nature of the considered phase transitions is rather unexpected and impressive as well.

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Author contributions  FJJ proposed and supervised the project, and wrote up the manuscript. YHT and YHT conducted the calculations and analyzed the data.

Data Availability Statement  This manuscript has associated data in a data repository. [Authors’ comment: Data are available from the corresponding author on reasonable request].

Declarations

Conflict of interest  The authors declare no conflict of interest.

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