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A Study of the Scaling Behavior of the Two-dimensional Ising Model by Methods of Machine Learning

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Abstract. In the field of condensed matter physics, machine learning methods have become an increasingly important instrument for researching phase transitions. Here we present a method for calculating the universal characteristics of spin models using an Ising model that is exactly solvable in two dimensions. The method is based on a convolutional neural network (CNN) with controlled learning. The scaling functions prove the continuing type of phase transition for the 2D Ising model. As a result of the proposed technique, it has been possible to calculate correlation length directly.

Keywords: machine learning, convolutional neural networks, Monte Carlo methods, Ising model, scaling, correlation length, magnetic susceptibility.

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Machine learning methods over the last few years have proved as a good tool for analysing multicomponent complex systems [1–3]. Different machine learning methods have been developed for study such systems [4–6]. Convolutional neural networks (CNN) [7] are traditionally used to investigate phase transition classification problems where no prior knowledge is assumed. This method is well applicable to any spin models [8, 9] also.

Machine learning methods look like a "black box" and the typical problem is "how to prove CNN classification without traditional methods". Machine learning can test a fundamental features of critical phenomena [10, 11], such as the long-range ordering and scaling.

Using the two-dimensional Ising model [12] as a basis for analysing the critical behavior of a spin system, we propose an alternative methodology for studying the critical behaviour of spin systems through the use of machine learning techniques [12].

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1. Model and methods

We calculate the system using the classical representation. Ising model Hamiltonian with spin states $S = \pm 1$ on a square lattice.

$$H = -\frac{J}{2} \sum_{\langle i,j \rangle}^{N} S_i S_j, \tag{1}$$

where $J = 1$ is the exchange interaction constant, $J > 0$ for the ferromagnetic model. A linear lattice size of L determines the number of spins in the system, and $N = L \times L$.

We used a CNN model with controlled learning to study the universal characteristics of spin systems. This CNN model is divided into two sets of convolutional layers by a pooling layer — followed by a dense layer with a softmax activation function. The neural network output layer contains two nodes whose values are real numbers in the interval [0;1] and correspond to the probability of detecting the system state in the high-temperature (HT, $T > T_C$) or low-temperature (LT, $T < T_C$) phases.

$$M^{\infty} = \begin{cases} 1, & T < T_c - \text{low-temperature phase, (LT)} \\ 0, & T > T_c - \text{high-temperature phase, (HT)} \end{cases}. \tag{2}$$

A supervised type of training is used, for which a large number of configurations are generated. The neural network training process was performed on the data set of correlation matrices, the values of which were determined for each spin configuration. The correlation matrices were obtained using the next equation (3).

$$C_i = \frac{1}{2} \left(S_{x,y} S_{x+L/2,y} + S_{x,y} S_{x,y+L/2} \right), \tag{3}$$

where the correlation function takes into account the interaction of spins at a distance equal to half of the lattice.

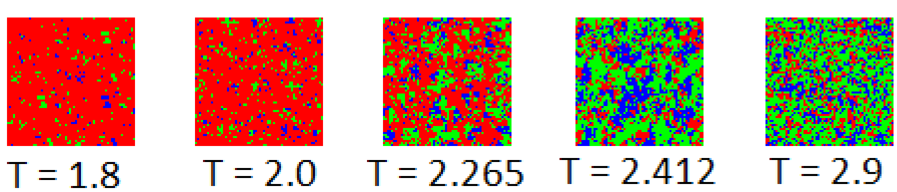

Fig. 1. Example of correlation matrices for training a neural network at different temperatures for linear size L = 64

The Binder cumulant of 4-th order (4), which is commonly used to find the critical temperature, was taken to construct the scaling relationship by Monte Carlo methods.

$$U_4(T) = \frac{1}{2} \left[3 - \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} \right]. \tag{4}$$

The methodology proposed for the calculation of universal characteristics using CNNs allows us to calculate the correlation length functio [10] describing the stepped recession near the critical point of the phase transition.

The results obtained with CNN were compared with the results of classical Monte Carlo calculations to confirm the correctness of the results obtained with the help of CNN. The correlation length function is presented in the equation (5).

$$\xi/L = \frac{1}{2\sin\frac{\pi}{2}}\sqrt{\frac{\langle M^2\rangle}{\langle\Phi\rangle}}, \tag{5}$$

where

$$\Phi = \frac{1}{2}\sum_{n=1}^{2}\left|\sum_i S_i e^{iq_n x_{nj}}\right|^2. \tag{6}$$

The method proposed by us also allowed us to calculate the temperature dependence of the magnetic susceptibility

$$\chi(T) = \frac{1}{N}\frac{\langle m^2\rangle - \langle m\rangle^2}{T} \tag{7}$$

a comparison with the classical calculations (eq. 7) was also carried out to check the correctness of the CNN results [10].

The calculation of two cases was carried out to verify the successful applicability of the proposed methodology and to identify the distinctive features of machine learning techniques:

- A low number of temperature steps (150) and a large number of Monte Carlo steps for relaxation (30 000 MCS/s) and averaging (50 000 MCS/s).
- A large number of temperature steps (2 000) and a small number of Monte Carlo steps for relaxation (3 000 MCS/s) and averaging (5 000 MCS/s).

The training dataset consisted of 200 statistical configurations, of which training was performed on 100 configurations.

2. Result of machine learning technique

Using the predicted values from the low-temperature phase, the scaling function, correlation lengths, and magnetic susceptibility calculations have been developed based on the low-temperature phase. We carried out the calculations using classical Monte Carlo methods, including the Metropolis algorithm, simultaneously with the derivation of the correlation matrices [13].

Fig. 2 and Fig. 3 show the scaling functions for different modeling cases. It can be clearly seen that for the two cases, the constructed scaling dependencies reflect the universal behavior of the model at different linear dimensions. It is worth noting that the smoothest function is observed in the case of a large number of temperature steps and small Monte Carlo times.

As a result of the calculations of scaling dependency, we have been able to demonstrate that machine learning methods are able to demonstrate universality in the same way that Monte Carlo calculations can demonstrate universality. The convolutional neural network on the other hand requires more temperature steps for smooth dependence as well as a small number of time steps, which results in a significant reduction in the calculation time of the model.

Using machine learning methods, we studied universal features of the spin model, and were able to find dependences between correlation length and magnetic susceptibility. These thermodynamic quantities provide a detailed description of the behavior of the system near the phase transition.

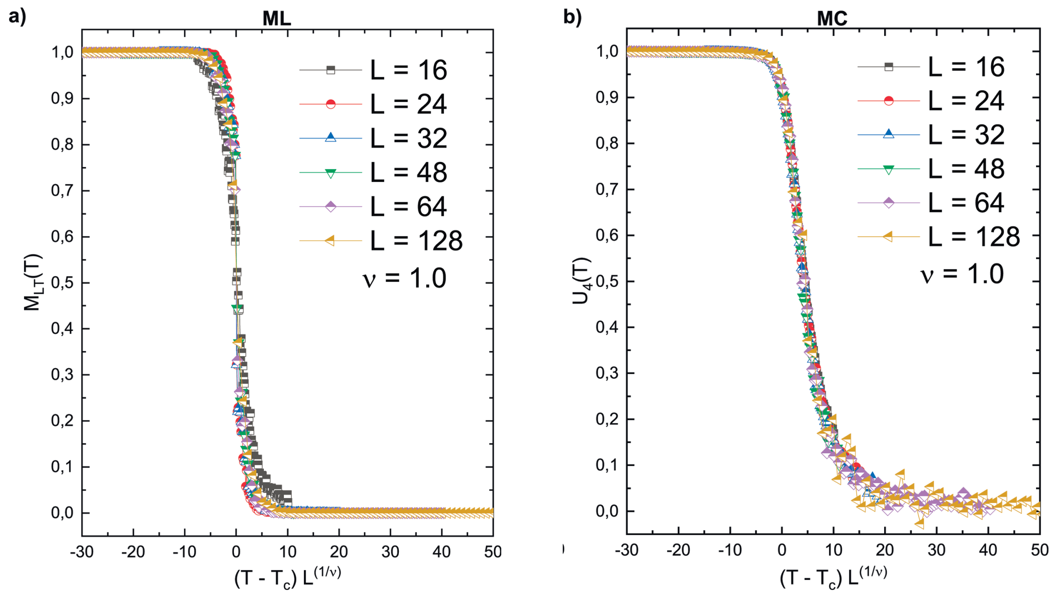

Fig. 2. The scaling relationships of the two-dimensional Ising model for 150 temperature steps constructed: a) by machine learning methods; b) by Monte Carlo methods

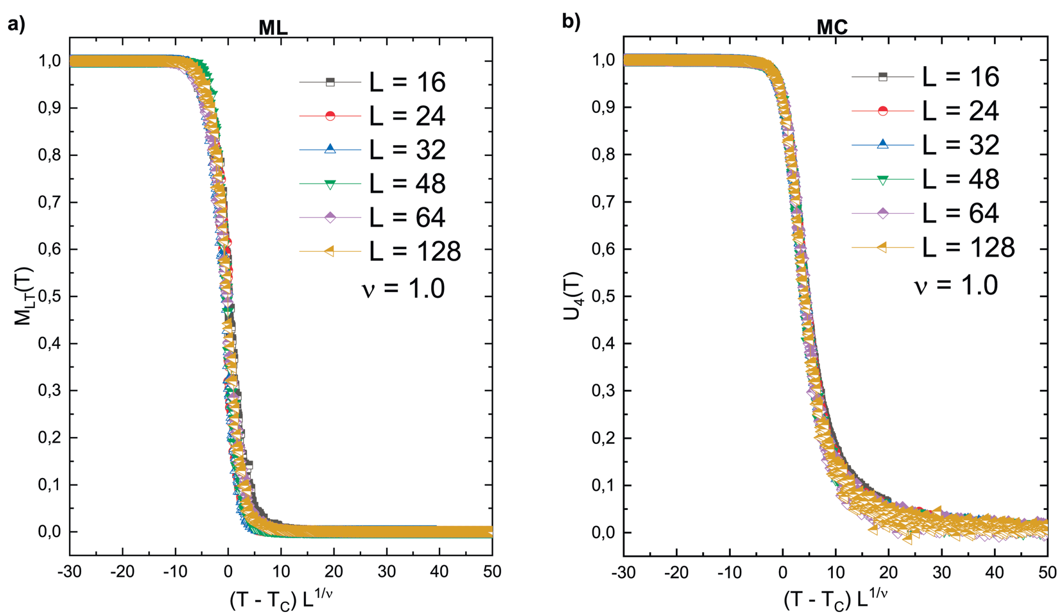

Fig. 3. The scaling relationships of the two-dimensional Ising model for 2000 temperature steps, constructed: a) by machine learning methods; b) by Monte Carlo methods

Figs. 4 and 5 show the correlation length calculations for each linear dimension for the two cases considered. It is worth noting that in both cases considered, the machine learning method performs well, although it is subject to fluctuation effects. The influence of fluctuations is much smaller in the case of a large number of temperature steps.

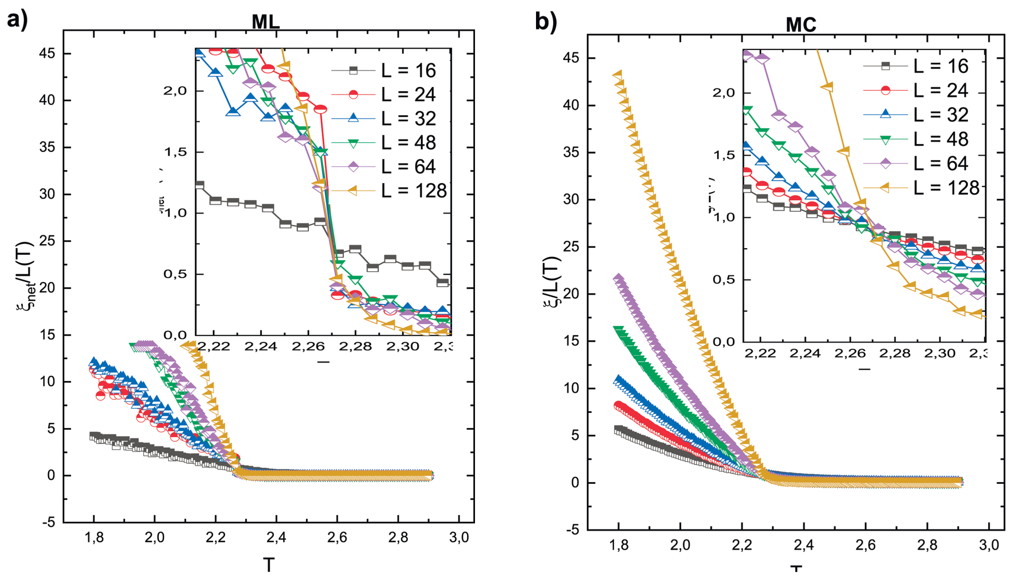

Fig. 4. The temperature relationships of the functions ξ_{net}/L and ξ/L for 150 temperature steps, plotted using: a) machine learning methods; b) Monte Carlo methods

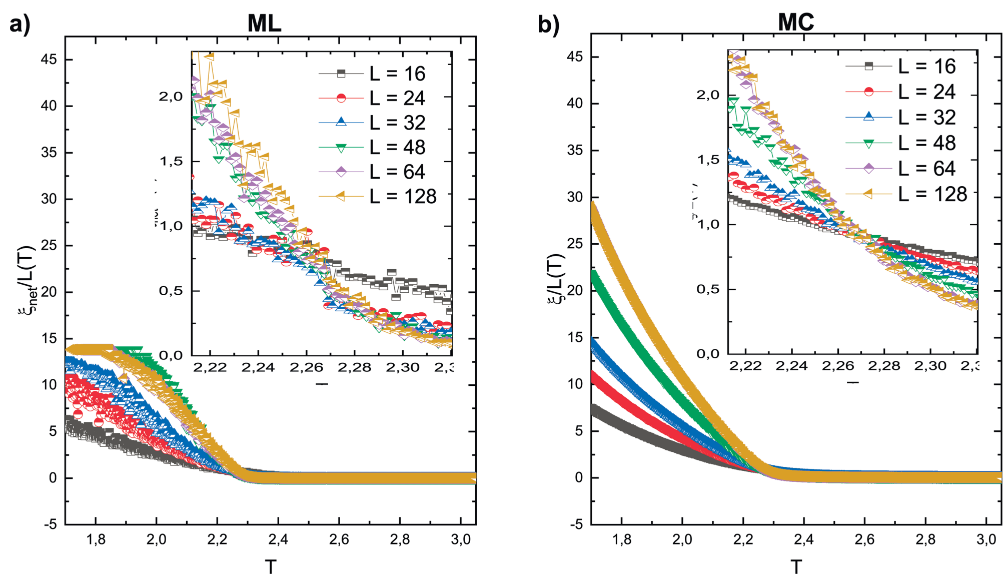

Fig. 5. The temperature relationships of the functions ξ_{net}/L and ξ/L for 2000 temperature steps, plotted using: a) machine learning methods; b) Monte Carlo methods

In constructing the temperature dependence of magnetic susceptibility (Fig. 6 and Fig. 7), it was noticed that CNNs show rather high peaks in the critical temperature region compared to the Monte Carlo results. It is worth noting that the machine learning results weakly demonstrate a property of the two-dimensional Ising model — as the linear size increases, there is a noticeable shift on the temperature scale to the exact value.

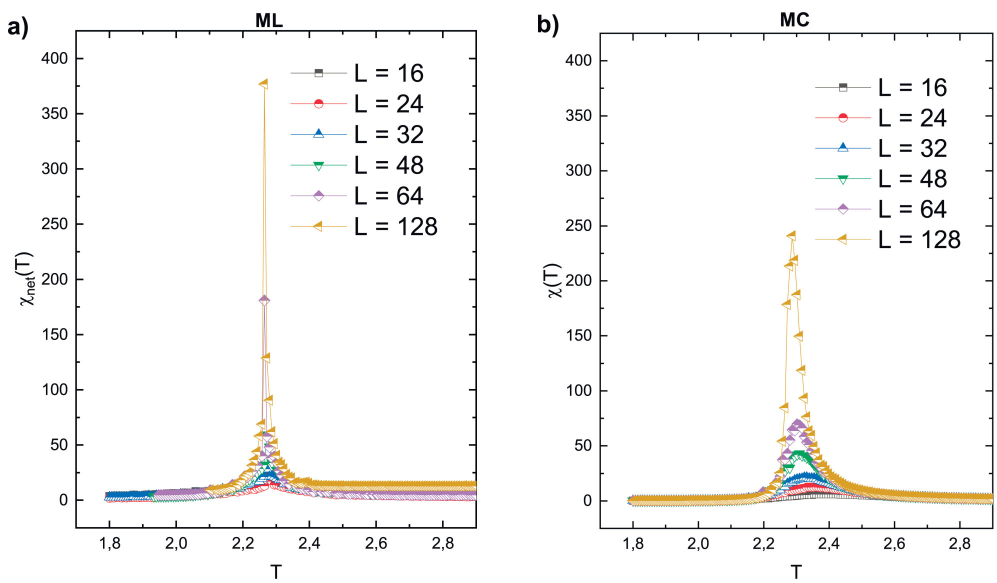

Fig. 6. The temperature relationships of the susceptibility $\chi_{net}(T)$ and $\chi(T)$ near the critical temperature for 150 temperature steps, constructed a) by machine learning methods; b) by Monte Carlo methods

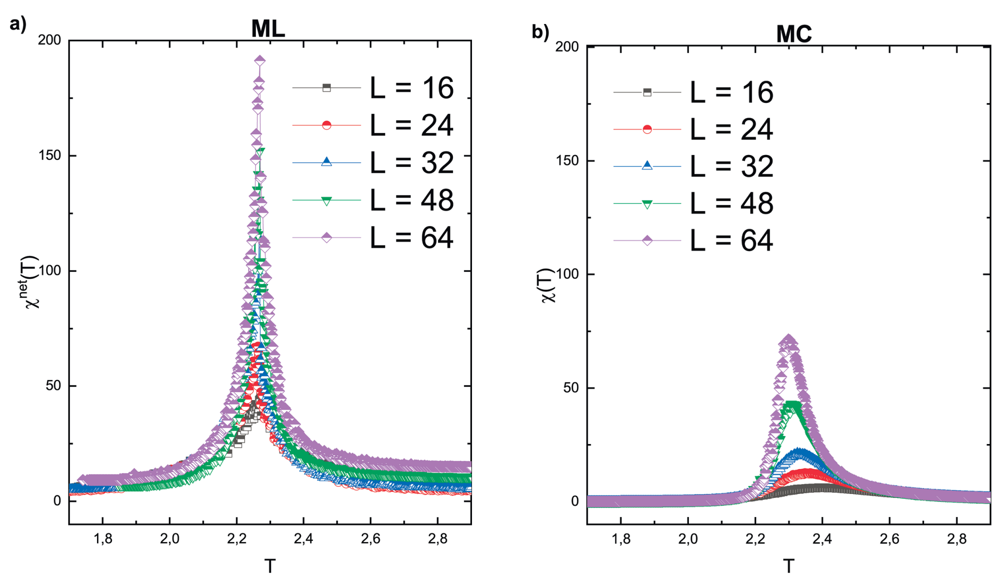

Fig. 7. The temperature relationships of the susceptibility $\chi_{net}(T)$ and $\chi(T)$ near the critical temperature for 2000 temperature steps, constructed a) by machine learning methods; b) by Monte Carlo methods

Conclusion

A universal technique for calculating the universal characteristics of spin systems is presented in the paper by using the method of convolutional neural networks on the example of a two-dimensional Ising model to calculate the universal characteristics of spin systems. A study that was carried out on spin systems uncovered that machine learning methods were an excellent tool for studying those systems. It was found that when classical calculations were compared to machine learning methods, it took significantly less time for the machine learning methods to make the universal characteristics calculations compared to classical calculations. Using the proposed method, in order to reflect the continuity of the phase transition, a scaling dependence was developed in order to reflect the continuity of the phase transition. This study was carried out using the CNN method in order to calculate the thermodynamic dependence of the correlation length and magnetic susceptibility.

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Исследование скейлингового поведения двумерной модели Изинга методами машинного обучения

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Аннотация. Методы машинного обучения стали новым быстро набирающим инструментом для исследования фазовых переходов в физике конденсированного состояния. В данной работе представлен метод расчета универсальных характеристик спиновых моделей на основе двумерной модели Изинга. Метод основан на использовании сверточной нейронной сети (CNN) с контролируемым обучением. Функции скейлинга доказывают непрерывный тип фазового перехода для двумерной модели Изинга. В результате применения предложенной методики стало возможным вычисление корреляционной длины.

Ключевые слова: машинное обучение, сверточные нейронные сети, методы Монте–Карло, модель Изинга, скейлинг, корреляционная длина, магнитная восприимчивость.