Limitations of transfer learning applicability for anisotropic phase transitions classification tasks

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1. Introduction

Transfer learning technique is ubiquitously used for computationally complicated tasks. Using a pre-trained neural network trained on one training data set, the information obtained during training is used on a new data set [1].

In this case, the application of transfer learning is possible if both data domains (the training and the test data domain to which training is to be transferred) have common properties. This approach is ideologically related to the definition of universality classes in statistical physics - some models, different from each other, have the same, universal properties, as a result of which they are united into classes.

In this work, we test the ability of neural networks to reproduce universal properties of models from the 2d Ising class. To do so, we train convolutional neural networks on the task of classifying Ising samples (snapshots) into ferromagnetic and paramagnetic phases, in the same way as in [2]. We then test the pre-trained network on samples of other models, but from the same universality class. Our main goal is to test how accurately we can estimate critical quantities, such as the critical exponent of the correlation length.

2. Methods

2.1 Models and data

We begin by training neural networks on samples of the Ising model on a square lattice with periodic boundary conditions: $H_I(\sigma) = -J\sum_{x,y=1}^{L}\sigma_{x,y}(\sigma_{x+1,y} + \sigma_{x,y+1})$. Values $\sigma_{x,y} = \pm 1$, so the data are black and white images.

We check transferability of learning on two other anisotropic models: $H_D(\sigma) = -\sum_{x,y=1}^{L}\sigma_{x,y}(J\sigma_{x+1,y} + J\sigma_{x,y+1} + J_d\sigma_{x+1,y+1})$ (diagonal anisotropy) and $H_O(\sigma) = -\sum_{x,y=1}^{L}\sigma_{x,y}(J_h\sigma_{x+1,y} + J_v\sigma_{x,y+1})$ (orthogonal anisotropy). Coupling constants $J \equiv 1$; J_d, J_v, J_h stands for diagonal/vertical/horizontal interactions, respectively. Both H_D and H_O models are in the 2d Ising universality class, but with different properties along diagonal or horizontal/vertical directions compared to the isotropic H_I model.

We use the Metropolis algorithm [3] to generate the data. Each snapshot is generated at a certain temperature T from range $T_c \pm 0.3$, where T_c is the critical temperature at which the phase transition between the ferromagnetic and paramagnetic phase occurs. The values of the critical temperature are known from the exact solution [4]. Depending on whether T is greater or less than T_c, each snapshot has a label 0 or 1.

2.2 Machine learning details

We apply convolutional neural network (CNN) with following architecture: Conv2d (N64, K2x2, S1) [5], MaxPool2d (2×2), ReLU, Linear $(64\times(L/2-1)\times(L/2-1), 64)$, ReLU, Linear $(64, 1)$. We use the binary cross entropy as the loss function, and Adam [6] as optimization algorithm. All CNNs we train for only 1 epoch so as not to lose the physics of the problem [7]. At the output of the network there is one neuron p_i, giving the probability of the snapshot from the input to belong to the paramagnetic phase.

Using notations from [1], we define $D_S = \{(x_{S_i}, y_{S_i})\}$ as source domain (training data set) where x_{S_i} is a snapshot of H_I isotropic model, y_{S_i} its label of phase, and $f_S(\cdot)$ is the source predictive function (CNN). Similarly, $D_T = \{(x_{T_i}, y_{T_i})\}$ is a target domain (testing data sets) where x_{T_i} are snapshots of models H_D or H_O, with corresponding labels y_{T_i}. Marginal distribution of D_S and D_T $P(X_S) \neq P(X_T)$ due to anisotropy in target domain data. Transfer learning then formally defined as $f_T(\cdot) = f_S(\cdot)$ when $D_S \neq D_T$.

2.3 Estimated quantities

Each snapshot is characterised by the temperature at which it was generated. There are N snapshots at each point over the entire temperature range. From the standard deviations of the forecast distribution p_i we construct a function of the second moments of the forecasts: $D(T;L)=\sqrt{\frac{1}{N}\sum_{i=1}^{N}(p_i(T;L))^2-\left(\frac{1}{N}\sum_{i=1}^{N}p_i(T;L)\right)^2}$.

For each linear size L, the function D has the form of a normal distribution with a peak in the vicinity of the phase transition [8]. Knowing the width σ of the distribution D, it is possible to extract the critical exponent from the neural network predictions.

From the theory of critical phenomena, it is known that correlation length ξ of the Ising model in critical regime and in the thermodynamic limit behaving like $\xi \propto (|T-T_c|/T_c)^{-1/\nu}$ where $\nu = 1$ is the critical exponent of correlation length. From finite-size scaling hypothesis [8] $\sigma(L)$ of distribution $D(T;L)$ is scalable: $\sigma(L) \propto AL^{-1/\nu}$. From this expression we construct estimates $1/\nu*$ and compare them with the exact solution.

3. Results

The results obtained are graphically depicted on the Fig. 1 and Fig. 2. On the plots, blue squares stands for relative error $|1/\nu^* - 1/\nu|/1/\nu$, orange triangles stands for relative error of the left half of the same distribution $D(T;L)$ (due to the asymmetry of Gaussians), and green stars stands the right half.

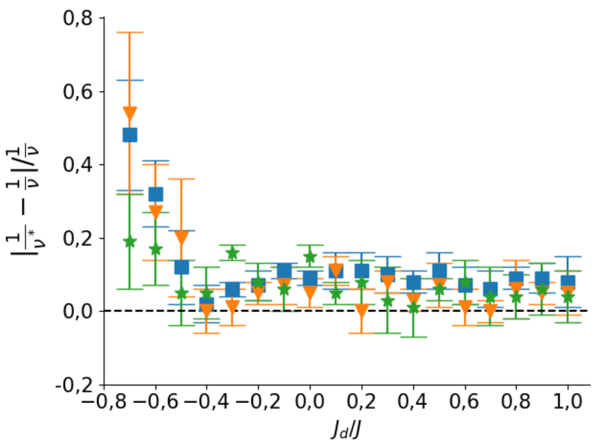

Fig. 1: Relative error of correlation length exponent estimation $1/\nu^*$, H_D model.

Fig. 1 shows results when training CNN on isotropic data H_I and testing on diagonally anisotropic data H_D. Similarly, Fig. 2 shows results when testing on orthogonally anisotropic data H_O. In both cases the growth of relative error is noticeable when the ratio of coupling constants decreases, i.e. the influence of anisotropic interactions on the system increases. Numerically, regions of strong anisotropy are $J_d/J < -0.4$ in H_D case and $J_v/J_h < 1/2$ in H_O case.

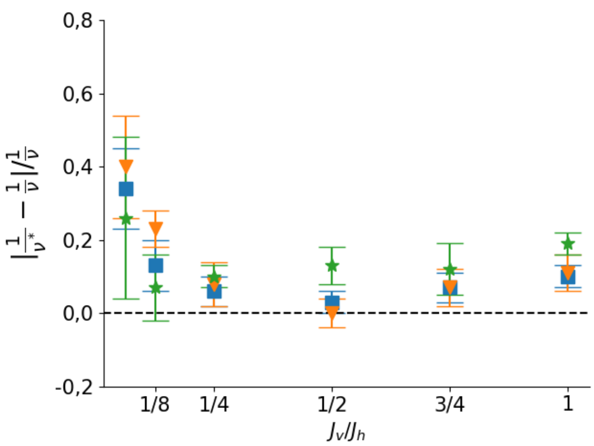

Fig. 2: Relative error of correlation length exponent estimation $1/\nu^*$, H_O model.

4. Discussion

In this work, the problem of reproducibility of universal properties of spin models by the method of transfer learning was investigated. We set limits of coupling constants where transfer learning reproduce universal properties in accordance with the theory.

One possible explanation for this effect is the presence of oscillations of the correlation function at strong diagonal anisotropy. The hypothesis about the occurrence of such an effect requires further investigation.

Details of diagonal anisotropy can be found in [9].

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