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Universality classes and machine learning

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Abstract. We formulate the problem of the universality class investigation using machine learning. We chose an example of the universality class of the two-dimensional 4-state Potts model. There are four known models within the universality class – the 4-state Potts model, the Baxter-Wu model, the Ashkin-Teller model, and the Turban model. All four of them together are not equivalent in the Hamiltonian representation, in the lattice symmetry, and the layout of spins on the lattice. We generate statistically independent datasets for all models using the same Monte Carlo technique. The machine learning methods will be used for the analysis of the universality class of models based on generated datasets.

1. Introduction

The deep machine learning technique was successfully applied to the Ising model on the triangular lattice with the network's training by the Ising model on the square lattice [6]. The magnetic moments (*spins*) sitting at the vertices have two values, $+1$ and -1 and can be represented by bits 0 and 1, or color white and black. The Ising model demonstrates a critical phase transition at temperature T_c in the limit of infinite lattice size (in the *thermodynamic limit*). The T_c separates the paramagnetic and ferromagnetic phases. In the paramagnetic phase ($T > T_c$), the temperature influence prevails the spin coupling, and spins take the random value for large values of temperatures. Authors of Ref. [6] used the fully connected and convolutional neural networks for training with the local magnetic moment snapshots at temperature T and provided with target labels for paramagnetic and ferromagnetic phases. The snapshot of the spin distribution looks grey in general. In the ferromagnetic phase, the spin coupling is larger than the randomizing influence of temperature at low enough temperature. All spins tend to have the same value, the 0 or the 1, with equal probability that the spin snapshot looks white or black. The phenomena named the *spontaneous magnetization* [15]. The Ising model in the square lattice was solved exactly by Onsager [14].

Using machine learning, Carasquilla and Melko [6] trained the networks on a broad range of data at temperatures above and below T_c using the square lattice Ising model. The trained network was applied to the testing set generated for the same model. Estimation of the critical temperature leads to the value $T_c^{ML} \approx 2.266(2)$ in good agreement with the exact value $T_c = 2/\ln(1+\sqrt{2}) = 2.269\ldots$, and estimation of the correlation length critical exponent $\nu^{ML} \approx 1.0(2)$ coincide not bad with the exact $\nu = 1$.

The next step of the Carasquilla and Melko [6] research was testing the data for the Ising model on the triangular lattice and estimating the critical temperature $T_c^{ML} \approx 3.65(1)$ close to the exact value $T_c = 4/\ln(3) = 3.64\ldots$ and $\nu^{ML} \approx 1.0(3)$. The estimation quality for the triangular model is less accurate than the estimation quality for the square model.

Several methodological questions arise. What is the regular procedure for high-quality estimation? How does the quality of estimation depend on the system's aspect ratio in the training and testing? How does the quality of estimation depend on the neural network type, and training procedure?

In the paper, we propose the more physical question - is it possible to catch the universality class properties with the machine learning methods? For that, we propose to investigate four different models in one universality class.

We choose four models belonging to the same universality class – four state Potts model [16], Baxter-Wu model [8], Ashkin-Teller model with some special relation of parameters [9], and Turban model [10]. Behaviour of all four models near the critical point belongs to the universality class named *4-state Potts universality class*. The numerical values of the critical exponents for 4-Potts universality class are known exactly [18, 19, 20, 21, 22]: heat capacity exponent $\alpha = 2/3$, magnetization exponent $\beta = 1/12$, magnetic susceptibility exponent $\gamma = 7/6$ and correlation length exponent $\nu = 2/3$.

2. Model parameters

We use lattices with the linear sizes $L \in \{12, 18, 48, 66\}$. Simulation was carried out at temperature distance ΔT in $[10^{-3}; 3{\cdot}10^{-1}]$ above and below the critical T_c. The exact expressions for the critical temperatures are presented in Table 1.

Table 1. Critical temperatures T_c for four models.

Model	4-Potts	Baxter-Wu	Ashkin-Teller	Turban
T_c	$1/\log(1+\sqrt{4})$ [16] $\approx 0.9102\ldots$	$2/\log(1+\sqrt{2})$ [13] $\approx 2.2691\ldots$	$4/\log(3)$ [9] $\approx 3.64095\ldots$	$2/\log(1+\sqrt{2})$ [10] $\approx 2.2691\ldots$

The total energy E, magnetization M, heat capacity C, and magnetic susceptibility χ are depended on the lattice size. We normalize them by the number of lattice vertices $N = L^2$ and obtain thermodynamic quantities per spin. The expressions for calculating these values are posted in Tables 2 and 3. For the Potts model, N_m is the maximum number of sites m when $\sigma_i = m$ and $m \in [0, 1, 2, 3]$. For the Baxter-Wu model, χ_- is susceptibility in the low-temperature phase and χ_+ susceptibility in the high-temperature phase. We fix the spin coupling energy $J = 1$ for simplicity.

Table 2. Expressions for energy E and magnetization M.

Model	Energy E	Magnetisation M
4-Potts	$-\frac{J}{N}\sum_{\langle i,j\rangle}\delta(\sigma_i,\sigma_j)$	$\frac{4N_m/N-1}{3}$
Baxter-Wu	$-\frac{J}{N}\sum_{\langle j,k\rangle}\sigma_{j,k}\sigma_{j+1,k+1}(\sigma_{j+1,k}+\sigma_{j,k+1})$	$\frac{1}{N}\sqrt{\sum_{m=1}^{3} m_i^2}$
Ashkin-Teller	$-\frac{J}{N}\sum_{\langle i,j\rangle}(\sigma_i\sigma_j+\tau_i\tau_j)+(\sigma_i\sigma_j\tau_i\tau_j)$	$M_q = \frac{1}{N}\sum_{i=0}^{N} q_i, q = \{\sigma,\tau\}$ $M = \sqrt{M_\sigma^2 + M_\tau^2}$
Turban	$-\frac{J}{N}\sum_{l} s_i s_j + -\frac{J}{N}\sum_{L}\prod_{k=1}^{3} s_k$	$\frac{1}{N}\sum_{i=0}^{N} s_i$

Table 3. Expressions for specific heat C and susceptibility χ.

Model	Heat capacity C	Magnetic susceptibility χ
4-Potts	$\frac{N}{T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$	$N\left(\langle M^2\rangle - \langle M\rangle^2\right)$
Baxter-Wu	$\frac{N}{T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$	$\chi_- = N\left(\langle M^2\rangle - \langle M\rangle^2\right)$ $\chi_+ = N\langle M^2\rangle$
Ashkin-Teller	$\frac{N}{T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$	$N\left(\langle M^2\rangle - \langle M\rangle^2\right)$
Turban	$\frac{N}{T^2}\left(\langle E^2\rangle - \langle E\rangle^2\right)$	$N\left(\langle M^2\rangle - \langle M\rangle^2\right)$

Simulations were carried using the Metropolis Monte Carlo method for all models. One step of the algorithm (1 MC-step) is the N attempts for spin flips. We use recommendations given in the lecture [17] in order to get uncorrelated samples. Autocorrelation time τ determines the statistical error ϵ that is of order $\sqrt{\tau/n}$, where n is a number of MC-steps. Closer to the critical point, critical slowing-down leads to the simulation difficulties, with autocorrelation time τ increased by a factor of L^z, where z is a dynamic critical exponent of the algorithm. The full protocol of simulations is as follows.

- Run model for N_{relax} MC-steps to reach thermodynamic equilibrium and discard collected data from further research. The empirical recommendation [17] for parameter $N_{relax} = 20\tau$.
- In equilibrium compute N_{mc} effective MC steps. Calculate thermodynamic quantities using expressions in the Tables 2 and 3. The parameter N_{mc} controls the statistical error and the available computational resources.

Table 4. Simulation parameters and integrated correlation time τ.

Model	L	ΔT	N_{relax}	N_{mc}	τ
4-Potts	12 18 48 66	$2\cdot10^{-3}$	$5\cdot10^6$	$2\cdot10^7$ 10^8 $2\cdot10^8$ $2\cdot10^8$	190 430 3700 7300
Baxter-Wu	12 18 48 66	$2\cdot10^{-3}$	10^7	10^8 10^8 10^8 $4\cdot10^8$	170 410 3200 6500
Ashkin-Teller	12 18 48 66	$2\cdot10^{-3}$	10^7	10^8 10^8 10^8 $4\cdot10^8$	170 400 3300 6700
Turban	12 18 48 66	$5\cdot10^{-3}$	10^7	$4\cdot10^8$	110 270 2300 4300

In the Table 4 we post the following parameters of simulations: autocorrelation time τ for a temperature at distance ΔT from the critical point, number of MC steps to reach equilibrium N_{relax} and number of effective MC steps N_{mc} for different lattice sizes L.

Table 5. Numerical results

Model	α	β	γ	ν
4-Potts	0.676(3)	0.092(3)	1.224(19)	0.676(3)
Baxter-Wu	0.686(11)	0.08(2)	1.154(15)	0.657(4)
Ashkin-Teller	0.665(1)	0.085(1)	1.165(1)	0.667
Turban	0.777(40)	0.079(1)	1.065(37)	0.611(20)
Exact	0.667	0.083	1.167	0.667

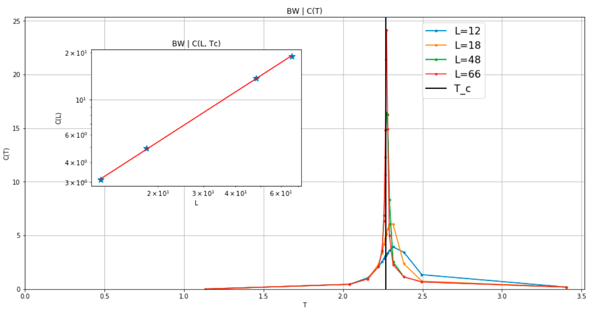
3. Results

The lattices of the models are

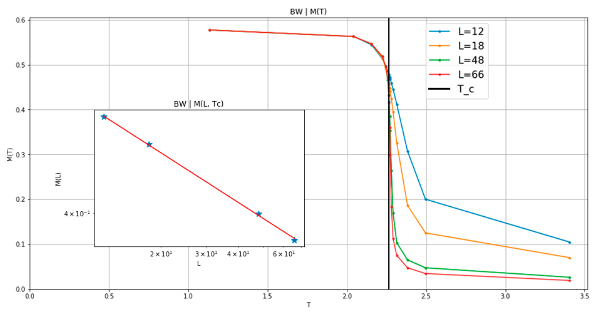
- *4-Potts* - the square lattice of linear size L,
- *Baxter-Wu* - the triangular lattice with the linear size L,
- *Ashkin-Teller* - the square lattice of linear size L,
- *Turban* - the square lattice with horizontal size $2L$ and vertical size L.

We estimate the ratio of the critical exponents α/ν, β/ν, and γ/ν from specific heat, magnetization, and magnetic susceptibility variation, respectively, as a function of the linear lattice size at the critical point. Values of ν estimated using the scaling relation $\nu = 2(d + \alpha/\nu)$. The results are posted in Table 5 and coincide rather well with the exact ones.

We provide an example of the critical behavior for the case of the Baxter-Wu model. Figure 1 demonstrates the critical behavior of the specific heat and magnetization as a function of the temperature for several lattice sizes. The procedure for the estimation of the critical exponents is shown in the insets – it is finite-size dependence of the specific heat $C(T_C)$ at the critical temperature (1-a)) and of the magnetization $M(T_C)$ at the critical temperature (1-b)). The slopes of the lines in the log-log presentation are the estimation of α/ν and β/ν, respectively.



a) Specific heat of the Baxter-Wu model. The vertical solid line marks the critical temperature T_C.



b) Magnetization of the Baxter-Wu model. The vertical solid line marks the critical temperature T_C.

Figure 1. Critical behaviour of the Baxter-Wu model with the linear lattice sizes L. Insets: dependence on the L of a) critical specific heat values $C(T_C)$ and b) magnetization $M(T_C)$.

4. Conclusion

In the paper, we stand the possibility of extracting the statistical mechanics model's critical behavior from the neural network trained with data from another model in the same universality class. As the first step of the research, we apply the same Monte Carlo method to four models in one universality class – the 4-state Potts model, the Baxter-Wu model, the Ashkin-Teller model, and the Turban model. We check the accuracy of the thermodynamic quantities estimation, comparing them with the exact results. So, we have developed the protocol for generating sample data, that is not correlated, which is necessary to avoid overfitting in the training procedure.

The question is not trivial. It is known that models can demonstrate some non-universal properties connected with the geometrical properties, such as the aspect ratio of the system sizes [23] or non-diagonal interactions [24]. We hope to examine how the four models' different interactions and geometrical properties are reflected in the training and accuracy of testing results.

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