Using *SVM* to determine critical temperature

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ABSTRACT

Condensed-matter physics implies dealing with a very large space of states, called the "curse of dimensionality". This is a problem for machine learning algorithms. However, there are techniques for applying machine learning to analyse such complex data sets. In this project, we will use Support Vector Machines (SVM) to find the critical temperature, which is a key parameter of macroscopic physical systems of matter. Its simulation is useful in research related to the superfluid state, Bose-Einstein condensation, superconductors, or magnetism. For this purpose, a complex matter system will be simulated using the Monte Carlo method for the Ising Model. The system will be trained at very low and very high temperatures.

Keywords

Support Vector Machine, Ising Model, critical temperature, machine learning

1. INTRODUCTION

There are many carefully designed tools to study the various properties and parameters of condensed matter[2]. One of the most frequently chosen is Monte Carlo simulations, which are based on the application of the laws of statistics and probability for large data sets. Such simulations consist of two stages: a stochastic importance sampling over state space, and the evaluation of estimators for physical quantities calculated from these samples. The selection of estimators is based on the conditions of a specific case, e.g. the availability of an experimental measurement. The Ising Model is one of the most popular and commonly used statistical models in calculations and scientific reports. Determining its critical temperature is a key parameter for macroscopic physical systems. In our project, the Monte Carlo simulation will be extended, and we will use the Machine Learning tool called Support Vector Machine to determine the critical temperature of the system. SVM gives the possibility of using the kernel function, and therefore appropriate mapping of points in the spin's table to a new abstract space, where it will be possible to linearly separate the ground states and excited states, and therefore their classification.

2. 2D ISING MODEL

The Ising Model is a statistical model of a ferromagnetic or antiferromagnetic body, very well known and mostly used for magnetism calculations. It can be used as a 3-dimensional model, but for our goal a 2-dimensional (2D) system is sufficient. This model is a representation of a square lattice of size $L \times L$ with spin interaction, shown as spin up and down or values $+1$ and -1, as respectively shown on matrix S and Fig. 1. Lattice of the model is considered as all spins occur at every vertex and can interact with its neighbours. This simplification can be used because forces between random spin and its next-nearest neighbours and next-next-nearest neighbours are significantly smaller than these between its nearest neighbours (nn).

$$S = \begin{pmatrix} 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & 1 \end{pmatrix}$$

In Ising Model spins configuration depends on temperature[4], i.e. for low temperatures all spins get the same value, it's called order phase for which all or almost all spin are correlated and take the same "direction", whereas for temperature larger than critical temperature ($T > T_c$) it goes into disordered phase and all spins are in fully random state (-1 or $+1$). These two phases might be seen as microstates of the system, magnetized for temperatures below critical temperature and with zero magnetization for larger temperatures. Transition between these two phases occurs at critical temperature (also called Curie temperature) T_c. Increase of temperature in the system decrease order which results in lack of preferred alignment of spins.

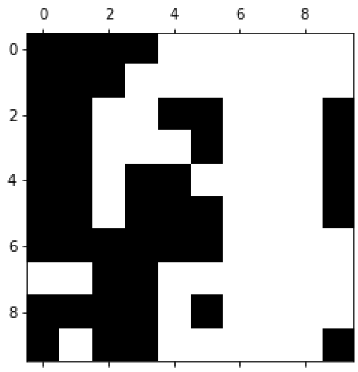


Figure 1: 2-dimensional spin configuration of Ising Model for lattice size 10×10 for reduced temperature $T > T_c$. Black squares represent spins up (or $+1$ values) and white squares show spins down (values -1)

2.1 Theory of 2D Ising Model

The system is a 2-dimensional square lattice with spins in every vertex of this lattice. In Ising Model, $i-th$ spin takes value $s_i = +1$ or -1 which correspond to up and down, respectively. Interaction appears only at nearest neighbours level[2]. Figure 2 represents a section of square lattice. Dots represent spins, which are placed at vertexes of the lattice. In red are spins considered once at the time, i.e. in Ising Model calculations are performed for nearest neighbours which are marked as red dots.

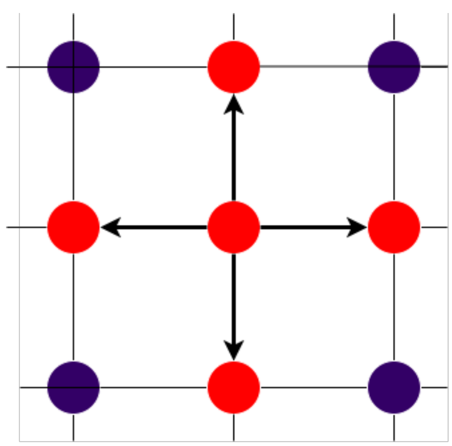


Figure 2: 2-dimenional lattice used in Ising Model. Spins are dots in intersections, red colour correspond to nearest neighbours and their interaction is shown as arrows between them.

For considered Ising Model, we can denote Hamiltonian of our system in dependence of nearest neighbours spin configurations:

$$H = -\frac{J}{2} \sum_{i,j=nn(i)}^{N} s_i s_j \tag{1}$$

where: N is a value equal to the lattice size $L \times L$, J corresponds to interaction strength between nn spins and $s_{i,j}$ is a value of spins, namely ± 1. Summation goes through all spins and its nearest spins, which corresponds to $nn(i)$ and due to fact that, every interaction is calculated twice appears division over 2 with J. Value of J depends on considered model, if case of our study would be anti-ferromagnetic, J would be equal -1, but for simulations we used $J = 1$ which determines that our model is ferromagnetic.

One of the most important feature of Ising Model is magnetisation which can be calculated as sum of all spins in the systems divided by their quantity N:

$$M = \frac{1}{N} \sum_{i=0}^{N} s_i \tag{2}$$

For lower temperatures, magnetisation is equal or very close to values 1 or -1, therefore while increasing value of temperature magnetisation decrease, but correlations between spins are still available to observe, and for values over Curie temperature magnetisation goes to 0, due to absolute randomness of spins. If temperature is greater than the critical temperature, the system is in disordered phase, whereas if temperature is below so-called critical point, the system is in ordered phase. Critical point might be considered as the point separating these two phases[1].

2.2 Monte Carlo simulations

We analysed our problem assuming a zero external magnetic field ($h = 0$), and for the sake of simplicity, we have assumed that $J \pm 1$ and $k_B = 1$. Thus, the theoretical value of the critical temperature of our system amounts to:

$$T_c = \frac{2}{ln(1+\sqrt{2})} = 2.2692. \tag{3}$$

To extract this quantity, the order parameter must be examined. For this purpose, we simulate successively for different reduced temperatures, from $T = 0.1$ to $T = 4.0$ with step 0.1. For each of them, we perform 50,000 Monte Carlo steps, where one Monte Carlo step is defined as going through a square array representing the examined particle system. Our simulation was performed successively on three tables: $L = 10$, $L = 20$ and $L = 30$. During this transition, we reverse the spins for the next particles, provided that the energy of a given network node in the vicinity of the nearest neighbours is < 0 or if it is > 0, but a randomly selected number from 0 to 1 each time is less than $\exp(-\frac{E}{T})$.

3. SUPPORT VECTOR MACHINE AND CRITICAL TEMPERATURE

Our goal was to find the critical temperature of the system simulated with the Monte Carlo method, which was described above. We used the machine learning model - Support Vector Machine (SVM)[6], which was used to classify successive spin configurations into appropriate phases. First, it was trained with extreme temperature data ($T = 0.1$ and $T = 4.0$), which resulted in an effectiveness of around 100% for the test data.

3.1 Method I

The first method of determining the critical temperature was based on the analysis of the dependence of the averaged phase adjustment on the temperature. To this end, we performed additional simulations near the phase transition temperature to obtain additional data and ultimately obtain a more accurate result. The generated data were then analyzed by the SVM model that performed the classification. After averaging the results, we obtained the temperature dependence of the phase adjustment. As we know, the phase transition takes place at the critical temperature, so we can easily calculate T_c from this relationship, using linear regression. We also expect, that it will be possible to calculate the critical temperature, which will be at the point of the breakdown of the plot.

3.2 Method II

The second method we used to predict the critical temperature was closely related to Mean Squared Error (MSE). This function has a value close to zero at low temperatures. We have postulated that it is possible to determine the critical temperature based on the temperature dependence of MSE. According to our expectations, the dependence of MSE on temperature will increase rapidly at the critical temperature. For this, it was necessary to assign the individual configurations to the respective phases in order to be able to assess the correctness of the assignment by the SVM. We therefore counted the magnetization, which is non-zero below the critical temperature and zero above..

4. RESULTS

Following the described methodology, we determined the value of the critical temperature of the simulated system using two methods. In the case of the method based on the analysis of the Mean Squared Error function, we obtained the following results:

The graph of MSE values behaves similarly for different network sizes and in each case, we have observed a sharp increase in the error value, which, according to our expectations, should occur in the place of the critical temperature. The 3 graph shows the increase in MSE value for each tested system as a function of temperature. The analysis of the results and SVM, and above all the shortages in computational resources, did not allow us to obtain an accurate answer to the question of what is the critical temperature in specific Ising models. As a result, this method of calculating the critical temperature is still an open question when using the SVM machine learning model. At this point, we can only give approximate values of the critical temperature for the systems:

System size L	10	20	30	40	50
Critical temperature	2.7	2.5	2.4	2.3	2.3

Table 1: Table of critical temperature values for various system sizes obtained with MSE.

In line with our original assumptions, the value of the critical temperature approaches the theoretical value as the size of the systems increases. With this method, T_c drops from 2.7 for $L = 10$ to 2.3 for $L = 40$ and 50. The value of 2.3, although it is only an approximate value, is giving us very general knowledge about the phase transition moment in a ferromagnet, can be used as a reference point in further studies to which SVM or other machine learning models can be applied. It will then be worth focusing on testing the temperature around 2.3 for larger systems.

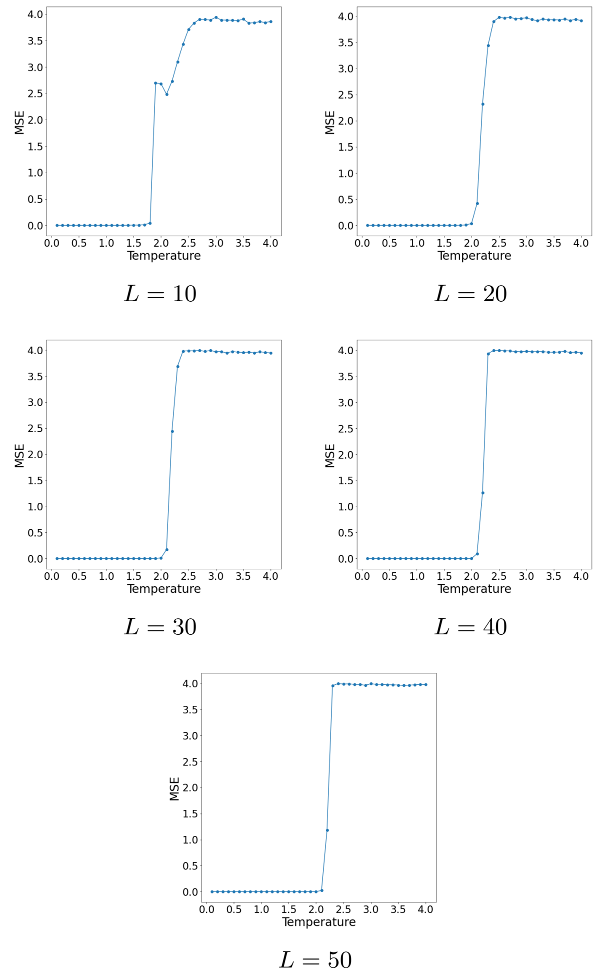
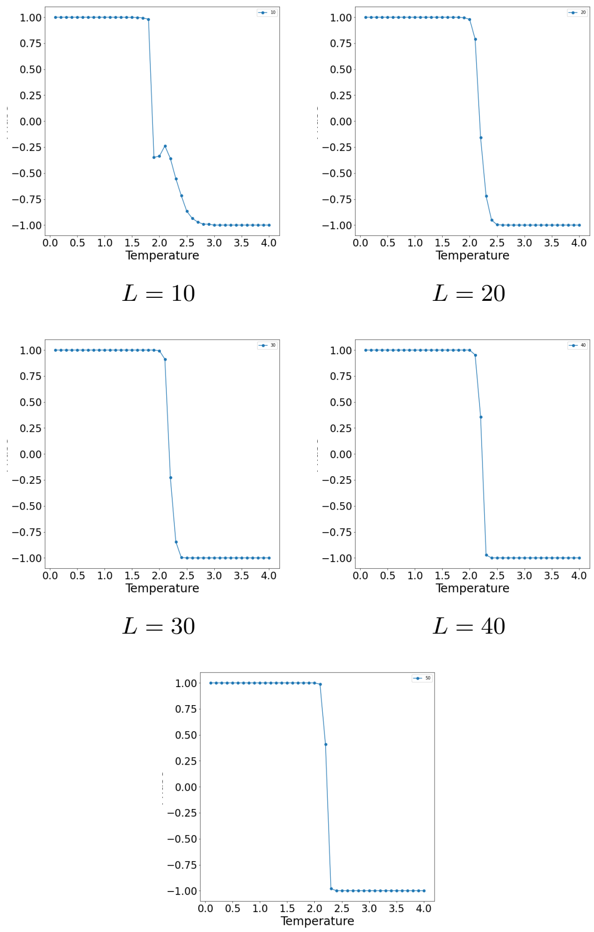


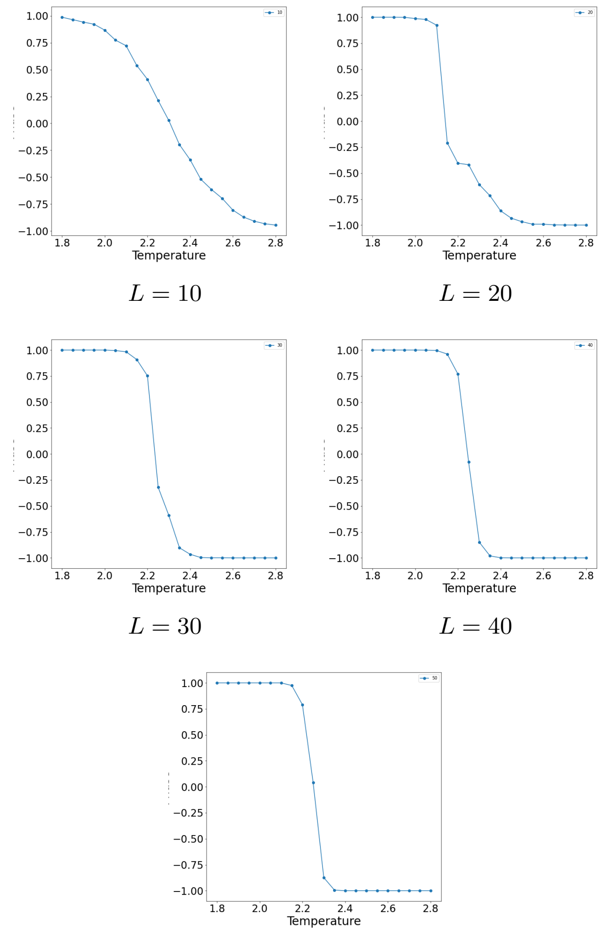
Figure 3: The dependence of MSE on temperature for the tested network sizes.

The next step was the analysis using the first method, but to be able to use it, it was necessary to check and analyze the phase diagrams for all tested system sizes.



$L = 10$ $L = 20$ $L = 30$ $L = 40$ $L = 50$

Figure 4: Dependence of the averaged phase adjustment on temperature for the tested network quantities.



$L = 10$ $L = 20$ $L = 30$ $L = 40$ $L = 50$

Figure 5: Dependence of the averaged phase adjustment on temperature for the tested network quantities.

From the above phase graphs, we noticed that the transition for all network sizes is in the temperature range of 1.8 to 2.8. To make our results and analysis more accurate, additional configurations were generated in this range with increments of $\Delta T = 0.05$. This allowed us for better results in the area of interest. As expected, the way of transition between the cold phase and the warm phase changes from a smooth way to an almost stepwise one as the size of the tested system increases.

However, when analyzing the dependence of the average value of the adjustment on the temperature, we obtained the following results:

System size L	10	20	30	40	50
T_c	2.3009	2.1407	2.2165	2.2390	2.2520

Table 2: Critical temperature value table calculated using linear regression for different system sizes.

The values obtained with the use of linear regression for phase diagrams allowed us to obtain satisfactory results. For smaller sized systems, the calculated critical temperature values showed a greater difference between the nominal critical temperature (2.2692) than for larger sized systems, except for $L = 10$, for which the calculated critical temperature value turned out to be quite accurate. In the tested system with the size $L = 50$ through analysis, the critical temperature was equal to $T_c = 2.252$, and therefore slightly lower than the expected value.

According to the dependence of the critical temperature on the size of the system presented in the diagram 6, it can be expected that obtaining a configuration for larger systems, e.g. 100 or 500, and then using SVM and the linear regression method would allow obtaining much more accurate results. An additional fact supporting this reasoning is the results of [3] research, which for large systems gave very good values of the critical temperature, almost equal to 2.2692.

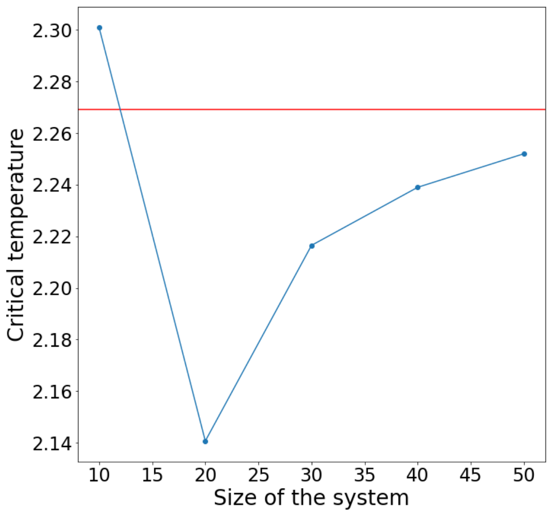


Figure 6: The dependence of T_c on the size of the network in the linear regression method.

5. CONCLUSIONS

The first method used by us with satisfactory accuracy allowed us to determine the critical temperature of the simulated system. Not surprisingly, an error at this point would clearly indicate that our simulation was incorrect or that the SVM model was incorrectly trained.

The results obtained using our new method based on the analysis of the dependence of the Mean Squared Error function on temperature seem to be more interesting. In the case of our data, the result is close to the theoretical value, but everything indicates that with the help of more computing resources it is possible to determine a more precise value. In our opinion, tests should be carried out for a larger system and a smaller temperature range with a smaller jump between successive test points. It can be seen, however, that this method is correct and can be effectively used both to determine the critical temperature and to study the behaviour of the system near critical point for ferromagnetic systems.

6. REFERENCES

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