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 analyze 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. 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 3-dimensional model, but for our goal 2-dimensional (2D) system is sufficient. This model is a representation of a square lattice of size LxL 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 neighbors. This simplification can be used because forces between random spin and its next-nearest neighbors and next-next-nearest neighbors are significantly smaller than these between its nearest neighbors (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, 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.

2.1 Theory of 2D Ising Model

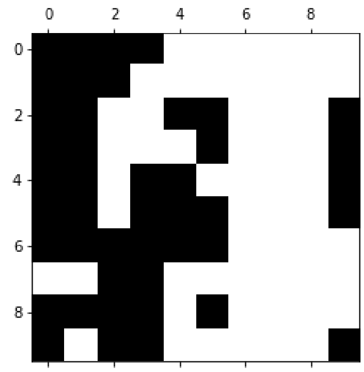

Figure 1: 2-dimensional spin configuration of Ising Model for lattice size $10x10$ for reduced temperature $T > T_c$. Black squares represent spins up (or +1 values) and white squares show spins down (values -1)

The system is 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. 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.

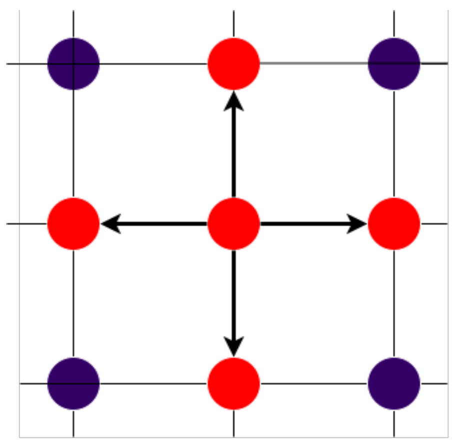

Figure 2: 2-dimenional lattice used in Ising Model. Spins are dots in intersections, red colour correspond to nearest neighbours and their interaction is shown as arrows between them.

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 LxL, 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.

2.2 Monte Carlo simulations

We analyzed 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:

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

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 neighbors 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

4. RESULTS

5. CONCLUSION

6. REFERENCES