Studying the effect of spin removal in the Ising model

Praagya Agrawal

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The Ising model is an exactly solvable statistical system at one or two dimensions that exhibits phase transitions and critical phenomena[1]. This paper explores the effect of the removal of lattice sites from the centre and the corners on the system being modelled. To simulate the Ising model, the Metropolis Algorithm is used. This paper will show that the number of sites and the location of the sites are important parameters, since sites at some locations have a higher interaction.

Introduction

The Ising model is the simplest representation that can model the essential features of real systems, such as the critical point2. The Ising model was proposed in the 1920s, and named after Ernst Ising. It is used to numerically solve the phase transitions that occur when changes in a certain parameter result in a large-scale change in the entire system being simulated.

The mathematical framework of the Ising model starts by creating a lattice that contains a set of equally spaced points. These points are referred to as *lattice sites*. Lattice sites share bonds, and if two sites are connected by a bond, they are called *nearest neighbours*. Ising models can be one-dimensional, two-dimensional, or three-dimensional.

Lattice sites are denoted by $\sigma_i, i = 1, \cdots, N$; where N is the number of lattice sites in the system. Each site σ_i takes either of two values, ± 1, which represent two possible states of the site. The assignment of states $(\sigma_1, \cdots, \sigma_N)$ is referred to as a *configuration* of the system. Fig 1, 2, and 3 show lattices formed by their lattice sites in one-dimensional, two-dimensional, and three-dimensional Ising model respectively.[2]

Fig. 1 A one-dimensional Ising model.

Ernst Ising's study focused on simulating ferromagnetism, as this paper will. In this system, at 2 or 3 dimensions, each lattice site represents an atom, which has a spin that can be either "up" or "down." The net spin of the system determines its magnetic properties. The simulation used in this paper, however, focuses on the net spin itself and not the type of magnetic properties.

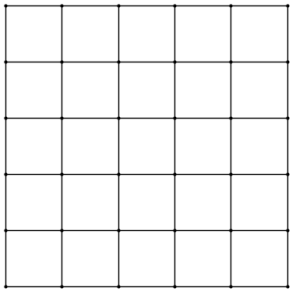

Fig. 2 A two-dimensional Ising model.

An important component of the Ising model is to find the total energy of a system, which is given by its *Hamiltonian*. For this, we assume that only two factors affect the total energy: (1) interactions of nearest-neighbour lattice sites and (2) interactions between an external field and the lattice sites[3]. The Hamiltonian is then given by

$$H(\sigma) = -\sum_{<i,j>} E\sigma_i\sigma_j - \sum_i J\sigma_i \tag{1}$$

where $\sigma = (\sigma_1, \cdots, \sigma_N)$. The first term is the summation over all nearest neighbours and E is a parameter corresponding to the energy associated with nearest-neighbour interactions. The second term is the summation over all lattice sites and J is a parameter corresponding to external field interactions. The system prefers configurations with lower energy levels, and thus finding its energy is an essential component of simulating its equilibrium[4].

Here, J can be expressed as a product of two terms:

$$J = \mu m \tag{2}$$

Where μ is the atomic magnetic moment and M is the strength of the external magnetic field. The Hamiltonian can then be expressed as

Table 1

Sites removed from	Parameter	R2 Score	Coefficient	Intercept
Whole lattice	Average spin	0.064	-0.113	-8.805
Whole lattice	Net energy	0.888	0.978	-0.012
Centre only	Average spin	-0.378	-0.067	0.0001
Centre only	Net energy	0.829	0.874	-0.023
Outside centre only	Average spin	-0.064	0.131	-0.0001
Outside centre only	Net energy	0.264	0.449	-0.062

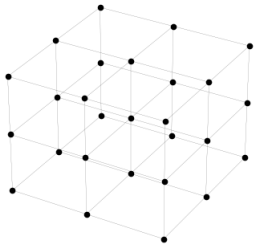

Fig. 3 A three-dimensional Ising model.

$$H(\sigma) = -\sum_{<i,j>} E\sigma_i\sigma_j - \mu m\sum_i \sigma_i \tag{3}$$

The energy of the ith atom, e_i, can then be given by

$$e_i = -\frac{E}{2}\sum_{N}^{k=1} \sigma_k\sigma_i - \mu M\sigma_i = -\mu M_{eff}\sigma_i \tag{4}$$

Where M_{eff} is the effective magnetic field given by[5]

$$M_{eff} = M + \frac{E}{2\mu}\sum_{N}^{k=1} \sigma_k \tag{5}$$

In the model, the partition function, given by

$$Z = \sum_{\pm 1} e^{-\beta H(\sigma)} \tag{6}$$

where $\beta = \frac{1}{k_B T}$; k_B is the Boltzmann's constant and T is the temperature, and Z is the summation over all 2^N possible ± 1 assignments to each lattice site, serves as a normalization constant for the probability of being in any given configuration $\sigma = (\sigma_1, \cdots, \sigma_N)$ over the Boltzmann distribution which is given by[6]

$$P(\sigma) = \frac{1}{Z}(e^{-\beta H(\sigma)}) \tag{7}$$

This probability also suggests that the probability of being in a state with a lower Hamiltonian (and thus energy) is greater than the probability of being in a state with a higher Hamiltonian, which means that the system prefers lower energy levels.

The Ising model is capable of showing the effect of magnitude of the parameters of the system: initial energy of the lattice E, temperature T and thus also β, and the external field interactions as denoted by J. As an example, it can show that average spin is close to 0 when temperature (T) is high and is closer to 1 when the temperature (T) is low. The Metropolis algorithm is covered in detail in the Results section.

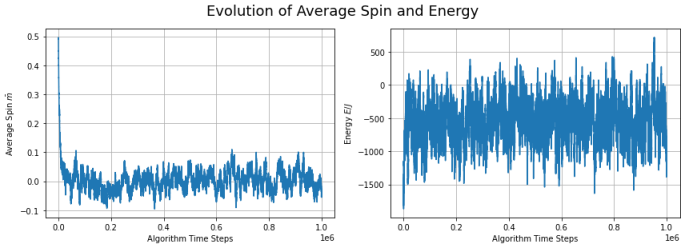

Fig. 4 Results for high temperature.

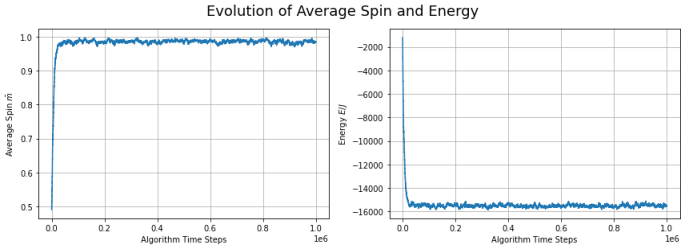

Fig. 5 Results for low temperature.

This paper analyses the effect of the removal of lattice sites on the system, by observing the changes in the evolution of spin and energy, with parameters E,J and β staying constant.

Results

It is difficult to manually mathematically solve the system since there are 2^N possible configurations, in cases where no removal is used (and therefore there is no 0 state in any lattice

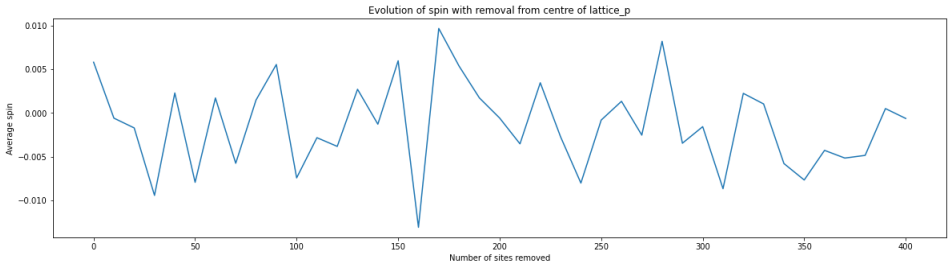

Fig. 6 Effect of the removal of the central lattice sites on average spin.

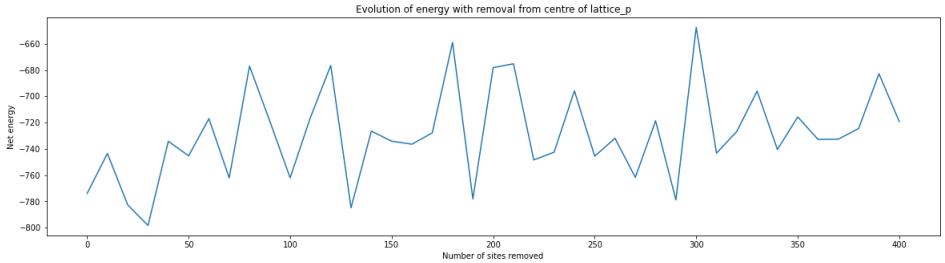

Fig. 7 Effect of the removal of the central lattice sites on net energy.

site), where N is the number of lattice sites. For this reason, a simulation is used instead. The type of simulation chosen is Monte Carlo.

The Monte Carlo algorithm used is the Metropolis Algorithm, which is used to simulate a series of states of the system and reach an equilibrium. It starts with an initial lattice with a given size and configuration, along with its net spin and energy. The average spin is calculated by simply adding the spin of every individual lattice site and dividing it by the number of lattice sites. The net energy is calculated using the Hamiltonian. Then, it picks a random site in the lattice and proposes a flip in its spin (i.e., -1 to +1 or +1 to -1), by creating a temporary lattice with the spin reversed, and calculates the change in energy ΔH that would be caused by the flip. If $\Delta H < 0$, the spin flip is accepted, since the system prefers lower energy levels. If $\Delta H > 0$, a random number r is generated from the range $0 < r < 1$. If $r < e^{-\beta H(\sigma)}$, the spin flip is accepted. Else, it is rejected. If the proposed spin is accepted, the original lattice is overwritten by the temporary lattice, and the new net spin and energy of the lattice is stored. This process is repeated for a given number of Monte Carlo steps, until equilibrium is reached[7]. In this paper, 1000000 Monte Carlo steps are used in our simulation on a 50×50 lattice. In addition, the removal of lattice sites has been added to the metropolis algorithm before computing equilibrium. For this, given number of randomly chosen sites have their values set to 0. The code used for the simulation can be found on reference[8].

Table 2

Sites removed from	$S(\sigma_{max})$	$E(\sigma_{max})$
Whole lattice	269.05%	-
Centre only	325.86%	16.35%
Outside centre only	314.81%	26.9%

First, the paper will analyze the effect of removing particles from the centre of the lattice on the evolution of average spin and net energy on a system with no external magnetic field. The size chosen is 50×50, and the centre was considered to be in the range of $15 \leq x \leq 35$ and $15 \leq y \leq 35$. The values chosen for the parameters are $E = 4$ and $\beta = 0.05$. No external magnetic field is considered. The parameter R represents the number of sites removed. The simulation was performed for a lattice initialized with 75%of sites as $+1$ (lattice p).

The results shown below are averages from 10 simulations.

The figures suggested that it might be possible to predict the average spin and net energy of the configuration $\sigma(R)$, that is achieved at equilibrium when R sites are removed, from their values at $\sigma(R-x)$ where x is some constant. When removing sites from only the centre or outside the centre, a total of 400 sites were removed and x was chosen to be 10. When removing sites from the whole lattice, a total of 2000 sites were removed and x was chosen to be 50. A model was then trained on this data, and the accuracy with which $\sigma(R)$ could be predicted by $\sigma(R-x)$ were then calculated, by using the R2 score of the model. The results are summarized in the table below:

The results suggest that the net energy of $\sigma(R)$ can be pre-

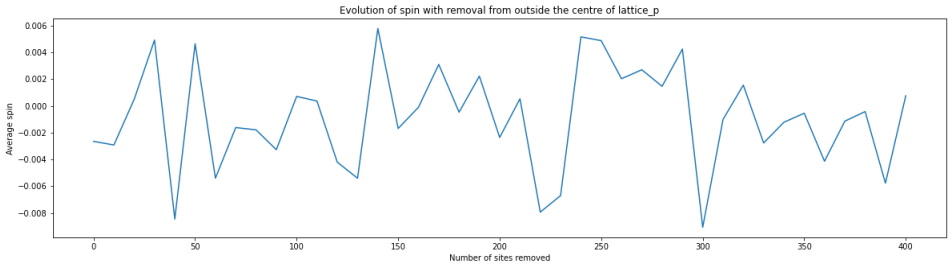

Fig. 8 Effect of the removal of the non-central lattice sites on average spin.

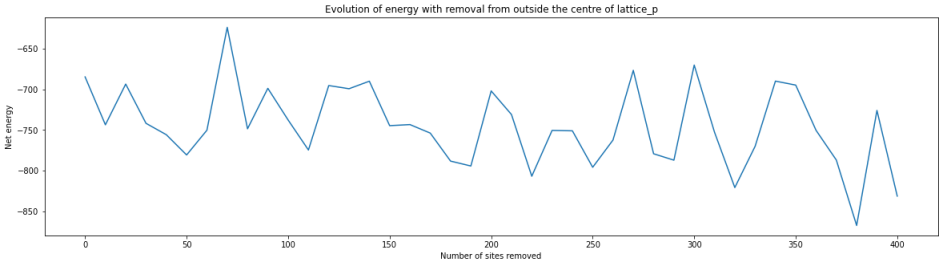

Fig. 9 Effect of the removal of the non-central lattice sites on net energy.

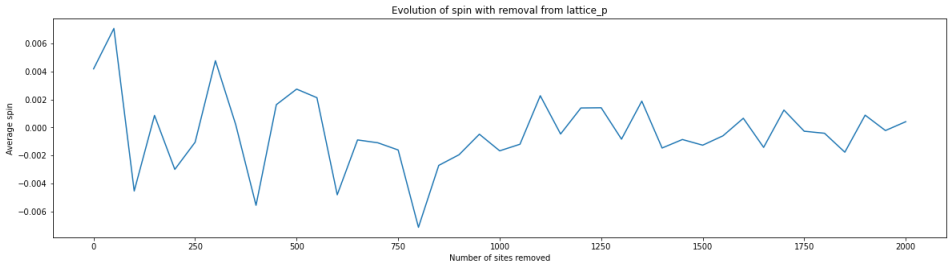

Fig. 10 Effect of the removal of the lattice sites from the entire lattice on average spin.

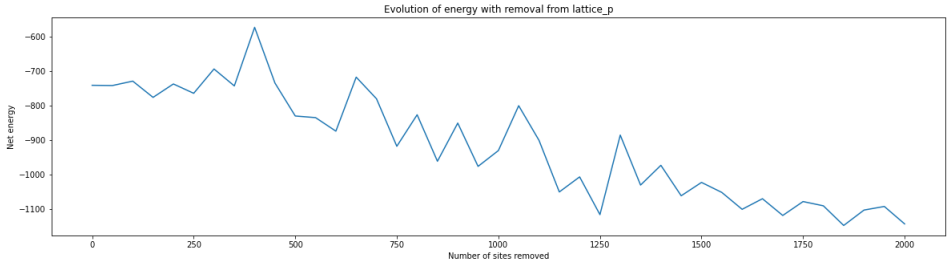

Fig. 11 Effect of the removal of lattice sites from the entire lattice on net energy.

dicted by the net energy of $\sigma(R-x)$ with over 80% accuracy when sites are removed from the whole lattice or the centre only, but with only 26% accuracy when sites are removed from outside the centre only. In all cases, the average spin of $\sigma(R)$ is not accurately predicted by the average spin of $\sigma(R-x)$.

The percentage maximum variation of average spin and net energy when $R > 0$, $S(\sigma_{max})$ and $E(\sigma_{max})$ respectively, from the average spin and net energy when $R = 0$ was measured in all 3 cases. $E(\sigma_{max})$ was not used for removal from the whole lattice as the larger values of R and the downward trend of net

energy would skew the results. The results are shown below:

From these results we can observe that the location of the removed sites does have an impact, and sites seem to have different interactions. However, $S(\sigma_{max})$ is not very different between except for when sites are removed from the whole lattice. This suggests that since sites in an area interact with each other, removing sites from a restricted area will have a larger impact than removing sites randomly.

Discussion

While the Ising model undoubtedly has applications in theoretical and computational physics, its uses spread beyond that. D. Stauffer showed that the Ising model can compute socioeconomic systems, such as business confidence, racial segregation, and the replacement of the dominant language spoken in an area[9]. C. Daskalakis, N. Dikkala, G. Kamath also showed that the Ising model has applications in both synthetic and real-world social networks[10]. The results of this paper can perhaps be taken forward by applying removal of sites from such systems, representing exiting or temporary inactivity of agents in socioeconomics systems or social networks.

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