Determination of ground states in the Ising Hamiltonian from genetic algorithms.

Kennet J. Rueda Espinosa ⋆
Universidad Nacional de Colombia, Facultad de Ciencias
Introduction to artificial intelligence - Project
Github repository.

December 2022

Abstract
In this work, a method for determining base states for the Ising Hamiltonian using genetic algorithms is presented. This work allows for the classification of the magnetic behavior of materials with known structure but unknown spin states.

Key words: Ising Hamiltonian – Genetic algorithms – Magnetization

1 Introducción

The Ising model was formulated by Wilhelm Lenz in 1925 to study the magnetic behavior of materials at the microscopic level using a simplified model that considers the individual magnetic interactions of atoms with their neighboring atoms. Simon (2017). Since its formulation, the Ising model has been a common part of developments in statistical mechanics for magnetism Wood (2021), which have allowed for the identification of phase transitions and an understanding of the behavior of ferromagnetic, antiferromagnetic, and more recent spin glasses and spin liquids Balents (2010), which have opened up new areas of research in physics and a range of new technological developments.
The model in question, for a 2-dimensional case, is described by the hamiltonian of the equation 1

$$H = -\sum_{i,j} J_{ij}\sigma_i\sigma_j + h\sum_i \sigma_i \tag{1}$$

where the terms J_{ij} quantify the effective magnetic interaction or coupling between the spins, while σ_i and σ_j are the spins that in this case take values $\sigma = 1$ or -1. Additionally, the Hamiltonian considers the application of an external magnetic field h that interacts individually with each spin σ_i.
Based on the principle of minimum energy, it is expected that for a case free of perturbations and external interactions, a physical system described by this Hamiltonian will naturally tend towards the state of minimum energy, that is, the configuration of variables and parameters that minimize H. 1.
In this work, we will consider the case where the crystal structure of the system is well defined, that is, when it is clear which are the neighboring atoms that each atom interacts with and the value of interaction J_{ij} is known for each coupling, which in practice comes from solving a different problem using experimental techniques Lokhov et al. (2018). This means the variables are the spins of each atom, and the problem of finding the minimum energy state is reduced to finding the set of spin values σ_i for each atom i in the system that minimizes H.
In the context of the use of artificial intelligence, this problem can be framed as a Constraint search problem or combinatorial optimization with constraints, in which we say that each site can take a single spin value and where we have a heuristic function to minimize H.
In this work, we will use genetic algorithms to search for the configurations of variables (spins) that minimize the evaluation function H of the problem.

2 Methodology

As mentioned in the previous section, we will use genetic algorithms to search for the minimum energy configuration. These algorithms are based on an analogy to the evolutionary behavior of genes. In the context of this problem, this can be presented as follows:
A set of Ng possible spin configurations (e.g., $[-1, 1, ..., -1]$) is generated in an initial iteration $t = 0$, then the evaluation function (e.g., the system's Hamiltonian) is evaluated on each configuration Ng_i. Then, based on a set of probabilities, which could follow a softmax distribution, pairs of configurations Ng_j and Ng_k are selected, prioritizing those with the best value of the evaluation function. Next, a "crossover" process occurs in which a percentage of the genes from Ng_j and Ng_k are mixed to generate two new configurations Ng_l and Ng_m that evolutionarily are considered the "children" or resulting generation of a "parent" configuration.
The resulting generations of configurations undergo a mutation process in which, with a certain probability, a spin in the chain takes on the opposite value of its current one.
The result of this process is a new generation of N'_g spin chains, resulting from a combination of their parents and mutation.
From here, the next iteration $t = 1$ begins, and the process is repeated until a number N_{iter} of repetitions is completed. Through the N_{iter} generations, we store in memory the configuration of variables that reports the minimum evaluation value over the entire process and report this value at the end.
For this work, we used the implementation of Solgi (Solgi) of the algorithms.

2.0.1 *Multiplicity of solutions*

Although we obtain a solution to the problem with the previous process, we know from the physical approach that there are systems in which the ground state has a multiplicity that may be different from zero, so we can expect more than one solution. It is important to try to identify these cases as they allow us to identify physical cases of interest such as frustra-

⋆ kruedae@unal.edu.co

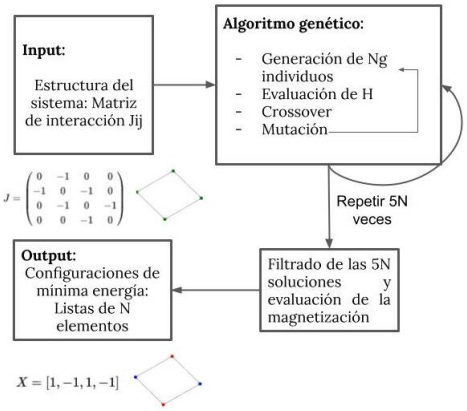

Figure 1. Block diagram of the proposed solution

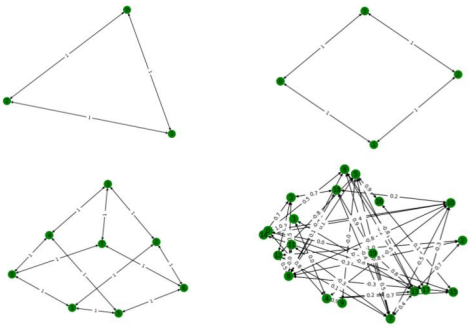

Figure 2. Test configuration with a.$N = 3$, b.$N = 4$, c.$N = 8$ and d.$N = 20$. The values of the interactions appear between the vertices.

tion, which we will discuss in the next section.
To do this, we propose that the genetic algorithm solution process be repeated $N * 5$ times, where N is the number of spins, in order to give the process the opportunity to converge on the different configurations that have the same energy.

The complete process above is summarized in the image 1

2.0.2 Experimental configuration

To test the algorithm, we decided to test 3 known base systems in the literature Simon (2017) with N = 3, N = 4, and N = 8, and a random system with N = 20. A scheme of these systems, as a representation of graphs, is shown in the figure. 2
For the first three systems, the expected results are well known, so it was possible to verify the resolution of the problem, which is shown in the following section.
Likewise, for all results, the behavior of the algorithms in the optimization process and the computation time were studied.

2.1 Resultados

We begin by studying the case of the square system b.2. For this case, we consider two scenarios in which the interactions J are all positive or all negative.
According to the literature, if the interactions are positive, the configuration that minimizes the energy is one in which all the spins have the same orientation. This is expected from the form of 1. On the other hand, when the interactions are negative,

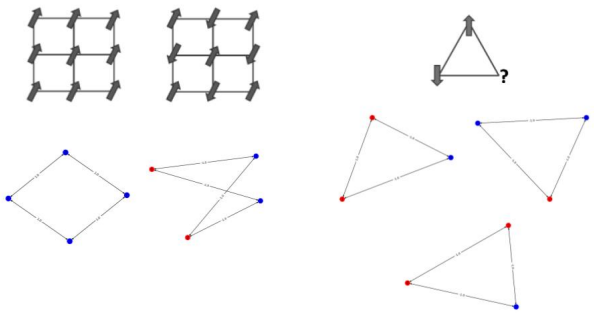

Figure 3. Solutions to configurations a. and b.

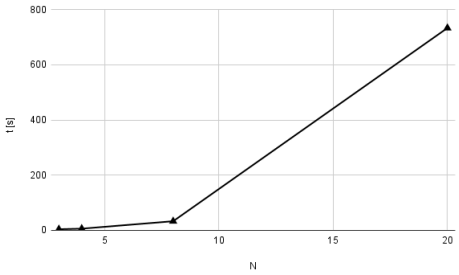

Figure 4. Computing time as a function of spin number

the configuration of minimum energy is one in which each spin is antiparallel to its neighbors. The results and what is expected in the literature are shown in figure 3.

The computation time for this case was 4 seconds. A summary of the times for each system is shown in 4.

In the b. configuration with $N = 3$, it is shown that for negative J interactions, multiple solutions appear because it is not possible to make completely antiparallel interactions between pairs, this impossibility is what is considered a "frustrated system". Frustrated systems are the principle of new areas of physics that include spin liquids and are of recent interest.
Similarly to the previous one, in figure 5, the solutions are compared with what is presented in the literature. Here we see that there are 4 equivalent solutions, with similar topologies but where the spins that do not manage to fulfill a null interaction between pairs are different. This material is antiferromagnetic because it has an equal number of parallel and antiparallel spins.

In figure 6, the optimization process for an iteration of the algorithms for 3 configurations is presented. Here it is observed that with respect to the maximum iterations of each case, the algorithm seems to converge quickly and appears to need as many iterations as proposed. Now that known cases have been explored, let's consider a currently unknown case in which we consider a random system. For configuration d., the result is shown in figure 7, and the result of the agent shows that for this particular configuration, 11 of the spins are antiparallel $s = -1$ and 9 are parallel $s = 1$. Physically, this means that we should expect this "random material" to have a very low magnetization, approaching the behavior expected for an antiferromagnetic material (in which all the spins would be antiparallel).

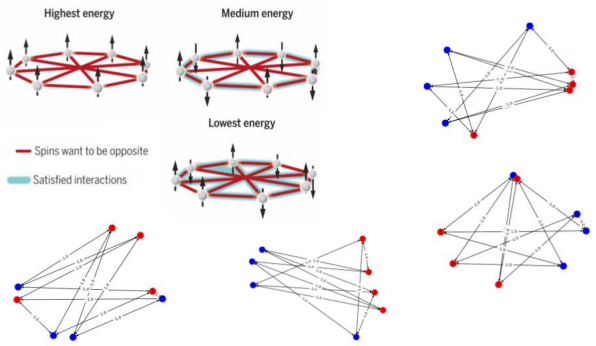

Figure 5. On the left above is an image from the literature with the solution of the system for N=8. Around it are shown the solutions found by the agent.

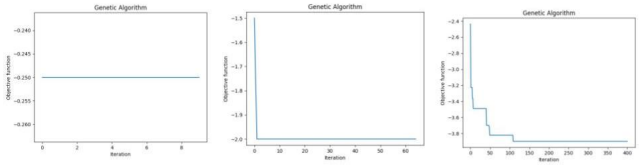

Figure 6. Optimization process for N=3,8 and 20

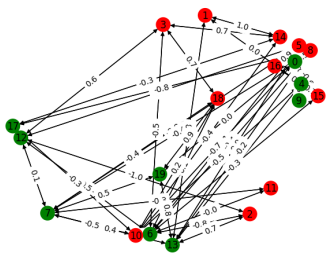

Figure 7. Solution to random configuration

3 Conclusiones

In this work, we proposed a way to solve the problem of the ground state of an Ising Hamiltonian where the spins are the variables, using genetic algorithms. The problem of multiplicity was considered and it was shown that the algorithm reproduces expected results for N=3,4 and spins. Then, an evaluation of an unknown case was carried out, allowing us to classify the "test material" as antiferromagnetic. In computational terms, the computation time seems to scale inefficiently with N, so in its current state, the algorithm does not seem to be able to be used on large systems. However, it is notable that the number of iterations used can be reduced and possibly also the number of times the genetic algorithms are run, currently $5N$, can be reduced to improve the application of the problem.
For future work, it would be academically interesting to test cases where magnetic fields are applied (where the second term of Equation 1 is used) and to explore phase transitions from the algorithm. It would also be interesting to consider models where the temperature and the statistical nature of the perturbation of states are taken into account.

References

Balents L., 2010, Nature, 464, 199
Lokhov A. Y., Vuffray M., Misra S., Chertkov M., 2018, Science Advances, 4, e1700791
Simon S. H., 2017, The Oxford solid state basics. Oxford University Press
Solgi R., , geneticalgorithm 1.0.2, https://github.com/rmsolgi/geneticalgorithm
Wood Charlie s., 2021, The cartoon picture of magnets that has transformed science, https://www.quantamagazine.org/the-cartoon-picture-of-magnets-that-has-transformed-science-2020