Assignment#5

CH5650: Molecular Data Science and Informatic
Jan-May, 2025

Due Date: April 25, 2025 (Online Submission, https://courses.iitm.ac.in/)

The Ising model, which originated as a model for understanding magnetism, is relevant to a range of materials, optimization, and graph theory problems. Because of this generality and because its ground state is analytically known, this model has long served as a benchmark for testing new optimization and machine learning algorithms. In its most general form, the Ising model consists of a grid or lattice arrangement of elements, which are called spin variables. A spin has two states and interacts with neighboring spins only. The total energy of the Ising model is then $E = \sum_{i,j}^{N} J_{ij} S_i S_j$, where $S_i = +1$ or -1 and J_{ij} is the interaction between the ith and jth spins. Let's assume $J_{ij} = 1$ for neighboring spin and 0 otherwise. Develop and employ a genetic algorithm to identify the ground state (lowest energy state) of a 100 spins 1D Ising model. Treat the system periodic. Submit your code along with a report. In the report, you should plot the lowest energy as a function of the evolution cycle. Choose different selection strategies—random selection, biased selection, and elitism—as well as various crossover and mutation strategies. Examine the performance of the optimizer for each of these strategies.

A GA code can be found in the following link.
https://github.com/patra-group/GA-code