2-d Ising Model (MCMC)

EESHAN BEOHAR

19036762014

Problem Statement:

The purpose of this project is to introduce Markov Chain Monte Carlo algorithms (focusing on Metropolis) and try to simulate an Ising system using it.

Ising Model:

The Hamiltonian of the Ising Model (h=0) can be written as

$$H = -\sum_{i,\,j} J S_i S_j$$

where J represents the spin-spin interaction and S_i are the individual spins on each of the lattice sites. Sum is over all pairs of neighbouring lattice sites (a.k.a. bonds), it represents the interactions between spins which is either -1 or +1.

A physical quantity Q can be calculated as a statistical mean from the partition function:

$$\langle Q \rangle = \sum_i^N Q_i\, e^{-\beta H} / \sum_i^N e^{-\beta H} = \sum_i^N Q_i\, e^{-\beta E_i} / \sum_i^N e^{-\beta E_i}$$

Numerical Techniques Used:

Markov Chain Monte Carlo: A Markov process, or a
Markov chain, is a stochastic process which, given the system in a state *u*, puts the system in a new state *v* in such a way that it has the *Markov property*, i.e. that it is memoryless. This forms a “Markov chain” which can be thought of as a generalized random walk, such that at any step x_i, probability of transition to x_{i+1} step depends on x_i only.
The transition probabilities must be “ergodic”.

Detailed Balance Condition:

Let X_0, X_1... be a Markov chain with stationary distribution π. The chain is said to be reversible with respect to π or to satisfy detailed balance with respect to π if $\pi_i * p_{ij} = \pi_j p_{ji}$, for all i,j., where p_{ij} is the transition probability of going from i to j. Basically, the conservation of rate of change of probability.

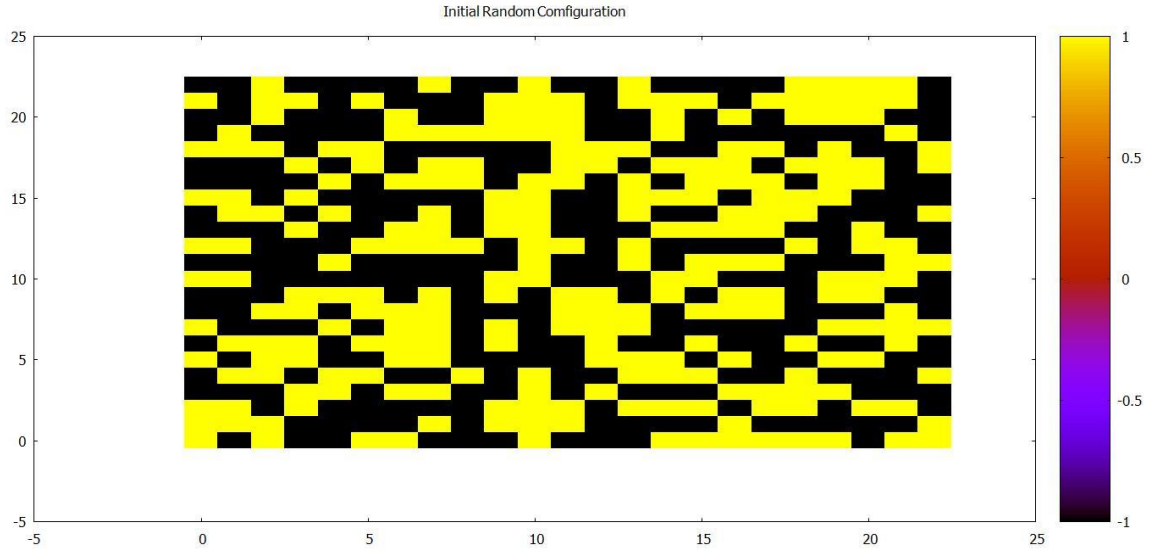
Metropolis–Hastings's algorithm:

The process in this method is similar to Rejection sampling. But here, a proxy distribution (like in importance sampling) function is represented by a conditional (correlation) probability $q(x|x_i)$, and the random number v is generated from a uniform distribution on [0,1]. The basic algorithm is as follows:

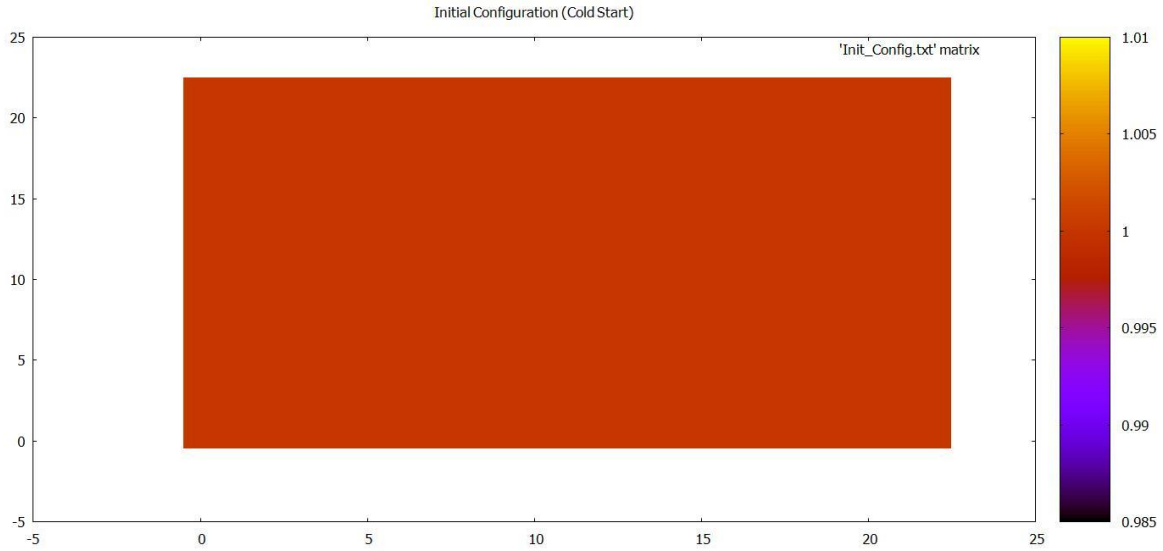
- generate a random number x' from a proxy distribution $q(x|x_i)$. This x' is called a *proposal point*.
- generate a random number v from a uniform distribution on [0, 1]. This v will be used to evaluate the proposal point, whether to be fine considering generated from p(x).
- If $v \leq p(x')q(x_i|x')/(p(x_i)q(x'|x_i))$, then x' is accepted as a random number generated by p(x), else, x' is rejected.

Implementation:

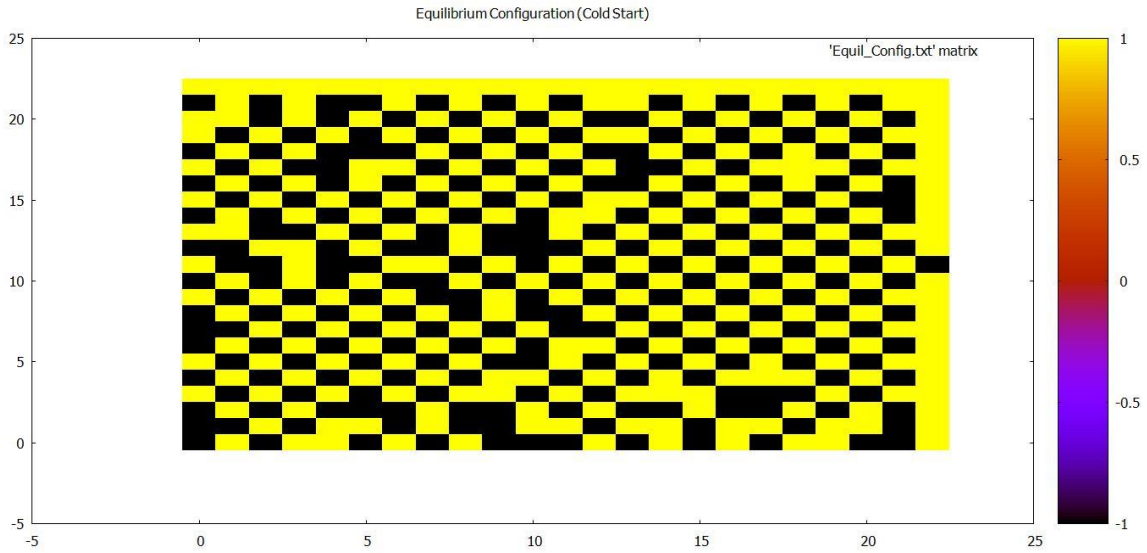
1. Initialization
    - Enter the number of linear sites L
    - Total number of sites N = L x L, 2-d spin array = spin [L][L]
    - (Hot Start) Initial Random Configuration: Randomly assign a spin +1 or -1 for each of the N sites.



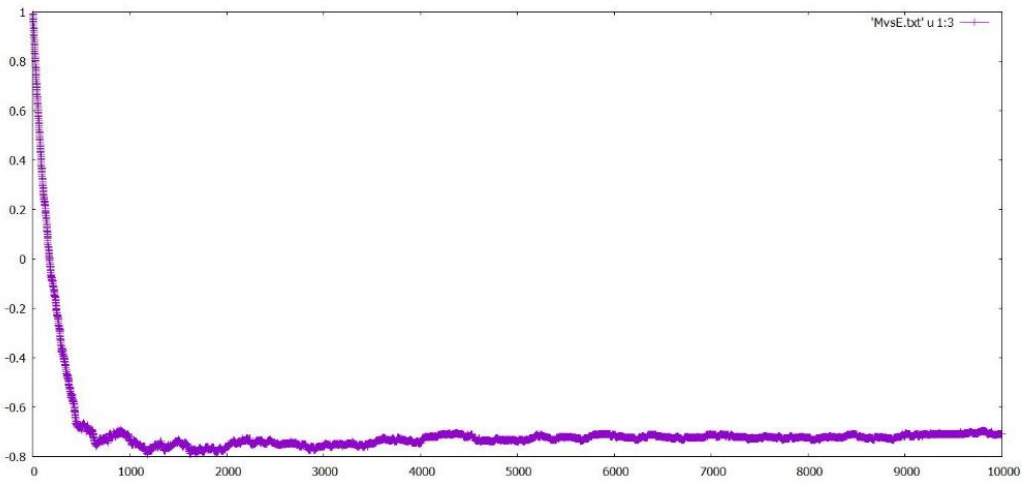
- Cold Start Initial Configuration: Assign all N sites spin +1.



2. Thermalization: Let the system come to a state of “Equilibrium” by initially running “n_equil” Metropolis cycles.



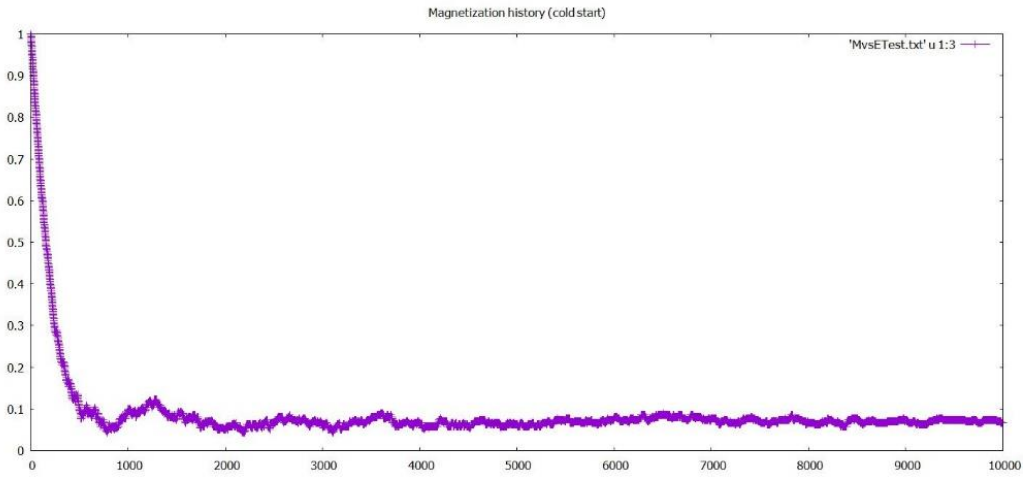
“Equilibrium State” and the required number of cycles can be visualized by looking at MC Energy/site(E) history:



E/site vs. Cycles

After ~1500 cycles, energy/site merely oscillates about an equilibrium value and hence it is safe to set n_equil = 2000.

Magnetization history:



M/site vs. cycles

3. Sampling: After reaching equilibrium, we can now take samples and form a markov chain. For a suitable “mcs” number of total cycles prior to “n_equil”, for every “Nskip” cycles, we measure the mean energy E and magnetization M per site. Sample output for (23 x 23) Cold Start:

Effective Temperature (J/Kb) = 2.0

Mean energy per spin = -0.513

Mean squared energy per spin = 1394.213

Mean magnetization per spin = 0.006511

Mean squared mag. per spin = 0.238087

Repeat the simulation for different lattice size, reduced temperatures.

Caution and Limitations:

The corelations among sites disrupt the simulation results and need to be taken care of.

Make sure to run the simulation for large number of cycles after thermalization.

Use of pointers is favourable for a smooth run.