Stochastic Simulations
Homework 2: Markov chain Monte Carlo

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December 9, 2020

From the problem sheet, we have that the energy function $H(\boldsymbol{S})$ is defined as:

$$H\left(\boldsymbol{S}\right) = -\sum_{i,j=1}^{m} \left(\frac{1}{2} J s_{ij} \left(s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1}\right) + B s_{ij}\right) \tag{1}$$

where J is a magnetic coupling constant and B is a constant describing the external magnetic field. We also have these boundary conditions: $s_{0,j} = s_{j,0} = s_{m+1,j} = s_{j,m+1} = 0$.

The probability of obtaining a specific system state is given by the Boltzmann distribution with probability mass function (PMF):

$$f(S) = f_{\beta}(\boldsymbol{S}) = \frac{1}{Z_{\beta}} e^{-H(\boldsymbol{S})\beta} \tag{2}$$

where $\beta = \frac{1}{k_B T}$.

As a result, for the discrete case, we have that Z_{β} can be computed as follows=

$$Z_{\beta} = \sum_{\boldsymbol{S} \in K} e^{-H(\boldsymbol{S})\beta} \tag{3}$$

where K = $\{-1, 1\}^{m \times m}$.

The system's total magnetic moment corresponding to the configuration $\boldsymbol{S}$ is:

$$M\left(\boldsymbol{S}\right) = \sum_{i,j=1}^{m} s_{ij} \tag{4}$$

The exact expected value of the total magnetic moment $\bar{M}(\boldsymbol{S})$ as a function of the inverse temperature reads:

$$\bar{M}(\boldsymbol{S}) = \sum_{\boldsymbol{S} \in K} M(\boldsymbol{S}) f_{\beta}(\boldsymbol{S}) = \frac{1}{Z_{\beta}} \sum_{\boldsymbol{S} \in K} M(\boldsymbol{S}) e^{-H(\boldsymbol{S})\beta} \tag{5}$$

Instead of computing the energy as given in (1), we can simplify it taking into account the boundary conditions and indices manipulation, which leads to the following expression:

$$H\left(\boldsymbol{S}\right) = -\sum_{i,j=1}^{m-1} \left(J s_{ij} \left(s_{i,j+1} + s_{i+1,j}\right)\right) - \sum_{i,j=1}^{m} B s_{ij} \tag{6}$$

The sum for the second term on the right-hand side of the latter is for all m atoms.

Given that the transition matrix $Q(\boldsymbol{S})$ is symmetric, the Metropolis-Hastings acceptance rate can be expressed as:

$$\alpha\left(\boldsymbol{S}^{old}, \boldsymbol{S}^{new}\right) = \min\left\{1, f(\boldsymbol{S}^{new})/f(\boldsymbol{S}^{old})\right\} \tag{7}$$

where $f(\boldsymbol{S}^{new})/f(\boldsymbol{S}^{old})$ can be written in terms of a energy change as: $f(\boldsymbol{S}^{new})/f(\boldsymbol{S}^{old}) = \mathrm{e}^{-\Delta H \beta}$ and ΔH= $H(\boldsymbol{S}^{new}) - H(\boldsymbol{S}^{old})$

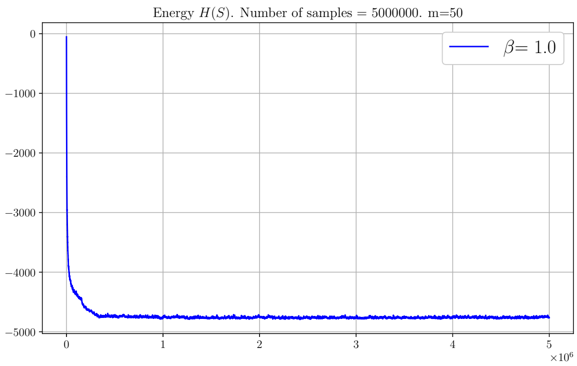
For all shown plots, blue represents a 1 (positive spin) and red a -1 (a negative spin).

1. The following picture shows a possible code implementation of the Ising Model. The full code is attached together with this document.

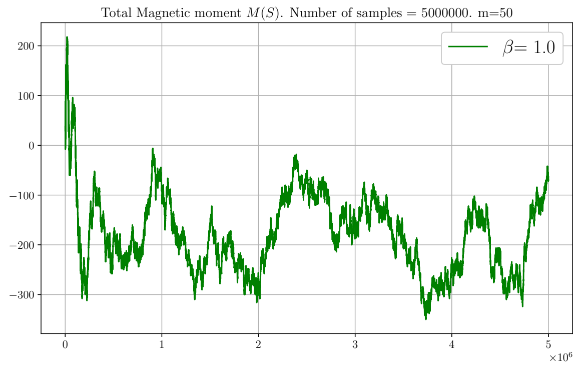
```python
def H_function(S, M, J, B):
    m = int(S.shape[0])
    t1 =np.sum( S[ : , :m-1] * S[ : ,1: ] )
    t2 = np.sum( S[ : m-1, : ] * S[1:, :] )
    return -J*(t1+t2) - B*M

def IsingModel(m, n, beta, J, B, S0):
    # n is the number of runs, so n represents the number of different
    # states we have
    H = np.zeros(n+1)
    M = np.zeros(n+1)

    #initial energy H and magnetic moment M
    S = S0
    M[0] = np.sum(S)

    H[0] = H_function(S, M[0], J, B)

    for k in range(n):
        S_new = np.copy(S)
        indices = np.arange(m, dtype = int)
        a = int(np.random.choice(indices))
        b = int(np.random.choice(indices))

        S_new[a,b] = -1* S[a,b]

        M_new = np.sum(S_new); #new magnetic moment
        H_new = H_function(S_new,M_new,J, B ) # new energy

        M_diff = M_new - M[k]
        H_diff =np.sum( H_new - H[k])

        alpha = np.min([1, np.exp(-H_diff*beta)])
        U = np.random.random()
        if U < alpha:
            S = S_new # new configuration
        else: #no change
            M_diff = 0
            H_diff = 0

        H[k+1] = H[k] + H_diff
        M[k+1] = M[k] + M_diff
    return S, H, M
```

Figure 1: Ising model implementation.

2. We ran our code for $m = 50, J = 1, B = 0, \beta = \frac{1}{3}, \beta = 1$. We obtained the following:

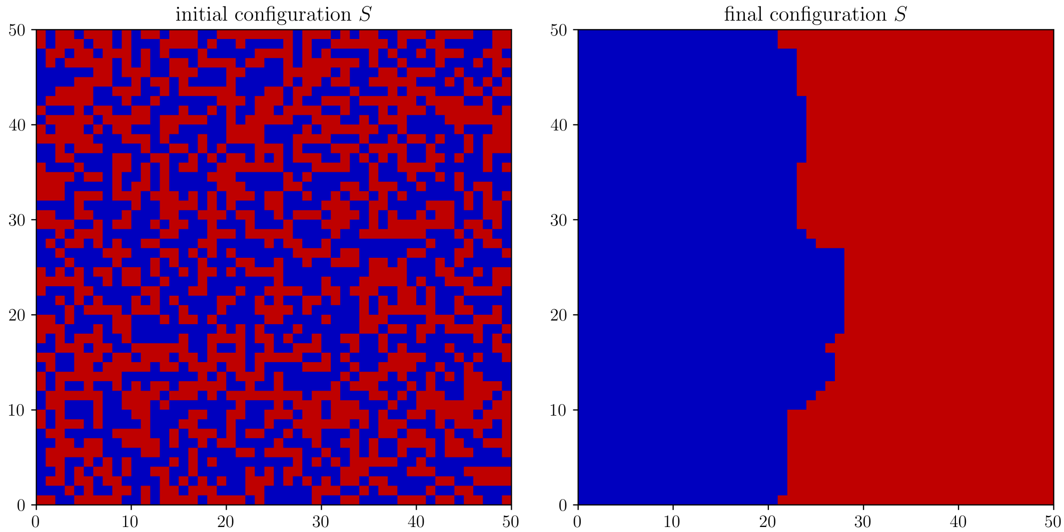


(a) Energy $H(\boldsymbol{S})$.



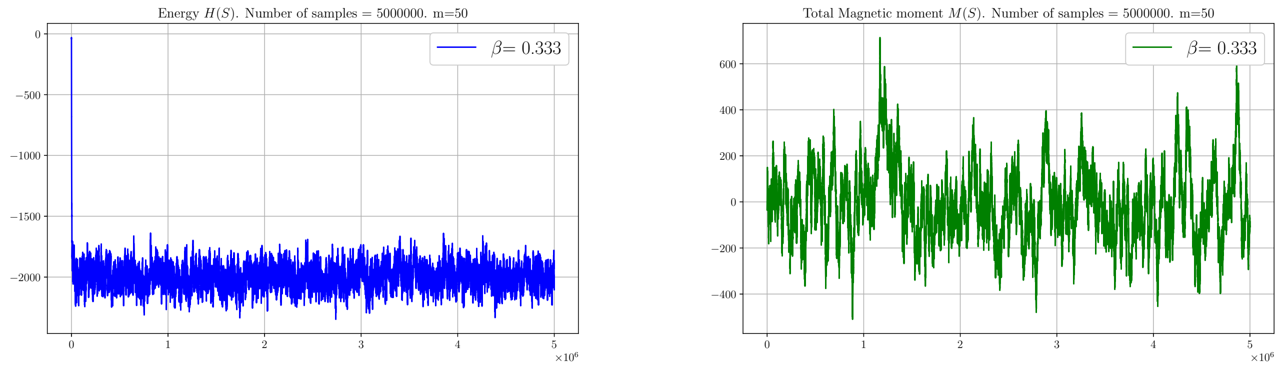
(b) Total magnetic moment $M(\boldsymbol{S})$.

Figure 2: Results for $m = 50, \beta = 1$.



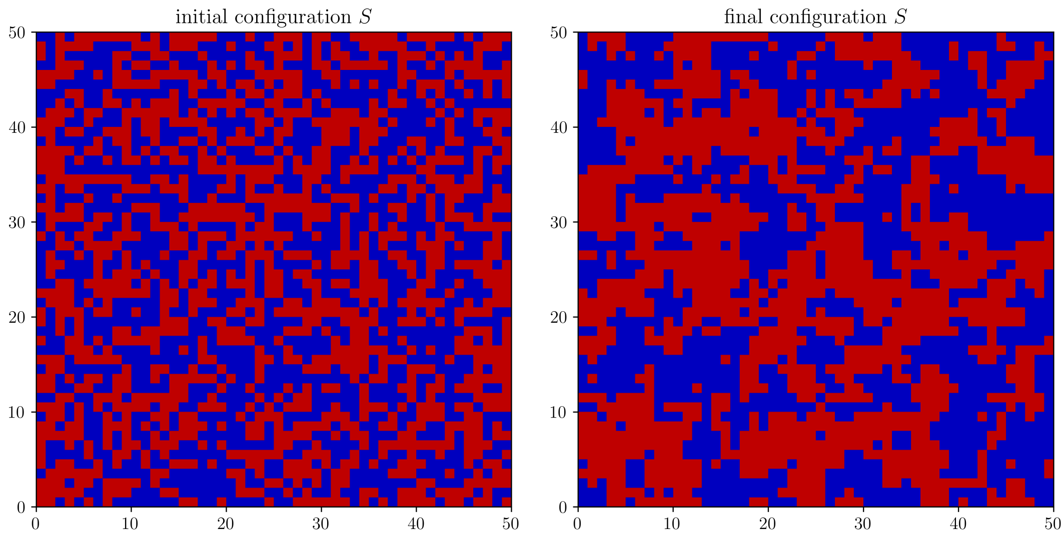
(a) Initial $\boldsymbol{S}$. (b) Final $\boldsymbol{S}$.

Figure 3: Initial and final $\boldsymbol{S}, \beta = 1$.



(a) Energy $H(\boldsymbol{S})$. (b) Total magnetic moment $M(\boldsymbol{S})$.

Figure 4: Results for $m = 50, \beta = 1/3$.



(a) Initial $\boldsymbol{S}$. (b) Final $\boldsymbol{S}$.

Figure 5: Initial and final $\boldsymbol{S}, \beta = 1/3$.

We observed that if $\beta = 1$ the final configuration is more polarized towards to either 1 or -1. On the contrary, when $\beta = 1/3$, the final configuration of our system is more homogeneous.

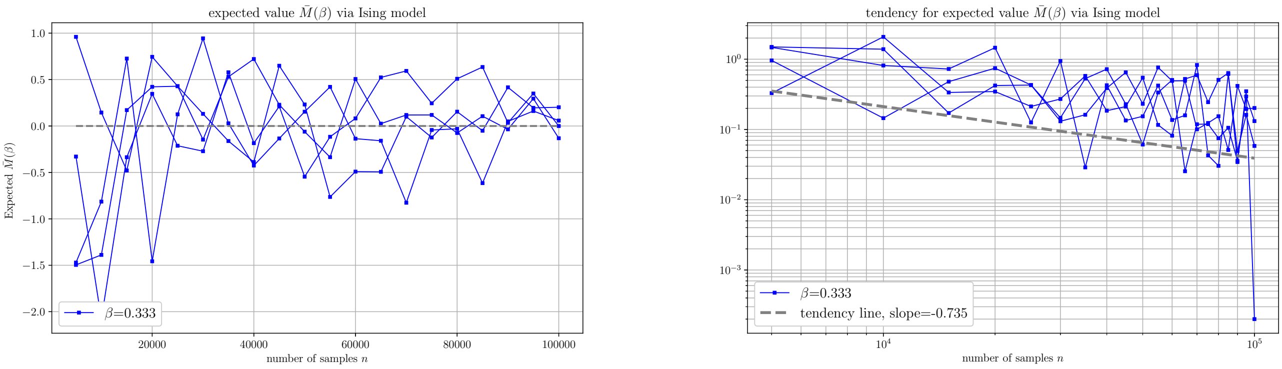
3. As stated in the problem sheet, we compute Z_β for the following parameters: $m = 4, J = 1, B = 0, \beta = \frac{1}{3}$.

   From equation (3), we can see that even if the number of atoms in the lattice is really small ($m = 4$), we must compute 2^{16} distinct configurations $\boldsymbol{S}$, which means we evaluate (3) for 65536 different $\boldsymbol{S}$. This is why computing the exact value is computationally expensive. Furthermore, we must evaluate our function $H(\boldsymbol{S})$ for each of these different configurations.

   Consequently, by using (3), we obtained $Z_\beta = 270990.1904$.

   Taking this, using (3), the expected total moments reads: $\bar{M}(\beta) = 2.14796 \times 10^{-16} \approx 0$.

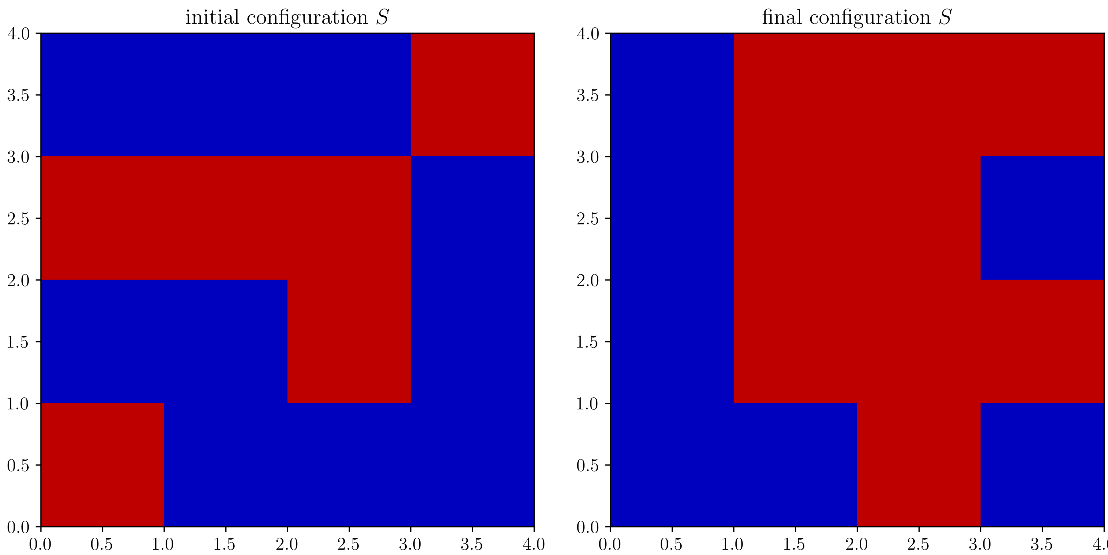
   When using the Ising model, we ran our algorithm 4 times for $n = 5000...100000$ each, which gives the following plots:



(a) Expected value for 4 runs $\bar{M}(\boldsymbol{S})$. (b) Tendency for $\bar{M}(\boldsymbol{S})$ to the true value.

Figure 6: Results for $m = 4$.

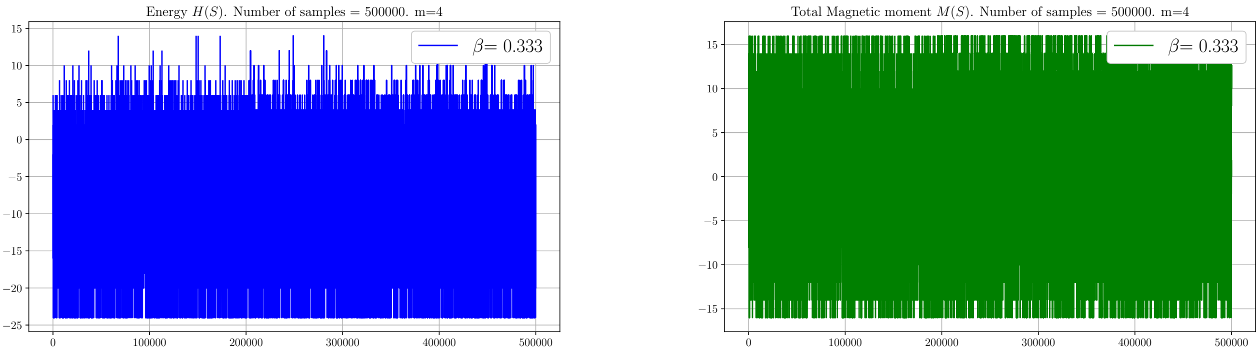
The initial and final $\boldsymbol{S}$ are given as:



(a) Initial $\boldsymbol{S}$ (b) Final $\boldsymbol{S}$

Figure 7: Initial and final $\boldsymbol{S}$, $m = 4$.

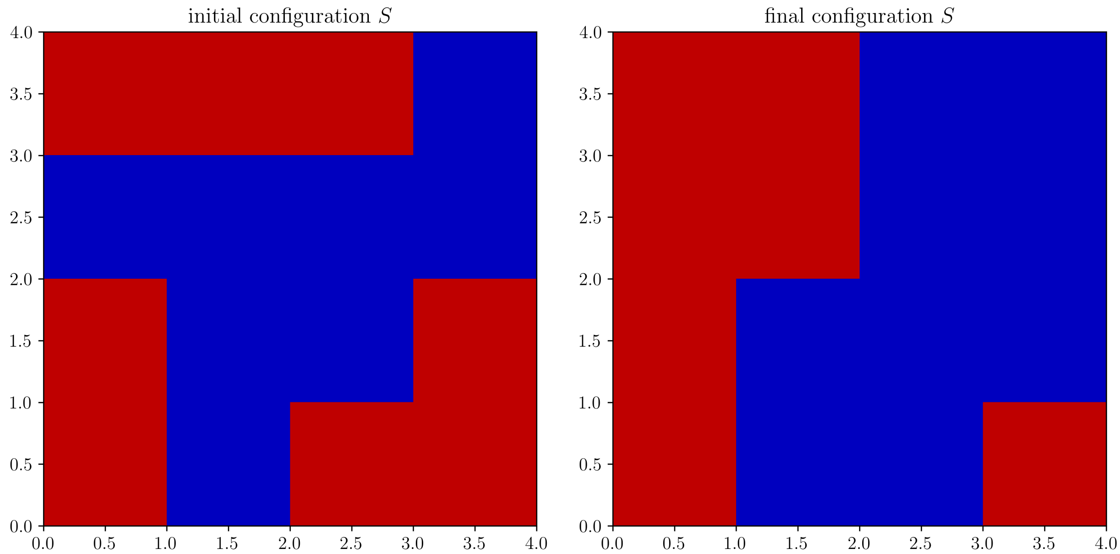
For a single run with $n = 500000$, we obtained the following plots:



(a) Energy $H(\boldsymbol{S})$.

(b) Total magnetic moment $M(\boldsymbol{S})$.

Figure 8: Results for $m = 4$, single run.



(a) Initial $\boldsymbol{S}$

(b) Final $\boldsymbol{S}$

Figure 9: Initial and final $\boldsymbol{S}$, $m = 4$, single run.

To estimate the convergence to the true $\bar{M}(\boldsymbol{S})$ as a function of the number of samples n, we computed the equation in logarithmic scale of the dashed line in (6). Then, we solved for the vertical axis equals 10^{-16}. From this and from picture (6), we observe that we will need approximately $n = 10^7$ samples to obtain the exact values of $\bar{M}(\beta)$. This is computationally expensive. In the same figure, we see that the $\bar{M}(\beta)$ is around 0.

From these plots, we see that the total expected magnetic moment computed via the Ising model is close to zero. Nevertheless, the rate of convergence is slow, as given by the slope in figure (6).

As the exact value for $\bar{M}(\boldsymbol{S})$ is really close to 0, we would need infinity number of samples to obtain the true value via the Ising model.

Regarding point 2, for example, if a change in energy from one state to another is negative, the change in energy is positive, then the system will state at the same configuration. As a consequence, the initial configuration of the system has a great effect on the system's evolution.

Besides, the initial states are randomly chosen. This randomness can originate that at the very beginning of the simulation, the matrix $\boldsymbol{S}$ is filled with many -1's or vice-versa, or can have one half of each.

We observed that the final state $\boldsymbol{S}$ is clearly divided into one zone with all 1's and the other with -1's when $\beta = 1$. On the other hand, when $\beta = 1/3$, $\boldsymbol{S}$ could be a mixture of 1's and -1's. This is due to the physical properties of the system itself and the effect of β on it.

From figures (2) to (5), we see that the value of energy $H(\boldsymbol{S})$ stabilizes or is around a specific number, which presents a random behavior. The sing of the final total magnetic moment is random too. This means that we can have a final state $\boldsymbol{S}$ filled with -1 and, after running our code once again, we could get a $\boldsymbol{S}$ filled with 1. This is the case when β is close to 1. In this case, when we could state that the system is much more polarized in its final configuration. When $\beta = 1/3$ the magnetic moments looks like having a homogeneous distribution around the final value.

What one can do is, first, to run the code and take the value for which the physical quantities tends to be at a stable state. Afterwards, we can use this values of n as a starting point for a second simulation.

Finally, for point 3, the results computed via the Ising model converged to zero as n gets larger, but with a slow tendency.