Stochastic Simulation
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Week of 2025-11-17 to 2025-11-21

Lab 10 of Thursday 20th November 2025

We recall some concepts on the theory of Markov chains on a discrete state space X.

Irreducibility

Let P be be a transition matrix on X. We say that a state $x_i \in X$ communicates with a state $x_j \in X$ if $\mathbb{P}(X_n = x_j, \text{ for some } n \mid X_0 = x_i) > 0$; equivalently, if $\exists n \geqslant 0$ such that $P_{i,j}^{(n)} > 0$. A Markov chain is *irreducible* if every state x_j communicates with every other state x_i, i.e.,

$$\forall i, j, \quad \exists n \geqslant 0 \text{ such that } P_{i,j}^{(n)} > 0.$$

Recurrence

A state $x_i \in X$ is *recurrent* if $\mathbb{P}(X_n = x_i \text{ infinitely often }) = 1$, that is, x_i is visited infinitely-often with probability 1. A Markov chain $\{X_n\}$ is recurrent if every state is recurrent. It is known that every irreducible recurrent Markov chain $\{X_n\}$ on a discrete state space has a (not necessarily finite) invariant distribution π that is unique up to a multiplicative constant. However, if the state space is *finite*, every irreducible Markov chain $\{X_n\}$ is recurrent and has a unique invariant probability distribution.

Aperiodicity

The *period* of a state x_i is the largest integer d satisfying the following property: $P_{i,i}^{(n)} = 0$, whenever n is not divisible by d. The period of x_i is given by $d(i)$. We say that if $d(i) > 1$, then the state x_i is *periodic*. We say that the state x_i is *aperiodic* otherwise. If a Markov chain $\{X_n\}$ is irreducible and has an aperiodic state, then all states are aperiodic, in which case we say that $\{X_n\}$ is aperiodic. In particular, an irreducible Markov chain $\{X_n\}$ is aperiodic if there exists a state $x_j \in X$ such that $P_{jj} > 0$. It is known that an irreducible Markov chain $\{X_n\}$ on a *finite* state space X converges to π, i.e., $\pi_j = \lim_{n\to\infty} \mathbb{P}(X_n = x_j)$, $x_j \in X$, if and only if $\{X_n\}$ is aperiodic.

Exercice 1.

A random walk on the integers $I = \{0, 1, 2 \dots\}$ can be constructed in the following way. For $0 < p < 1/2$, let $Y_0, Y_1, \dots$ be i.i.d random variables with $P(Y_i = 1) = p$ and $P(Y_i = -1) = 1 - p$. Define two random walks as (1) $X_n = \max\{X_{n-1} + Y_n, 0\}$ and (2) $Z_n = |Z_{n-1} + Y_n|$.

1) Show that (X_n) and (Z_n) are Markov chains.

2) Show that an invariant measure of the chains (X_n) and (Z_n) is given by

$$\hat{\pi} = \left[1, \left(\frac{p}{1-p}\right), \dots, \left(\frac{p}{1-p}\right)^k, \dots\right] a_0, \quad k \geqslant 0$$
$$\bar{\pi} = \left[1, \frac{1}{1-p}, \frac{p}{(1-p)^2}, \dots, \frac{p^{k-1}}{(1-p)^k}, \dots\right] b_0, \quad k \geqslant 1,$$

respectively. Find a_0, b_0 such that the expressions above are probability distributions.

3) Let $p = 1/8$. Assess numerically the convergence of both Markov chains to their invariant distribution by simulating multiple (independent) chains of length $n = 100$, each starting in 0 (i.e. $\lambda = \delta_0$). That is, plot the empirical distribution of X_n, Z_n vs $\hat{\pi}$ and $\bar{\pi}$, respectively. Repeat your experiments for $m = n + 1$. Explain your results.

4) Discuss the periodicity of both chains.

Solution

1. This follows from the definition of Markov chain, since X_{n+1} only depends on X_n. Thus,

$$\mathbb{P}(X_{n+1} = x_{n+1} | X_1 = x_1, \dots, X_n = x_n) = \mathbb{P}(X_{n+1} = x_{n+1} | X_n = x_n).$$

2. Recall that π is an invariant distribution of a Markov chain with transition matrix P if

$$\pi P = \pi.$$

Thus, we will verify this for our case. Consider the two Markov transition matrices P and Q given by

$$P = \begin{pmatrix} 1-p & p & 0 & 0 & 0 & \dots \\ 1-p & 0 & p & 0 & 0 & \ddots \\ 0 & 1-p & 0 & p & \ddots & \ddots \\ 0 & 0 & 1-p & \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}, \quad Q = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \dots \\ 1-p & 0 & p & 0 & 0 & \ddots \\ 0 & 1-p & 0 & p & \ddots & \ddots \\ 0 & 0 & 1-p & \ddots & \ddots & \ddots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}, \tag{1.1}$$

where P corresponds to the transition matrix of the chain generated by $X_{n+1} = \max\{0, X_n + Y\}$ and Q corresponds to that of $Z_{n+1} = |Z_n + Y|$. We will show that to P and Q there correspond invariant distributions

$$\hat{\pi} = \left[1, \left(\frac{p}{1-p}\right), \dots, \left(\frac{p}{1-p}\right)^k, \dots\right] a_0, \quad k \geqslant 0,$$
$$\bar{\pi} = \left[1, \frac{1}{1-p}, \frac{p}{(1-p)^2}, \dots, \frac{p^{k-1}}{(1-p)^k}, \dots, \right] b_0, \quad k \geqslant 1.$$

respectively. We begin with P. For simplicity, denote the $i-$th column of P by P_i. Notice that for P_1, we have $\hat{\pi}P_1 = [(1-p) + (1-p)p/(1-p)]a_0 = a_0 = \hat{\pi}_1$. Moreover, for the $k-$th column we have

$$\hat{\pi}P_k = \hat{\pi}_{k-1}P_{k-1,k} + \hat{\pi}_{k+1}P_{k+1,k} = p\left(\frac{p}{1-p}\right)^{k-1} a_0 + (1-p)\left(\frac{p}{1-p}\right)^{k+1} a_0$$
$$= \left(p + \frac{p^2}{1-p}\right)\left(\frac{p}{1-p}\right)^{k-1} a_0 = \left(\frac{p - p^2 + p^2}{1-p}\right)\left(\frac{p}{1-p}\right)^{k-1} a_0 = \left(\frac{p}{1-p}\right)^k a_0 = \hat{\pi}_k, \tag{1.2}$$

and as such, the chain with transition matrix P is invariant with respect to $\hat{\pi}$.

As for Q, we have that for Q_1, $\bar{\pi}Q_1 = (1-p)/(1-p)b_0 = b_0$, for Q_2, we have $\bar{\pi}Q_2 = b_0 + p/(1-p)b_0 = \bar{\pi}_2$. Moreover, for Q_k, $k > 2$, we have

$$\begin{aligned}
\bar{\pi}Q_k &= \bar{\pi}_{k-1}p + \bar{\pi}_{k+1}(1-p) \\
&= p\frac{p^{k-2}}{(1-p)^{k-1}}b_0 + (1-p)\frac{p^k}{(1-p)^{k+1}}b_0 \\
&= \frac{p^{k-1}}{(1-p)^{k-1}}b_0 + \frac{p^k}{(1-p)^k}b_0 \\
&= \frac{p^{k-1}}{(1-p)^k}b_0 = \bar{\pi}_k
\end{aligned}$$

which implies that $\bar{\pi}$ is an invariant distribution for the Markov chain with transition matrix Q.

Notice that for both chains to be probability distributions, the sum of the components of $\hat{\pi}$ and $\bar{\pi}$ must add to 1. On the case of $\bar{\pi}$, and a_0 must be chosen such that

$$a_0 \sum_{k=0}^{\infty} \left(\frac{p}{1-p}\right)^k = 1.$$

Notice that the previous sum is finite if $p/(1-p) < 1$, which occurs for any $p < 1/2$. In turn, it can be shown that (by computing the value of the previous geometric series) in this case, the normalization constant is

$$a_0 = \frac{1-2p}{1-p}.$$

A similar approach can be applied to Q to obtain

$$b_0 = \frac{1-2p}{2-2p}. \tag{1.3}$$

3/4. Python code is attached. We repeat our experiments $N = 10000$ times starting at $X_0 = Z_0 = 0$. Figure 1 shows the empirical CDF of X_n (left) and Z_n (right) for $n = 100$ and $n = 101$. As we can see, the chain with transition matrix P converges to its invariant distribution, while the one with transition matrix Q does not. This is due to the chain with transition matrix Q not being aperiodic; notice that if the chain is at state 0, the chain will move to state 1 with probability 1 and only returns to 0 after an even number of steps.

Python code

```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import rc

np.random.seed(42)

#-------------------------------------
rc('font',**{'family':'serif','serif':['Computer Modern Roman'],
     'size' : '12'})
rc('text', usetex=True)
rc('lines', linewidth=2)
plt.rcParams['axes.facecolor']='w'
```

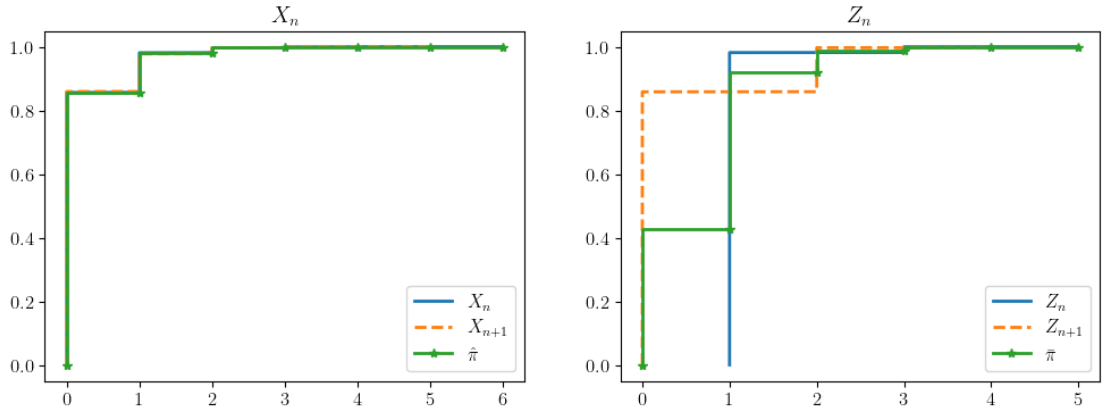

Figure 1: Empirical CDF of X_n (left) and Z_n (right) estimated from 10000 independent runs. As we can see, the process X_n converges to the true distribution, whilst Z_n does not. this is due to the periodicity of Z_n.

```
import matplotlib
latex_preamble = r'\usepackage{amsmath} \usepackage{amssymb}'
matplotlib.rcParams.update({
    'text.usetex': True,
    'text.latex.preamble': latex_preamble
})
#-----------------------------------------------
def chain1(n):
    xn=np.zeros(n)
    for i in range(n-1):
        u=np.random.random(1)
        if u <p:
            a=1
        else:
            a=-1
        xn[i+1]= np.max((xn[i] + a,0))
    return xn

def chain2(n):
    zn=np.zeros(n)
    for i in range(n-1):
        u=np.random.random(1)
        if u <p:
            a=1
        else:
            a=-1
        zn[i+1]= np.abs(zn[i] + a)
    return zn

#computes empirical cdf
def ecdf(data):
    """ Compute ECDF """
    x = np.sort(data)
    n = x.size
    y = np.arange(1, n+1) / n
    return(x,y)

#computes pi hat
def true_cdf_1(K,p):
```

```
    a0=(1-2*p)/(1-p) #this is the normalization constant
    pi_hat=(p/(1-p))**np.arange(K)*a0
    return pi_hat

#computes pi bar
def true_cdf_2(K,p):
    r=p/(1-p)
    b0=1/(1+(1/p)*(r/(1-r))) #this is the normalization constant
    print(b0)
    print(1/(1+1/(1-2*p)))
    pi_hat=(1/p)*(p/(1-p))**np.arange(1,K)*b0
    return np.concatenate([[b0],pi_hat])

n=100
p=1/8

N=10000
m1=np.zeros(N)
m2=np.zeros(N)
m3=np.zeros(N)
m4=np.zeros(N)
for i in range(N):
    m1[i]=chain1(n)[-1]
    m2[i]=chain1(n+1)[-1]
    m3[i]=chain2(n)[-1]
    m4[i]=chain2(n+1)[-1]

# computes empirical distribution
x1,e1=ecdf(m1)
x2,e2=ecdf(m2)
x3,e3=ecdf(m3)
x4,e4=ecdf(m4)

# computes the CDF for Xn
K1=np.max(x1) #highest value obtained
pi_hat=true_cdf_1(K1,p) #obtaines values of pi hat
cdf_pi_hat=np.cumsum(pi_hat) #computes cdf
cdf_pi_hat=np.concatenate([ [0],cdf_pi_hat]) # adds 0 for plotting

# Computes the CDF for Zn
K2=np.max([np.max(x3),np.max(x4)]) #highest value obtained
pi_bar=true_cdf_2(K2,p) #obtaines values of pi bar
cdf_pi_bar=np.cumsum(pi_bar) #computes cdf
cdf_pi_bar=np.concatenate([ [0],cdf_pi_bar]) # adds 0 for plotting

#fixes parameter for plotting
fig, axes = plt.subplots(nrows = 1, ncols = 2, figsize = (12,4))

# plots cdf of Xn
axes[0].plot(x1,e1);
axes[0].plot(x2,e2,'--');
axes[0].step(np.arange(K1+1),cdf_pi_hat,'-*')
axes[0].set_title(r'$X_n$')
axes[0].legend([r'$X_{n}$',r'$X_{n+1}$',r'$\hat{\pi}$'])

# plots cdf of Zn
axes[1].plot(x3,e3);
axes[1].plot(x4,e4,'--');
axes[1].step(np.arange(K2+1),cdf_pi_bar,'-*')
axes[1].set_title(r'$Z_n$')
axes[1].legend([r'$Z_{n}$',r'$Z_{n+1}$',r'$\bar{\pi}$'])
plt.show()
```

Exercice 2.

Given the transition matrix

$$P = \begin{pmatrix} 0.0 & 0.4 & 0.6 & 0.0 & 0.0 \\ 0.65 & 0.0 & 0.35 & 0.0 & 0.0 \\ 0.32 & 0.68 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.12 & 0.88 \\ 0.0 & 0.0 & 0.0 & 0.56 & 0.44 \end{pmatrix}, \tag{2.1}$$

and examine whether the corresponding chain is irreducible and aperiodic.

Solution

Notice that from the block structure of the matrix P, the chain is not irreducible since states 4 and 5 do not communicate with states $1, 2, 3$. Aperiodicity can be checked by definition.

Exercice 3.

Let us consider a 2D uniform square-lattice with atoms placed at each vertex, as is sketched in Figure 2. The atoms can have an upward (red arrow) or a downward (blue arrow) pointing

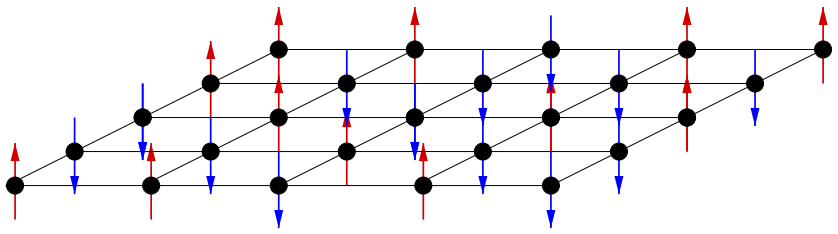

Figure 2: Sketch of 2D square-lattice Ising model.

magnetic moment (so-called *spin*). Specifically, let the lattice be made out of $m \times m$ atoms. Therefore the system's possible states are the 2^{m^2} possible spin choices for the m^2 atoms. That is, the spin of the atom at position (i, j) in the lattice is denoted with s_{ij}, $1 \leqslant i, j \leqslant m$, and can take a value in $\{-1, +1\}$. A specific system configuration is described by the matrix $S = (s_{ij}) \in \{-1, +1\}^{m \times m}$, containing the spin of each of the m^2 atoms.

The energy of a given system state of this Ising model is given by

$$H(S) = -\sum_{i,j=1}^{m} \left(\frac{1}{2} J s_{ij} (s_{i-1,j} + s_{i+1,j} + s_{i,j-1} + s_{i,j+1}) + B s_{ij} \right), \tag{3.1}$$

where J is a magnetic coupling constant and B is a constant describing the external magnetic field. To account for boundary effects, we set $s_{0,j} = s_{j,0} = s_{m+1,j} = s_{j,m+1} = 0$ in (3.1). The probability of obtaining a specific system state is then given by the *Boltzmann* distribution with Probability Mass Function (PMF)

$$f(S) \equiv f_\beta(S) = \frac{1}{Z_\beta} e^{-H(S)\beta}, \tag{3.2}$$

where $\beta = 1/(k_B T)$ denotes the so-called inverse-temperature (or thermodynamic beta) with k_B being the Boltzmann constant and T the absolute temperature. Here, Z_β denotes the normalization constant that makes the target distribution $f_\beta \colon \{-1, +1\}^{m \times m} \to \mathbb{R}_+$ a proper PMF.

Let's denote by $M(S) = \sum_{i,j=1}^{m} s_{ij}/m^2$ the system's average magnetic moment corresponding to the configuration S. Notice that the random realizations of the configuration matrix S depend on the inverse temperature β. The expected value of the average magnetic moment $\overline{M}(\beta)$ as a function of the inverse temperature β thus reads

$$\overline{M}(\beta) = \sum_{S \in \mathcal{K}} M(S) f_\beta(S) = \frac{1}{Z_\beta} \sum_{S \in \mathcal{K}} M(S) e^{-H(S)\beta} \,, \tag{3.3}$$

where $\mathcal{K} = \{-1, 1\}^{m \times m}$ is the set of all possible system configurations. Since the explicit computation of the normalization constant Z_β is computationally expensive (Explain why!), we rely on the Metropolis–Hastings algorithm here. That is, at each step a candidate configuration is proposed by randomly choosing an atom, with uniform probability, and "flipping" its spin.

1) Write a `Python` function that implements the Metropolis–Hastings algorithm for the Ising model. The input parameters for your function are: the number of steps n of the chain that should be simulated, the number of atoms m^2, the inverse temperature β, the constants J and B, and the initial state of the system. The function should return a list of energies and mean magnetic moments computed for each step of the chain, as well as the final configuration of the system.

2) Use your `Python` function with $\beta = 1/3$ and for n, such that both the energy and the average magnetic moment appear to have reached stationarity. Plot also the final system configuration. Furthermore, compute the mean magnetic moment $\overline{M}(\beta)$ for different values of $\beta \in [\frac{1}{3}, 1]$ and $n = 5 \cdot 10^6$. Choose a lattice of 50×50 atoms, $J = 1$, and $B > 0$ for all simulations.

3) Show that the Markov Chain obtained via the Metropolis-Hastings algorithm in this case is irreducible.

Solution

Notice that the energy

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

contains the products $s_{ij}s_{i-1,j}, \ldots$ twice, so that we can rewrite the energy as

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

which is more amenable for an implementation (and, in fact, used below). It is noteworthy however, that also the evaluation of the energy in this rewritten form requires $\mathcal{O}(m^2)$ operations. That is, if m is large, the evaluation is computationally expensive!

However, in the Metropolis-Hastings algorithm, we only need to evaluate the energy difference between two different states. In particular, let us denote by S the current system configuration at step n of the algorithm and by S^c the proposed candidate configuration. Due to the particular proposal structure, it follows that the only difference between S and the candidate S^c is one spin. Suppose that this difference is at the atom in position (l, k), so that

$$S = (s_{ij}), \quad S^c = (s^c_{ij}), \quad \text{with} \quad s^c_{ij} = \begin{cases} s_{ij} \,, & \text{if} \quad i \neq l, \ j \neq k \,, \\ -s_{ij} \,, & \text{if} \quad i = l, \ j = k \,. \end{cases}$$

Consequently, we can write the energy difference conveniently as

$$\begin{aligned}\Delta H(\mathbf{S},\mathbf{S}^c) = H(S^c) - H(S) &= -J(s^c_{lk} - s_{lk})(s_{l-1,k} + s_{l+1,k} + s_{l,k-1} + s_{l,k+1}) - B(s^c_{lk} - s_{lk}) \\ &= 2Js_{lk}(s_{l-1,k} + s_{l+1,k} + s_{l,k-1} + s_{l,k+1}) + 2Bs_{lk}\ ,\end{aligned}$$

which simplifies the implementation. Notice that the proposal transition matrix $Q(\mathbf{S},\mathbf{S}^*)$ is symmetric. Indeed $Q(\mathbf{S},\mathbf{S}^*) = Q(\mathbf{S}^*,\mathbf{S}) = \frac{1}{m^2}$ if $\mathbf{S}$ and $\mathbf{S}^*$ differ by only one spin and $Q(\mathbf{S},\mathbf{S}^*) = 0$ if they differ by two or more spins. Hence the Metropolis-Hastings acceptance rate becomes

$$\alpha(\mathbf{S},\mathbf{S}^c) = \min\left\{1, \frac{f(\mathbf{S}^c)Q(\mathbf{S}^c,\mathbf{S})}{f(\mathbf{S})Q(\mathbf{S},\mathbf{S}^c)}\right\} = \min\left\{1, \frac{f(\mathbf{S}^c)}{f(\mathbf{S})}\right\} = \min\{1, \exp[-\beta\Delta H(\mathbf{S},\mathbf{S}^c)]\}. \tag{3.4}$$

A possible `Python` code that uses these formulas is shown below. Figs. 3, 4, 5 and 6 show the evolution of energy and magnetic moment as well as the state configuration for $\beta = 1/3$ and $\beta = 1$ respectively. For $\beta = 1/3$, the configuration plot shows the formation of spin-up or spin-down clumps. The expected total magnetic moment is expected to be zero, and we get an estimated value of 4.17. For $\beta = 1$, the configuration plot shows a phase transition, namely that the spins all align eventually in the same direction. The absolute value of the expected total magnetic moment of the invariant distribution is 2500 in theory, and we get an estimated value of approximately 1968 since we have not excluded any burn-in time from the calculation of the mean. We use the ergodic estimator

$$\overline{M}(\beta) \approx \frac{1}{n}\sum_{k=0}^{n} M(\mathbf{S}_k), \tag{3.5}$$

where $\mathbf{S}_k$ denotes the state at the k^{th} step of the MH algorithm.

Lastly, we cover the irreducibility of the Markov Chain. Let $\mathbf{S},\mathbf{S}' \in \{-1,+1\}^{m\times m}$ be two arbitrary configurations of spins. Denote by

$$D = \{(i,j)\ :\ s_{ij} \neq s'_{ij}\}$$

the set of sites at which the two configurations differ. By flipping the spins in D one site at a time, we obtain a finite sequence of configurations

$$\mathbf{S} = \mathbf{S}^{(0)} \to \mathbf{S}^{(1)} \to \cdots \to \mathbf{S}^{(|D|)} = \mathbf{S}',$$

where each transition $\mathbf{S}^{(t)} \to \mathbf{S}^{(t+1)}$ consists of flipping exactly one spin. For a single spin flip at site (l,k), the energy difference is given by

$$\Delta H(\mathbf{S},\mathbf{S}^c) = 2Js_{lk}(s_{l-1,k} + s_{l+1,k} + s_{l,k-1} + s_{l,k+1}) + 2Bs_{lk},$$

so that $|\Delta H(\mathbf{S},\mathbf{S}^c)|$ is uniformly bounded. Hence the Metropolis acceptance probability

$$\alpha(\mathbf{S},\mathbf{S}^c) = \min\{1, \exp[-\beta\Delta H(\mathbf{S},\mathbf{S}^c)]\}$$

is strictly positive for every possible single–spin–flip move. Since the proposal kernel chooses every site with probability $1/m^2$, it follows that the transition probability

$$P(\mathbf{S},\mathbf{S}^c) = \frac{1}{m^2}\,\alpha(\mathbf{S},\mathbf{S}^c) > 0$$

whenever $\mathbf{S}$ and $\mathbf{S}^c$ differ by exactly one spin, which concludes the proof as the probability of moving from $\mathbf{S}$ to $\mathbf{S}'$ in finitely many steps is hence strictly positive. **Python code**

```
import numpy as np

def ising(n, m, beta, J, B, S0):
    # Allocate vectors derived from a system's state
    E = np.zeros(n+1)
    M = np.zeros(n+1)

    # Initialize system
    S = S0
    # Magnetic moment associated with the initial condition
    M[0] = S.sum()
    # Energy associated with the initial condition
    E[0] = - J * ( (S[:,:m-1] * S[:,1:]).sum() + (S[:m-1,:]*S[1:,:]).sum() ) - B * M[0]

    for k in range(n):
        # PROPOSAL : generate candidate state
        Sc = S.copy()
        # select randomly an atom on the lattice
        i = int( np.floor(m * np.random.random()) )
        j = int( np.floor(m * np.random.random()) )
        Sc[i,j] = - S[i,j] # flip the spin

        # Change in magnetic moment due to this flip
        dM = - 2 * S[i,j]

        # Change in the energy due to this flip
        dE = 0
        if i>0:
                dE = dE + S[i-1,j]
        if i < m-1:
                dE = dE + S[i+1,j]
        if j>0:
                dE = dE + S[i,j-1]
        if j<m-1:
                dE = dE + S[i,j+1]

        dE = 2*S[i,j]*(J*dE + B)

        # ACCEPT-REJECT STEP
        alpha = np.min([np.exp(-dE*beta),1])
        U = np.random.random()
        if U < alpha:
                S = Sc # Accept proposed candidate state
        else:
                dM = 0
                dE = 0

        # Update energy and magnetic moment
        E[k+1] = E[k] + dE
        M[k+1] = M[k] + dM

    return E, M, S
```

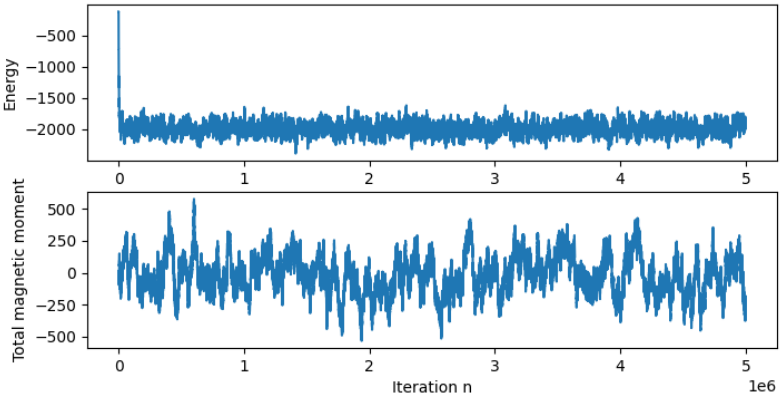

Figure 3: Evolution of energy and magnetic moment for $\beta = 1/3$.

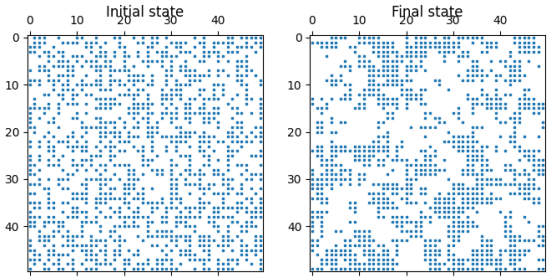

Figure 4: Snapshots of the configuration for $\beta = 1/3$.

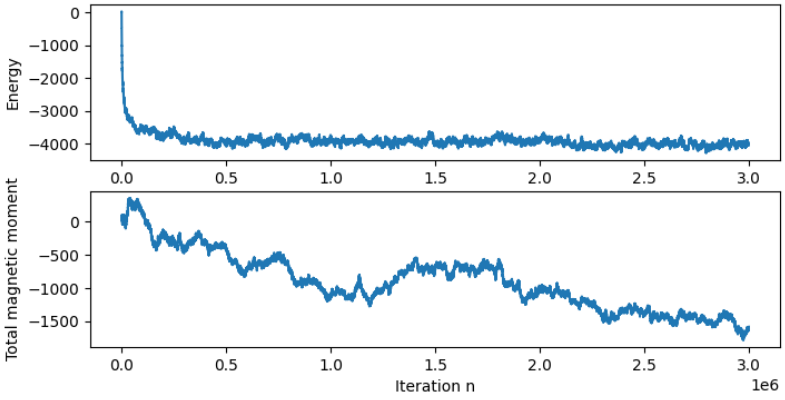

Figure 5: Evolution of energy and magnetic moment for $\beta = 1$.

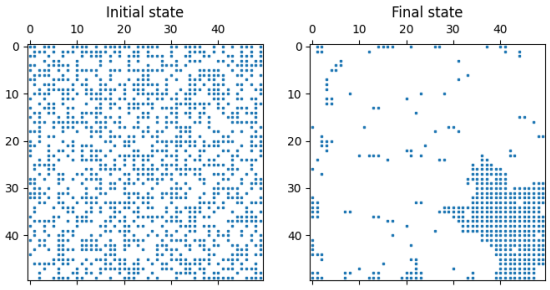

Figure 6: Snapshots of the configuration for $\beta = 1$.

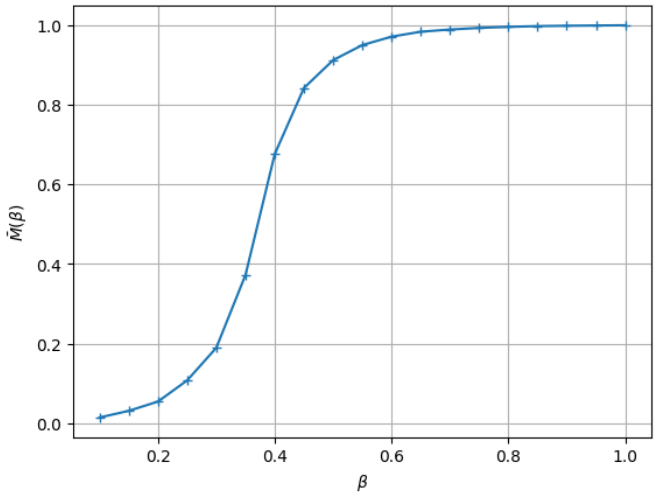

Figure 7: Mean magnetization versus β for $B = 0.1$

Exercice 4.

Consider a Random Walk $(X_n)_n$ on the integers $\mathbb{Z} = \{0, \pm 1, \pm 2, \dots\}$ with transition probabilities given by

$$\mathbb{P}(X_{n+1} = i + 1 | X_n = i) = p, \quad \mathbb{P}(X_{n+1} = i - 1 | X_n = i) = q = 1 - p,$$

where $0 < p < 1$. Address the following points.

1) Show that the chain is irreducible.

2) Conclude for each value of p if the chain is recurrent or transient by computing $\mathbb{E}(V_0)$, where V_0 denotes the number of visits of the state 0. (*Hint*: use Stirling's approximation $n! \sim (n/e)^n \sqrt{2\pi n}$.)

Now consider a symmetric Random Walk on $\mathbb{Z}^2$ with

$$\mathbb{P}(X_{n+1} = (i \pm 1, j)|X_n = (i, j)) = \mathbb{P}(X_{n+1} = (i, j \pm 1)|X_n = (i, j)) = \frac{1}{4}.$$

Address the following points.

3) Show that the chain is irreducible.

4) Conclude that the chain is recurrent by computing $\mathbb{E}(V_0)$, where V_0 denotes the number of visits of the state $(0, 0)$. (*Hint*: use the identity $\binom{2n}{n} = \sum_{i=0}^{n} \binom{n}{i}\binom{n}{n-i}$ and Stirling's approximation.)

Solution

1) Given two states $i < j \in \mathbb{Z}$ there exists the path which visits $i, i+1, \dots, j$ that has probability $p^{j-i} > 0$, so that $P_{ij}^{(j-i)} > 0$. Similarly, we can consider the path $i, i-1, \dots, j$ with probability $(1-p)^{j-i} > 0$ and conclude that $P_{ji}^{(j-i)} > 0$. Finally, for all $i \in \mathbb{Z}$, $P_{ii}^{(2)} > 0$ since the chain can jump to $i+1$ and back with probability $p(1-p) > 0$.

2) Denote $P_{ij}^{(n)}$ the probability of going from state i to state j in n steps. It is clear that the chain cannot come back to the state 0 in an odd number of steps, that is $P_{00}^{(2n-1)} = 0$ for $n = 1, 2, \dots$. On the other hand, in $2n$ steps the chain can come back to zero if and only if n of them are up, and the other n are down, in any order. Then, the probability of returning to zero in $2n$ steps is given by the binomial formula

$$P_{00}^{(2n)} = \binom{2n}{n} p^n q^n \sim \frac{(4pq)^n}{\sqrt{\pi n}}, \tag{4.1}$$

where we used Stirling's approximation. Hence, $\sum_{n=1}^{\infty} P_{00}^{n}$ will converge if and only if

$$\sum_{n=1}^{\infty} \frac{(4pq)^n}{\sqrt{\pi n}}$$

does. Now, $4pq \leqslant 1$ with equality if and only if $p = q = 1/2$. Hence, the chain is recurrent when $p = 1/2$ and transient if $p \neq 1/2$.

3) With a similar argument to the one in point (i), it is easy to show that the chain is irreducible.

4) The chain is recurrent if and only if the state $(0, 0)$ is. Now, after $2n$ steps, the chain will back in its original location if for some i, $0 \leqslant i \leqslant n$, the $2n$ steps consist in i steps to the left, i to the right, $n - i$ up, and $n - i$ down. Since each step will be either of these four types with probability $1/4$, it follows that the desired probability is a multinomial probability.

That is,

$$\begin{aligned} P_{00}^{(2n)} &= \sum_{i=0}^{n} \frac{(2n)!}{i!i!(n-i)!(n-i)!} \left(\frac{1}{4}\right)^{2n} \\ &= \sum_{i=0}^{n} \frac{(2n)!}{n!n!} \frac{n!}{i!(n-i)!} \frac{n!}{i!(n-i)!} \left(\frac{1}{4}\right)^{2n} \\ &= \left(\frac{1}{4}\right)^{2n} \binom{2n}{n} \sum_{i=0}^{n} \binom{n}{i} \binom{n}{n-i} \\ &= \left(\frac{1}{4}\right)^{2n} \binom{2n}{n} \binom{2n}{n}, \end{aligned}$$

where we used the combinatorial identity given in the hint. Now, using Stirling's approximation we have that

$$\binom{2n}{n} \sim \frac{4^n}{\sqrt{\pi n}},$$

so that

$$P_{00}^{(2n)} \sim \frac{1}{\pi n},$$

which shows that $\sum_n P_{00}^{(2n)} = \infty$, and thus the chain is recurrent.

Interestingy enough, even though the symmetric random walks in one and two domensions are recurrent, all high-dimensional (three or more) symmetric random walks turn out to be transient.