Ising Monte Carlo Simulation

May 21, 2022

[42]:
```
%matplotlib inline

import numpy as np
import matplotlib.pyplot as plt
plt.style.use(['science','notebook', 'grid'])
import numba
from numba import jit
from scipy.ndimage import convolve, generate_binary_structure
```

0.1 1. neg_lattice, pos_lattice = simulation_inputs()

0.1.1 fixes initialisation from system size, algorithmic time steps and random probability of up or down-ness

[219]:
```
# Global variables and Initialisation

def simulation_inputs():

    N = int(input("\n Enter the square system size: "))           # square␣
 ↪system size
    M = int(input("\n Enter the number of algorithm steps: "))    # Algorithm␣
 ↪time step
    R = .75                             # random probabiliy to initialise the␣
 ↪state


    init_random = np.random.random((N,N))     # A random N x N lattice is␣
 ↪initialised
    lattice_n = np.zeros((N, N))              # lattice of desire is N x N␣
 ↪matrix of Os

    lattice_n[init_random>=R] = 1             # If a site has greater value than␣
 ↪R in random initial state, put 1 or -1 otherwise
    lattice_n[init_random<R] = -1

    init_random = np.random.random((N,N))     # Likely construst a lattice with␣
 ↪equal random likelihood but with different majority
```

```
    lattice_p = np.zeros((N, N))
    lattice_p[init_random<=R] = 1
    lattice_p[init_random>R] = -1

    print("\n \n System of size ", N**2, " with randomness of ", R, "has been␣
 ↪initialised where simulation will run for ", M, "steps")

    return lattice_n, lattice_p, N, M, R
```

[208]:
```
n,p, N, M, R = simulation_inputs()


# n = negative lattice

# p = positive lattice

# N = square system's size

# M = Algorithm steps

# R = Random uniform distribution of spins as initial state
```

```
 Enter the square system size: 50

 Enter the number of algorithm steps: 100000


 System of size  2500  with randomness of  0.75 has been initialised where
simulation will run for  100000 steps
```

0.2 2. get_energy ()

0.2.1 returns value of energy of a certain configuration

[220]:
```
def get_energy(lattice):   # returns energy given a configuration [The␣
 ↪Hamiltonian function]

    kern = generate_binary_structure(2, 1)
    kern[1][1] = False
    arr = -lattice * convolve(lattice, kern, mode='constant', cval=0) # applies␣
 ↪the nearest neighbours summation
    return arr.sum()
```

0.3 3. spins, energies = metropolis (lattice, algo_timeStep, βJ, get_energy())

0.3.1 Runs the initial state towards equilibriation by

A. Randomly flipping one spin

B. Calculating corresponding energy value of the lattice

C. If energy is same or lower, directly accept the state, but if not accept with Boltzmannian weightage of their energy difference

D. Repeat to step A untill M number of iterations has been made

[210]:
```
@numba.jit("UniTuple(f8[:], 2)(f8[:,:], i8, f8, f8)", nopython=True, nogil=True)
def metropolis(spin_arr, times, BJ, energy):
    spin_arr = spin_arr.copy()
    net_spins = np.zeros(times-1)
    net_energy = np.zeros(times-1)
    for t in range(0,times-1):
        # 2. pick random point on array and flip spin
        x = np.random.randint(0,N)
        y = np.random.randint(0,N)
        spin_i = spin_arr[x,y] #initial spin
        spin_f = spin_i*-1 #proposed spin flip

        # compute change in energy
        E_i = 0
        E_f = 0
        if x>0:
            E_i += -spin_i*spin_arr[x-1,y]
            E_f += -spin_f*spin_arr[x-1,y]
        if x<N-1:
            E_i += -spin_i*spin_arr[x+1,y]
            E_f += -spin_f*spin_arr[x+1,y]
        if y>0:
            E_i += -spin_i*spin_arr[x,y-1]
            E_f += -spin_f*spin_arr[x,y-1]
        if y<N-1:
            E_i += -spin_i*spin_arr[x,y+1]
            E_f += -spin_f*spin_arr[x,y+1]

        # 3 / 4. change state with designated probabilities
        dE = E_f-E_i
        if (dE>0)*(np.random.random() < np.exp(-BJ*dE)):
            spin_arr[x,y]=spin_f
            energy += dE
        elif dE<=0:
            spin_arr[x,y]=spin_f
            energy += dE
```

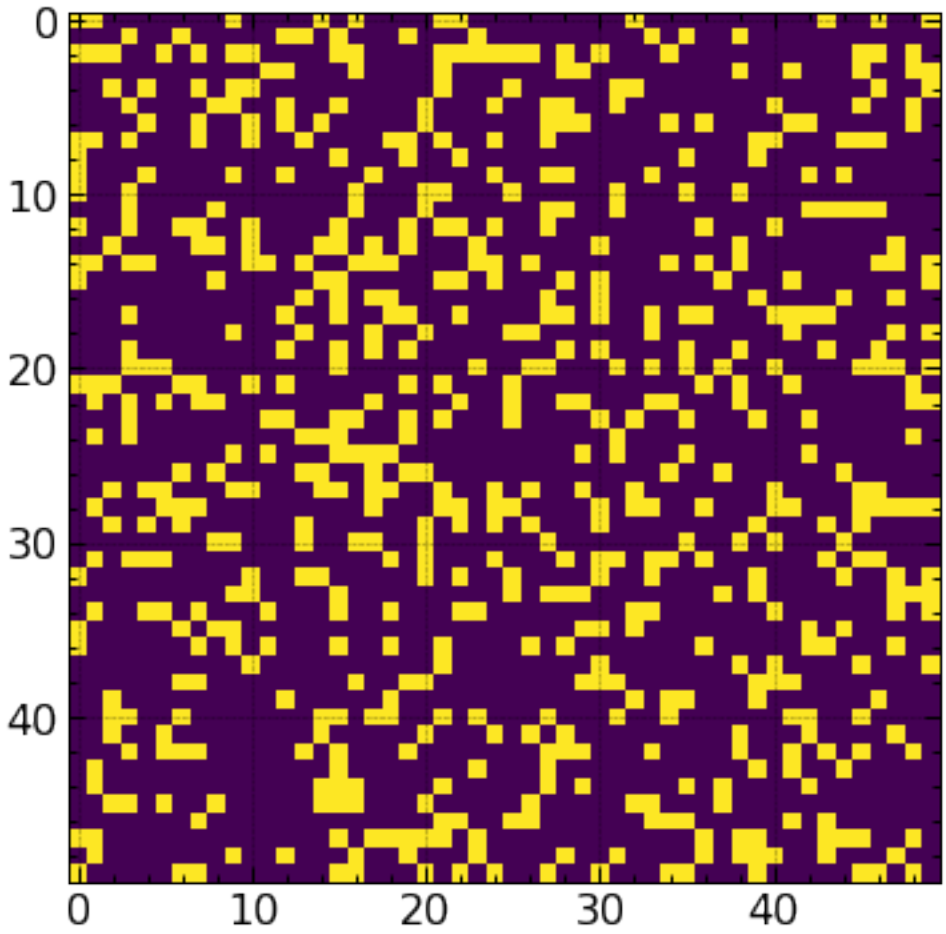
```
        net_spins[t] = spin_arr.sum()
        net_energy[t] = energy

    return net_spins, net_energy
```

All necessaryy functions are defined so we can start working with the functions

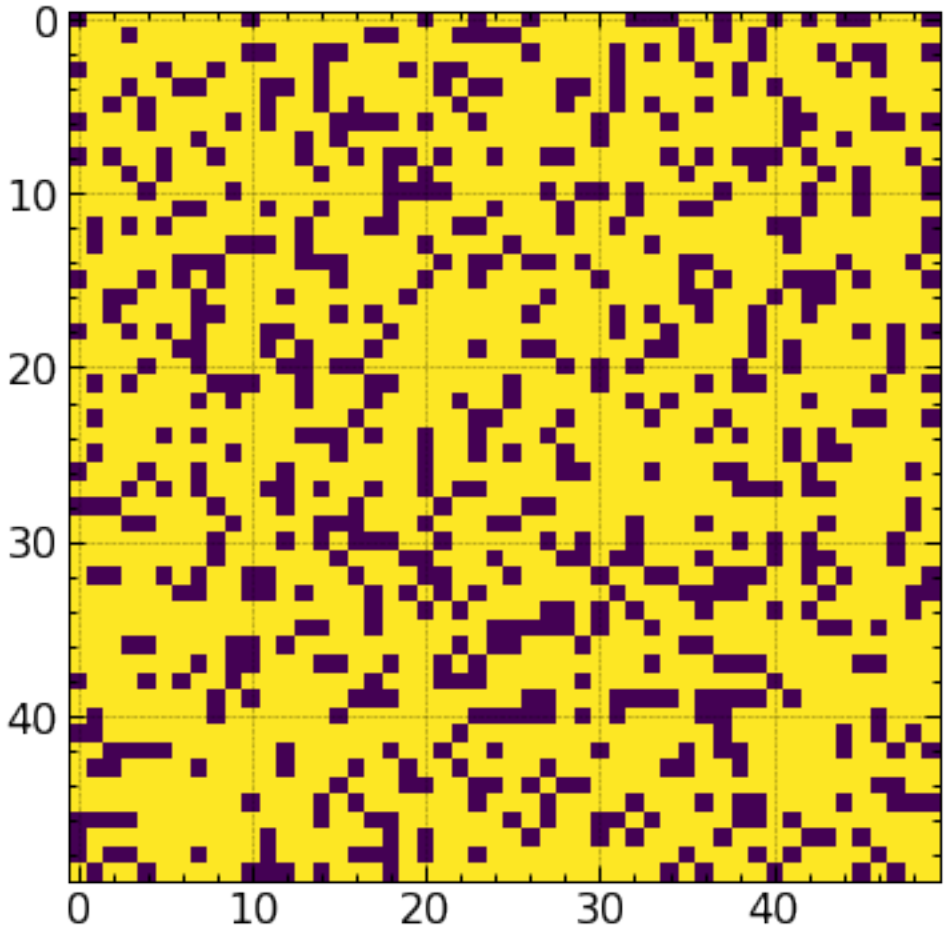
[224]:
```
plt.imshow(n)
```

[224]: <matplotlib.image.AxesImage at 0x7f0c23e56160>



[225]:
```
plt.imshow(p)
```

[225]: <matplotlib.image.AxesImage at 0x7f0c238b93d0>



[213]:
```
spins, energies = metropolis(n, M, .10, get_energy(n))    # assigning two lists␣
↪returning values of equilibriating state's information
```

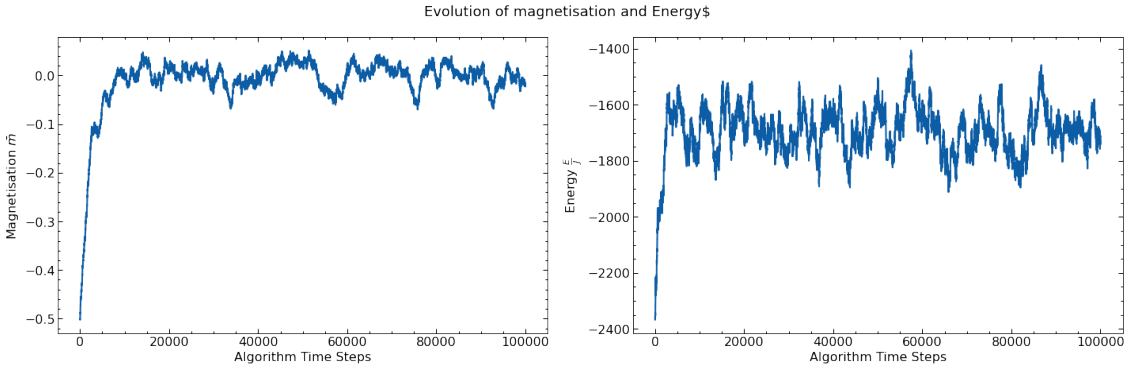
[214]:
```
%time metropolis(p, M, 0.5, get_energy(p))  # estimate time of computation
```

```
CPU times: user 376 ms, sys: 3.98 ms, total: 380 ms
Wall time: 383 ms
```

[214]:
```
(array([1232., 1232., 1234., …, 2076., 2076., 2076.]),
 array([-2320., -2320., -2324., …, -5216., -5216., -5216.]))
```

[215]:
```
fig, axes = plt.subplots(1, 2, figsize=(20,6))
ax = axes[0]
ax.plot(spins/N**2)
ax.set_xlabel('Algorithm Time Steps')
ax.set_ylabel(r'Magnetisation $\bar{m}$')
ax.grid()
ax = axes[1]
```

```
ax.plot(energies)
ax.set_xlabel('Algorithm Time Steps')
ax.set_ylabel(r'Energy $\frac{E}{J}$')
ax.grid()
fig.tight_layout()
fig.suptitle(r'Evolution of magnetisation and Energy$', y=1.07, size=18)
plt.show()
```



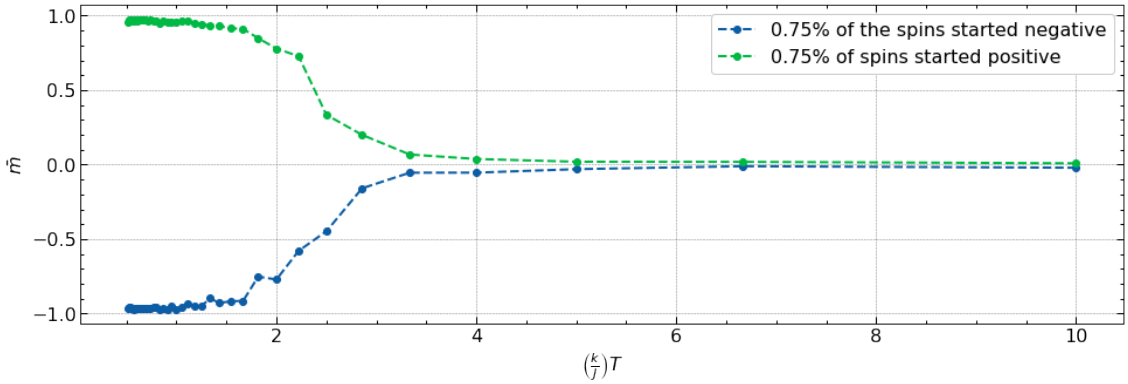
[216]:
```
def get_spin_energy(lattice, BJs):
    ms = np.zeros(len(BJs))
    E_means = np.zeros(len(BJs))
    E_stds = np.zeros(len(BJs))
    for i, bj in enumerate(BJs):
        spins, energies = metropolis(lattice, M, bj, get_energy(lattice))
        ms[i] = spins[-M:].mean()/N**2
        E_means[i] = energies[-M:].mean()
        E_stds[i] = energies[-M:].std()
    return ms, E_means, E_stds
```

[217]:
```
BJs = np.arange(0.1, 2, 0.05) # Setting temperature range and spacing in␣
 ↪simulation
```

[221]:
```
ms_n, E_means_n, E_stds_n = get_spin_energy(n, BJs)
ms_p, E_means_p, E_stds_p = get_spin_energy(p, BJs)
```

[222]:
```
plt.figure(figsize=(16,5))

plt.plot(1/BJs, ms_n, 'o--', label= str(R)+'% of the spins started negative')
plt.plot(1/BJs, ms_p, 'o--', label= str(R)+'% of spins started positive')
plt.xlabel(r'$\left(\frac{k}{J}\right)T$')
plt.ylabel(r'$\bar{m}$')
plt.legend(facecolor='white', framealpha=1)
plt.show()
```



[223]:
```
plt.figure(figsize=(16,6))

plt.plot(1/BJs, E_stds_n*BJs, label=str(R)+'% of spins started negative')
plt.plot(1/BJs, E_stds_p*BJs, label=str(R)+'% of spins started positive')
plt.xlabel(r'$\left(\frac{k}{J}\right)T$')
plt.ylabel(r'$C_v / k^2$')
plt.legend()
plt.show()
```