1 Ergocity breaking

Sequential algorithm consists of choosing particles in a increasing order (and restarting to 1 when the last particle is reached). It is not considered as an efficient simulation method and is sometimes non ergodic. The non-ergodicity is associated with the fact that the dynamics cannot explore the entire phase space, which appears as a set of disconnected parts. To highlight this point, consider a one-dimensional Ising model.

1. Starting from a staggered configuration of a line of 4 spins, using a sequential algorithm with a Metropolis rule and by considering the system at an infinite temperature, draw the sequence of configurations until the system goes back to the initial configuration.

> **Solution:** At infinite temperature, the new configuration is always accepted. Starting from a staggered configuration, one has the sequence ↑↓↑↓ →↓↓↑↓ →↓↑↑↓ →↓↑↓↓ →↓↑↓↑ →↑↑↓↑ →↑↓↓↑ →↑↓↑↑ →↑↓↑↓ To go back to the initial configuration, one has 8 different configurations. The total number of configurations is equal to $2^4 = 16$. 8 configurations are missing for instance the ground-state configurations.

2. Give an example of a configuration unreachable by using the sequential algorithm when one starts from the stagerred configuration. Consider all available configurations of the system and determine the number of independent trajectories. (A trajectory corresponds to a complete sequence of spin flips of the system where the system goes back to the initial configuration).

> **Solution:** Starting from a ground state ↑↑↑↑, one has the 8 other configurations in order to return to the initial configuration. We have two different trajectories.

3. Modify the previous algorithm as follows : at each step, one has a probability α of flipping the spin i and a probability $(1-\alpha)$ of keeping the same configuration. Show that the new algorithm is ergodic if $\alpha \neq 1$.

> **Solution:** If a flip is not accepted, for instance the first one, starting from a staggered configuration, one can reach the configuration ↑↑↓↑ which is a configuration of the second trajectory. If $\alpha \neq 1$, all configurations are reachable in a single trajectory and the ergodicity is restored

2 Unit vectors

1. By using the spherical coordinates, and the inverse transformation method, show how to obtain a set of unit vectors randomy and uniformly distributed on the sphere.

Solution: The spherical coordinates are

$$x = \cos(\phi)\sin(\theta) \quad (1)$$
$$y = \sin(\phi)\sin(\theta) \quad (2)$$
$$z = \cos(\theta) \quad (3)$$

For a uniform distribution on a sphere, the différential of the distribution is given by

$$\frac{\sin(\theta)}{4\pi} d\phi d\theta \quad (4)$$

By using the change of variable $u = \cos(\theta)$ one obtains

$$\frac{1}{4\pi} d\phi du \quad (5)$$

By using a couple of random numbers uniformly distributedd (u, v) between 0 and 1 one obtains

$$z = 2v - 1 \quad (6)$$
$$x = \cos(2\pi u)\sqrt{1 - z^2} \quad (7)$$
$$y = \sin(2\pi u)\sqrt{1 - z^2} \quad (8)$$

2. Write a Python script which gives a 3D configuration of unit vectors uniformly distributed on the sphere in order to obtain a figure similar to Fig.1

Solution:

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

fig = plt.figure(figsize=(6,6))
ax = fig.gca(projection='3d')
x=y=z=np.zeros(300)
eta1=2*np.random.uniform(0,1,300)-1
eta2=2*np.pi*np.random.uniform(0,1,300)
X=np.cos(eta2)*np.sqrt(1-eta1*eta1)
Y=np.sin(eta2)*np.sqrt(1-eta1*eta1)
Z=eta1
ax.quiver3D(x,y,z,X,Y,Z,arrow_length_ratio=0.1,length=1)
ax.set_xlim(-1.0,1.0)
ax.set_ylim(-1.0,1.0)
ax.set_zlim(-1.0,1.0)
```

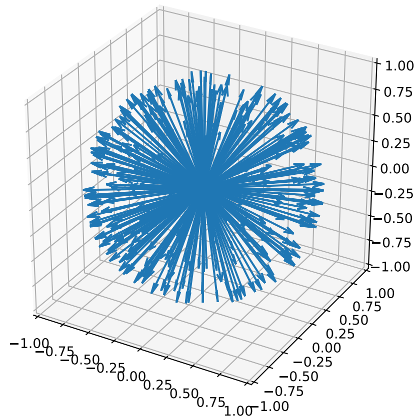

FIGURE 1 – Unit vectors

```
plt.savefig("sphere.pdf")
plt.show()
```

3 Glauber Dynamics

Let us consider the one-dimensional Ising model described by the Hamilonian

$$H = -J \sum_i \sigma_i \sigma_{i+1} \tag{9}$$

where σ_i is a Ising variable and i an integer index running the one-dimensional lattice.

To perform tractable calculations, one often uses the Glauber dynamics. That is a stochastic process where the transition rate between two configurations which differs by a spin flip at site i is given by

$$\Pi(\sigma_i \to -\sigma_i) = \frac{1}{2}(1 - \sigma_i \tanh(\beta h_i)) \tag{10}$$

where $h_i = J(\sigma_{i-1} + \sigma_{i+1})$ is the local field of the spin σ_i.

1. Show that the dynamics satisfies the detailed balance.

Solution: The energy difference is given by

$$\Delta E = 2\sigma_i h_i \tag{11}$$

Expanding

$$\frac{\Pi(\sigma_i \to -\sigma_i)}{\Pi(-\sigma_i \to \sigma_i)} = \frac{e^{\sigma_i h_i}}{e^{-\sigma_i h_i}} = e^{2\sigma_i h_i} \tag{12}$$

This corresponds to the ratio of the equilibrium probability.

2. Justify that the dynamics converges to equilibrium.

Solution: When detailed equation is satisfied, the balance equation is also satisfied and the system relaxes to equilbrium

3. By using the master equation, show that the mean value of σ_i evolves as

$$\frac{d < \sigma_i >}{dt} = - < \sigma_i > + < \tanh(\beta h_i) > \tag{13}$$

Solution: The master equation is given by

$$\frac{dP(\sigma_i)}{dt} = -\Pi(\sigma_i \to -\sigma_i)P(\sigma_i) + +\Pi(-\sigma_i \to +\sigma_i)P(-\sigma_i) \tag{14}$$

The mean value $\langle \sigma_i >= \frac{1}{N}\sum_{i=1}^{N} \sigma_i P(\sigma_i)$ By taking the first moment of the master equation, one obtains Eq.13.

4. Show that $\tanh(\beta h_i) = \gamma(\sigma_{i-1} + \sigma_{i+1})$ where γ is a function of βJ to be determined.

Solution: $h_i = \sigma_{i-1} + \sigma_{i+1}$. Therefore, one hase three case : $-2J, 0$ and 2J When $h_i = 2J$, one has $\gamma = \tan(2\beta J)$. Similarly when $h_i = 0$ and -2.

5. The mean values of all spins being identical, by using the fluctuation-dissipation theorem, the dynamic susceptibility $\chi(t)$ of the system is proportional to $\sum_i < \sigma_i(t) >$. Infer that the total susceptibility satisfies the differential equation

$$\frac{d\chi(t)}{dt} = -(1 - 2\gamma)\chi(t) \tag{15}$$

Solution: By using that $\langle \tan(\beta h_i) \rangle = 2\gamma \langle \sigma_i \rangle$ and inserting in Eq.13, one obtains Eq. 15 for the magnetization which also corresponds to the susceptibility due to the fluctuation dissipation theorem.

6. From the above equation and the expression of γ, show that the characteristic relaxation time of the susceptibility behaves as $\frac{1}{1-\tanh(2\beta J)}$.

Solution: Integrating the relaxation equation one obtains $\chi(t) \sim e{-}t/\tau$ where

$$\tau = \frac{1}{1 - \tanh(2\beta J)}$$

. The relaxation time diverges at low temperature.

Références

[1] Roy J. Glauber, *Time-Dependent Statistics of the Ising Model* J. Math. Phys.**4**, 294 (1963).