

## 1. Ising Model

We would like to apply the Metropolis algorithm to simulate the 1D Ising chain model:  $N$  magnetic dipoles fixed on a chain. Write a program following the Metropolis algorithm. A code skeleton is available in the code section of the homepage.

- (a) Use a *warm* start configuration (all spins are set randomly) as the initial condition. Set the number of dipoles to  $N = 20$ .
- (b) Pick one dipole randomly and flip its spin to create the new *trial* configuration. Calculate the energy of both the old and the trial configuration,  $E_i$  and  $E_{tr}$ , by using

$$E = -J \sum_{i=1}^N s_i s_{i+1}. \quad (1)$$

We will set  $J = 1$  to fix the energy scale. Use a periodic boundary condition for your chain.

- (c) Calculate the relative probability for the trial configuration following

$$\mathcal{P} = e^{-\Delta E/kT}, \quad \Delta E = E_{tr} - E_i. \quad (2)$$

Set  $kT = 0.1$  representing the low temperature case.

- (d) The trial configuration is accepted if it satisfies the condition  $\mathcal{P} \geq r_j$ , where  $r_j$  is a random number in the range  $[0, 1]$ . Convince yourself that this single condition corresponds to the Metropolis algorithm described in the lecture.
- (e) Continue your calculation for  $10N$  steps and observe your result. How is the alignment of spins? Does it change with different random start parameters?
- (f) Using now  $100N$  steps, try  $kT = 0.01$ ,  $kT = 0.1$ , and  $kT = 1$ .
- (g) Try also a *cold* start where initial spins are aligned (in this case you either have to do lots of steps or increase  $kT$ ).
- (h) Extend your program to the 2D model.
  - 1. How many steps are necessary for the 2D model?
  - 2. Store the result every  $n$  steps. How do you choose  $n$ ?
  - 3. Animate your results using the function `plotConfigurations` of `exercise_02.py` or save the frames to disk and join them to a movie with `frames_to_video.py`.
  - 4. Change the initial conditions and observe how your result changes.
  - 5. Increase  $kT$  in small steps. How does the spin alignment change?

## 2. Monte Carlo Integration

Compare the results of the different techniques for Monte Carlo (MC) integration for the following functions

$$f_1(x) = x^2 + x - 1, \quad x \in [-10, 10] \quad (3)$$

$$f_2(x) = \frac{\cos(x) \log(x)}{\sqrt{x}} \quad x \in [0, 1]. \quad (4)$$

As on the last sheet, calculate the integral by using both the rejection and the mean method and plot 1000 results (each with a different seed and 10000 sample points) for each function and each method into a histogram. Compare the mean of these histograms to the analytical values of the integrals. (*Compare the accuracy of the MC integration to that of the Simpson algorithm for the second function  $f_2$ . How many integration points should be used for the Simpson algorithm for a fair comparison?*)

### 3. Monte Carlo Model of Evolution

In [1], certain aspects of evolution are described with the help of a MC model. Read the article and verify its findings by implementing the introduced model yourself and compare your results to the results of the article.

1.  $N$  species are arranged in 1D line.
2. Assign a random barrier  $B_i$  in the range  $[0, 1]$  to each species.
3. Mutate the species with the lowest barrier by assigning a new barrier  $B_n$  for this species and its neighbouring species  $B_{n-1}$  and  $B_{n+1}$ .
4. Repeat this mutation for each iteration.
5. The real time of the mutation is proportional to  $\exp(B_n/T_{\text{car}})$ , where  $T_{\text{car}}$  is a characteristic time scale. (Use  $T_{\text{car}} = 0.01$  as it is done by the author of the article.)
6. Produce similar plots to those printed in the article.

## References

- [1] P. Bak and K. Sneppen, *Punctuated equilibrium and criticality in a simple model of evolution*, Phys. Rev. Lett. 71 (1993) 4083.