1 Monte Carlo simulation of the Ising model

In this exercise we will use Metropolis algorithm to study the Ising model, which is certainly the most thoroughly researched model in the whole of statistical physics. The Ising model is a model of a magnet. The essential premise behind it is that the magnetism of a bulk material is made up of the combined magnetic dipole moments of many atomic spins within the material. The model postulates a lattice (which can be of any geometry we choose; the simple cubic lattice in three dimensions is a common choice) with a magnetic dipole or spin on each site. In the Ising model these spins assume the simplest form possible, which consists of scalar variables σ_i which can take only two values ± 1, representing up-pointing or down-pointing dipoles of unit magnitude.

In a real, magnetic material the spins interact, and the Ising model mimics this by including terms in the Hamiltonian proportional to products $\sigma_i \sigma_j$ of the spins. In the simplest case, the interactions are all of the same strength, denoted by J which has the dimensions of an energy, and the Hamiltonian is defined by:

$$\mathcal{H}(\sigma_1 \dots \sigma_N) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i \tag{1}$$

where the notation $\langle ij \rangle$ indicates that the sum runs over nearest neighbours. The minus signs here are conventional. They merely dictate the choice of sign for the interaction parameter J and the external magnetic field B. A positive value for J signals a ferromagnetic model.

We want to study the equilibrium distribution of the model for N spins at temperature $T = 1/\beta$, that is the probability density:

$$\pi(\sigma_1 \dots \sigma_N) = \frac{1}{Z(\beta, B, N)} \exp\left(-\beta \mathcal{H}(\sigma_1 \dots \sigma_N)\right) \tag{2}$$

defined on the state space $E = \{(\sigma_1 \dots \sigma_N),\ \sigma_i = \pm 1\}$ containing 2^N possible configurations of spins. The denominator $Z(\beta, B, N)$ is the partition function of the model:

$$Z(\beta, B, N) = \sum_{(\sigma_1 \dots \sigma_N) \in E} \exp\left(-\beta \mathcal{H}(\sigma_1 \dots \sigma_N)\right) \tag{3}$$

In this exercise, we focus our attenrion to the simplest situation: the one-dimensional case. We adopt also periodic boundary conditions, defining:

$$\mathcal{H}(\sigma_1 \dots \sigma_N) = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - B \sum_{i=1}^{N} \sigma_i, \quad \sigma_{N+1} \equiv \sigma_1 \tag{4}$$

We will learn now how to implement the Metropolis algorithm to sample π. We will use the notation $\vec{\sigma} \equiv (\sigma_1 \dots \sigma_N)$ for the states, i.e. the configurations of the spins.

1.1 The Algorithm

1. **Inizialization**. We start choosing an initial state, that is an initial configuration for the spins $\vec{\sigma}_0$. For example, we can make all spins up-pointing.

2. **Trial move**. We propose a move $\vec{\sigma}_0 \rightsquigarrow \vec{\sigma}_{trial}$ as follows: we randomly choose a spin and flip it.

3. **Acceptation**. If we have flipped, say, the j^{th} spin, we have $\vec{\sigma}_0 = (\sigma_1, \dots, \sigma_j, \dots, \sigma_N)$ and $\vec{\sigma}_{trial} = (\sigma_1, \dots, -\sigma_j, \dots, \sigma_N)$.

   We evaluate the number:

   $$w = \frac{\pi(\vec{\sigma}_{trial})}{\pi(\vec{\sigma}_0)} = \exp\left(-\beta \left[\mathcal{H}(\vec{\sigma}_{trial}) - \mathcal{H}(\vec{\sigma}_0)\right][\right) \tag{5}$$

   that is:

   $$w = \exp\left(-2\beta B \sigma_j - 2\beta J \sigma_j (\sigma_{j-1} + \sigma_{j+1})\right) \tag{6}$$

   Then we generate a uniform random number $r \in (0, 1)$ and:

   (a) if $r \leq w$, accept the move, defining $\vec{\sigma}_1 = \vec{\sigma}_{trial}$;

   (b) if $r > w$, reject the move, defining $\vec{\sigma}_1 = \vec{\sigma}_0$.

4. **Iteration**. Then, we use $\vec{\sigma}_1$ as the new starting point, and go back to point 2.

We proceed with the process for, at least, $N_{MC} \simeq 10^5 - 10^6$ Monte Carlo steps.

In such a way we have a realization of a Markov chain:

$$\vec{\sigma}_0 \rightsquigarrow \vec{\sigma}_1 \rightsquigarrow \cdots \rightsquigarrow \vec{\sigma}_n \rightsquigarrow \ldots \tag{7}$$

and the Metropolis theorem ensures us that, for n large enough, the $\{\vec{\sigma}_n\}$ sample the probability π.

As the spins "move" exploring the state space, we can perform measurements on the system, actually like an experimentalist. We wish to evaluate the average magnetization:

$$\mathcal{M}(B, \beta) = \sum_{\vec{\sigma}} m(\vec{\sigma})\, \pi(\vec{\sigma}) \tag{8}$$

where:

$$m(\vec{\sigma}) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \tag{9}$$

The basic idea is to estimate it computing an empirical mean over the random walk:

$$\mathcal{M}(B, \beta) \simeq \frac{1}{N_{MC}} \sum_{n=0}^{N_{MC}-1} m(\vec{\sigma}_n) \tag{10}$$

for a number N_{MC} of Monte Carlo steps large enough.

Although the above estimation is justified by the ergodic theorem, in practice one wishes to modify it, to use the central limit theorem properly in order to provide an estimation together with a statistical uncertainty. Three empirical strategies are commonly adopted: equilibration, sparse averaging and datat blocking.

Equilibration actually means that we discard the first steps of the random walk, when the distribution of the sampled Markov chain has not yet reached its limit π. This is done empirically, monitoring, for example, the magnetization itself.

Sparse averaging means that we "measure" $m(\vec{\sigma}_n)$ not at each step, but we wait for a given number of steps between two "measurements". This is meant to reduce statistical correlations. The "waiting time" can be adjusted empirically or evaluated computing an autocorrelation time of the

magnetization (for those of you interested in such topic, in the directory you find a presentation explaining this point in some detail). In practice, we can safely decide to perform a measurement every N (number of spins) Monte Carlo steps: intuitively, we measure the magnetization after having moved, on average, all the spins.

Data blocking actually corresponds to perform many different independent simulations. We divide the simulation in large (this is empirical) blocks; for each bloch we provide an estimation of $\mathcal{M}(B, \beta)$. If the blocks are large enough, we may rely on the central limit theorem and interpret each estimation as a realization of a normal random variable; we can thus use mathematical statistic to provide a confidence interval for the average magnetization of the system.

2 Exercise

Measure the magnetization as a function of B for given β fot $N = 10$ spins in one-dimension, letting $J = 1$ in the hamiltonian. Choose first $\beta = 0.2$ and let B vary on a grid inside the interval $-20 < B < 20$. Then, choose $\beta = 0.02$ (higher temperature!) and let B vary on a grid inside the interval $-20 < B < 20$.

3 Analytic Results

You can compare your results with the analytic results for the Ising model in one-dimension. The explicit solution relies on the observation that the partition function can be written as:

$$Z(\beta, B, N) = Tr\left(\mathcal{T}^N\right) \tag{11}$$

where:

$$\mathcal{T} = \begin{pmatrix} e^{\beta(J+B)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} \end{pmatrix} \tag{12}$$

Thus, we have:

$$Z(\beta, B, N) = \tau_+^N + \tau_-^N \tag{13}$$

$\tau_\pm$ being the eigenvalues of the matrix $\mathcal{T}$. Explicitely:

$$\tau_{\pm} = e^{\beta J}\left(Ch(\beta B) \pm \sqrt{Sh(\beta B)^2 + e^{-4\beta J}}\right) \tag{14}$$

You can use this expressions to evaluate analytically the magnetization. The expression becomes simple in the thermodynamic limit $N \to +\infty$:

$$M(\beta, B) = \langle \sigma_i \rangle = \frac{Sh(\beta B) + \frac{Sh(\beta B)Ch(\beta B)}{\sqrt{Sh^2(\beta B)+e^{-4\beta J}}}}{Ch(\beta B) + \sqrt{Sh^2(\beta B) + e^{-4\beta J}}} \tag{15}$$

You can find the exact expression for the finite N case in the file *ising.pdf*.