

Topic 3: Monte Carlo Simulation of Magnetic Materials (continued)

Many systems are characterized by a very large number of *configurations* or *states* which occur with some well defined probability distribution. The Monte Carlo method *samples* this set of configurations randomly, for example by using a *Markov process* or *random walk*.

A Markov chain is a sequences of random variables in which the next variable is determined by the present variable but is independent of the way in which the present state arose from its predecessors.

Generating the Gaussian distribution using the Metropolis Method

Suppose the system is the set of all points $-\infty < x < \infty$ distributed according to the probability

$$P(x) = \frac{e^{-(x-c)^2/(2\sigma^2)}}{\sqrt{2\pi}\sigma},$$

where c is the center of the Gaussian peak and σ is its width.

The Metropolis algorithm is based on a *random walk* which generates a sequence (Markov chain) of points $x_i, i = 1, 2, \dots, N$. The random walker takes steps with random direction and magnitude less than some fixed maximum step size δ . Given the present position x_i of the walker, the next (future) position is determined by the Metropolis step algorithm:

- Let

$$x_{\text{trial}} = x_i + (2r - 1)\delta ,$$

where δ is a fixed maximum step size and r is a uniform deviate (i.e., a random number in the interval $[0, 1)$).

- If

$$\frac{P(x_{\text{trial}})}{P(x_i)} \geq r' ,$$

where r' is an independent random deviate, then

$$x_{i+1} = x_{\text{trial}} ,$$

else, the next position is identical to the current position

$$x_{i+1} = x_i .$$

Imagine that the probability function $P(x)$ represents the height of a one-dimensional landscape with hills and valleys. Notice that

- if the trial step is in the *uphill direction*, it is always accepted, but
- if the trial step is in the *downhill direction*, the step is accepted only if the decrease in probability is smaller than some randomly chosen amount.

Thus the walker moves uphill preferentially and spends more time near the peaks in the landscape.

This algorithm for taking a single step in the chain can be used to generate the probability distribution as follows:

1. Choose an initial position x_0 for the walker, and a fixed maximum step size $\delta > 0$.
2. Allow the walker to *thermalize* or come to equilibrium by taking some number N_0 of initial steps. These steps are discarded.
3. After the walker has thermalized, start taking data. The simplest procedure is to take N further Metropolis steps, and use these to sample the distribution and calculate average values

$$\langle A \rangle = \frac{1}{N} \sum_{i=1}^N A(x_i) ,$$

where $A(x)$ is some quantity whose average value is to be determined.

Some important considerations:

- Choice of initial position: If possible, this should be chosen close to where $P(x)$ has a maximum.

- Choice of step size: If δ is too small, then the walker may have trouble finding the peaks in the landscape because the probability of rejecting a step, i.e., moving preferentially in the uphill direction, becomes small. If δ is too big, then the walker may also have trouble finding the peaks! One useful criterion is to adjust the step size so that the *acceptance ratio*

$$R_{\text{acceptance}} = \frac{\text{Number of steps accepted}}{\text{Total number of steps}} \simeq 0.5 .$$

- Number of thermalization steps N_0 : This is usually determined by trial and error. With a bad choice of initial position x_0 it may take a long time for the walker to find the peaks in the distribution!
- Correlations: It sometimes happens that successive Metropolis steps are not sufficiently random and violate the Markov criterion. If this is the case, one can discard some number of intermediate steps between successive retained data steps.