Initial conditions

As we discussed, the ergodic theorem states that

time averages = sample averages

One can prove that:

1) For any starting condition the time average

$$\frac{1}{N+1}\sum_{n=0}^{N} f(X_n)$$

is a **biased** estimate of the sample average $\sum_x \pi_x f(x)$. The bias is of order $1/N$.

2) The bias vanishes if one starts in equilibrium.
From a rigorous point of view, "a start in equilibrium" corresponds to choosing the starting point according to the equilibrium distribution.
In practice, it means we start from a typical configuration.

Initialization: practical considerations

Initial-condition effects vanish as $1/N$.

Statistical fluctuations vanish as $1/\sqrt{N}$.

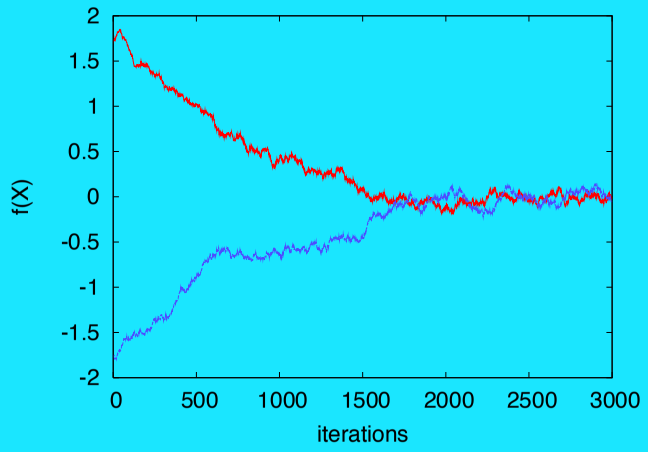
Initial conditions introduce a bias in the estimates which is particularly important for short runs and which become irrelevant as the number of iterations increases.

Contrary to what one might think, in high-precision Monte Carlo studies (of non disordered systems!!!) there is no need to be very careful about thermalization.

Useful check: repeat the simulation starting from two very different configurations and check when the two runs provide results that roughly agree.

For a spin system, one can perform a simulation that starts from a disordered configuration (at $t = 0$ the spins have random direction) and a second one starting from an ordered configuration (at $t = 0$ all spins are parallel).

For a fluid system, one can perform a simulation that starts from a disordered configuration (at $t = 0$ particles have a random position in the box) and a second one starting from an ordered configuration (at $t = 0$ all particles are set on a regular lattice).



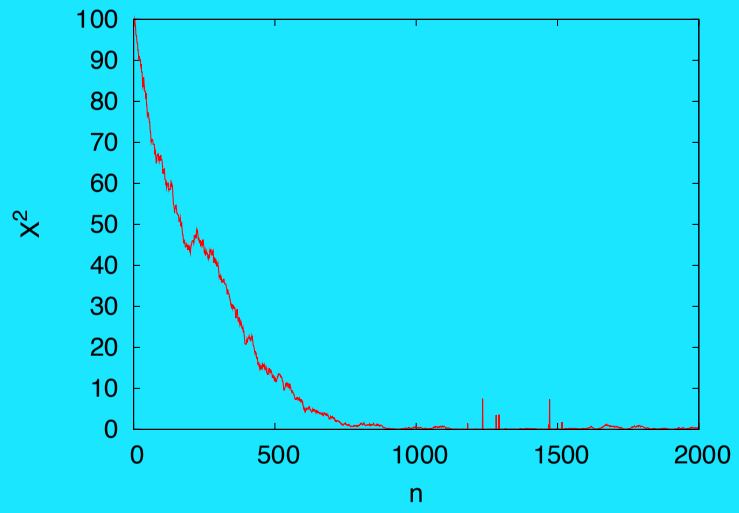
We consider a MC dynamics and plot $f(x_t)$ versus x_t.
To avoid the bias one looks at the data and discard all data that do not appear in equilibrium. For instance, in the case of the figure, one can discard 2000 iterations. After 2000, results are independent of the starting point.

To clarify the role of the initial conditions let consider a simple example. We consider the Gaussian probability $e^{-x^2}/\sqrt{\pi}$ on the real line.

A simple dynamic Monte Carlo algorithm for this distribution is the following (this is the algorithm discussed as an eaxmple of the **Metropolis** method):

1. If X_n is the value of x at the n-th iterations, propose $Y = X_n + p(U - 1/2)$, where p is a constant and U a random number uniformly distributed in $[0,1]$.
2. If $|Y| \leq |X_n|$ then $X_{n+1} = Y$. If $|Y| > |X_n|$ we draw a random number V uniformly distributed in $[0,1]$. If $U \leq \exp(X_n^2 - Y^2)$, then $X_{n+1} = Y$; otherwise $X_{n+1} = X_n$.

The algorithm is correct for any $p > 0$. In the following we shall use the value $p = 0.2$. Moreover, we will start very far from equilibrium taking $X_0 = 10$.



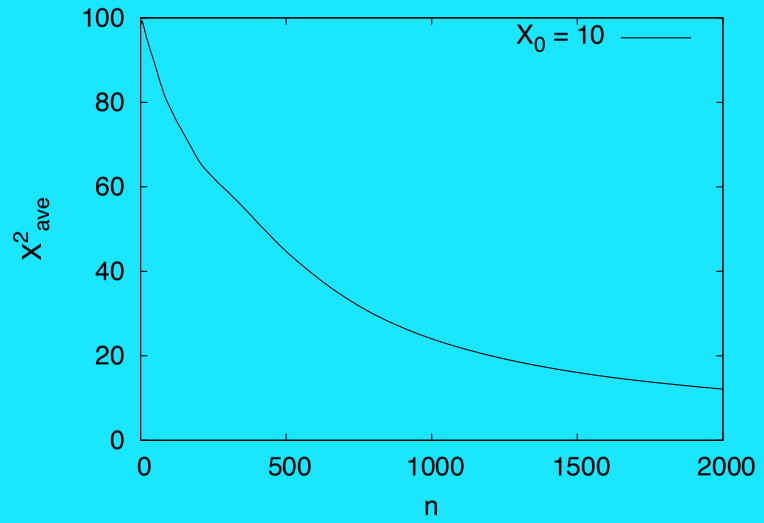
We report here the quantity X^2. Its average should converge to $1/2$. Equilibrium is reached after 1000 iterations. There is no bias if we discard the first 1000 iterations.

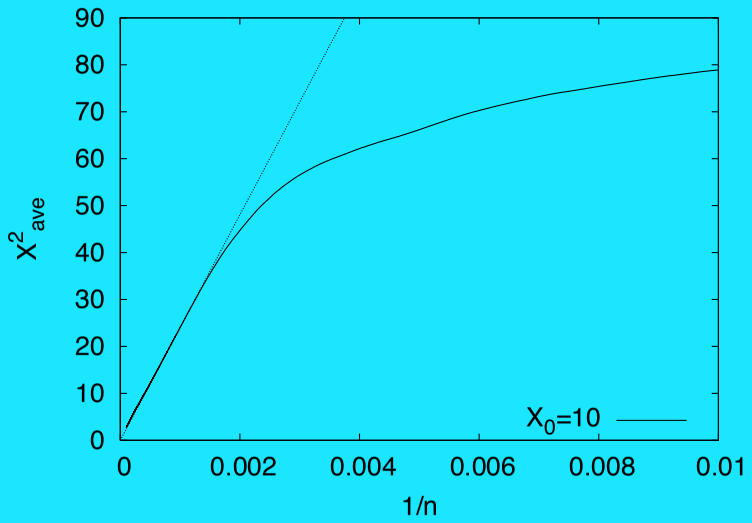
Now we report the sample mean computed using the first n iterations:

$$X^2_{\rm ave}(n) = \frac{1}{n+1}\sum_{i=0}^{n} X^2_n$$

Here we keep all data. For $n \to \infty$ it converges to the 1/2 (the average value in the distribution π)

Convergence is very slow (see below, left panel): even with 2000 iterations, the average value is very far from the asymptotic result 1/2. The bias is very large!
In the right panel, we plot the sample mean as a function of $1/n$. For $n \to \infty$ $(1/n \to 0)$ the behavior becomes asymptotically linear, as expected.





To avoid the problem we should discard the first 1000 iterations (we use the information obtained from the figure at p. 5). Results for 10000 iterations (average of all data and average of all data minus the first 1000 ones)

$$\frac{1}{10000}\sum_{i=1}^{10000} X_i^2 = 2.70 \qquad \frac{1}{9000}\sum_{i=1001}^{10000} X_i^2 = 0.33$$

The asymptotic result should be $1/2 = 0.5$.