Monte Carlo Simulation for classical 1D harmonic oscillator

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Goal: write a Monte Carlo program for a classical 1D harmonic oscillator, perform simulations at different temperatures and compare the resulting probability distribution with analytical results.

1. Analytical results

For a classical 1D harmonic oscillator, the restoring force is proportional to the displacement of a particle from the mean position and directed towards the mean position, so

$$\mathrm{F} = -kx$$

$$\frac{d^2x}{dt^2} + \omega^2 x = 0, where\ \omega^2 = k/m$$

Then we have

$$x = a\sin(\omega t + \varphi)$$

The potential energy and kinetic energy are

$$V(x) = \frac{1}{2}kx^2, K = \frac{1}{2}m\dot{x}^2$$

The total energy of the oscillator, which is a constant, is

$$E = \frac{1}{2}ka^2$$

The particle moves around in the classically allowed region: $|x| < a$. The time (*dt*) a particle spends in a little region *dx* depends on its speed *v = dx/dt*. The probability of finding the particle in *dx* is then proportional to the time it spends there is *dP = 2dt/T*, where *T* is the period of oscillation.

$$\mathrm{dP} = \frac{2\mathrm{dt}}{\mathrm{T}} = \frac{2}{\mathrm{T}}\left(\frac{1}{\mathrm{v}}\right)\mathrm{dx}, \mathrm{v} = \ \omega^2\sqrt{\mathrm{a}^2 - \mathrm{x}^2}$$

$$\mathrm{P(x)} = \frac{1}{\pi\sqrt{\mathrm{a}^2 - \mathrm{x}^2}}$$

P(x) is called probability density. Since we need to know the distribution under different temperatures, I assume *E = kT*, where *T* is the temperature now. So *P(x)* could be expressed using temperature and position *x*. By set force constant *k=1* and Boltzmann constant to be 1, we now have

$$\mathrm{a} = \sqrt{2\mathrm{T}}$$

The distributions for different temperature are shown in Figure 1.

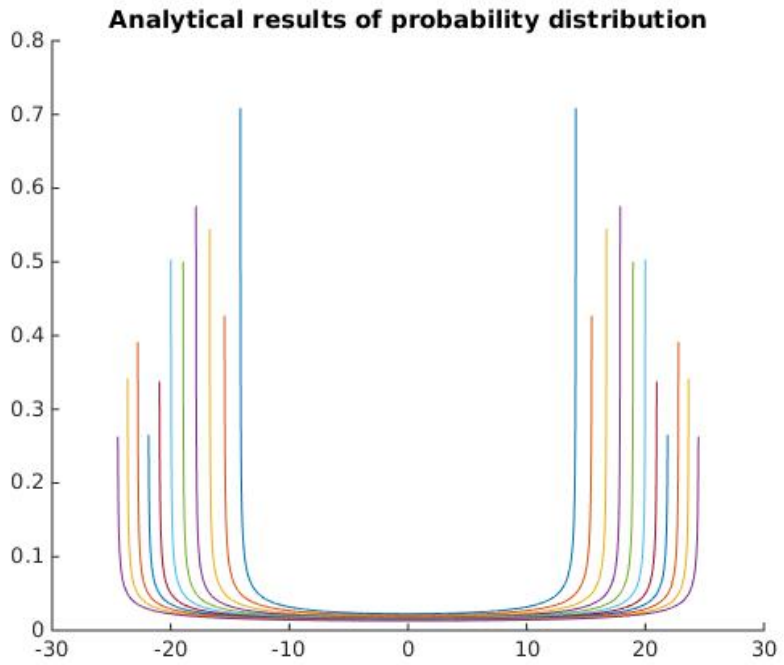

Figure 1. Analytical results of probability distribution under different temperatures.

2. Monte Carlo simulations

For an introduction, Monte Carlo methods are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results. Its core idea is to use random samples of parameters or inputs to explore the behavior of a complex system or process. There are problems that are too complex for an analytical solution – so they have to be evaluated numerically. If the exhaustive numerical evaluation is prohibitively slow, Monte Carlo simulation could be used to find solutions.

Monte Carlo simulations sample from a probability distribution for each variable to produce hundreds or thousands of possible outcomes. The results are analyzed to get probabilities of different outcomes occurring.

Here in this little project, potential energy is used to calculate the energy difference between different tries. Metropolis algorithm is used to accept or reject the next state.

To get started, Monte Carlo simulation needs an initial value as the starting point. 0 is chosen. The next position is randomly chosen from $-a$ to a. By randomly choosing this point, the detailed balance requirement is satisfied. Then the energy difference between the current position and the next position is computed. It accepts or rejects it according to Metropolis algorithm. 10000000 samples are sampled for each single temperature. Histogram graphs are plotted as curves, which are shown in Figure 2.

We can see that the curves don't agree with the analytical results at all. The reason for this, I think, is because classical 1D harmonic oscillator takes the kinetic energy into consideration, while there is no velocity in MC simulation. To accurately simulate 1D harmonic oscillator, we may need MD simulation for

classical 1D harmonic oscillator. Or we could just use MC to simulation quantum 1D harmonic oscillator.

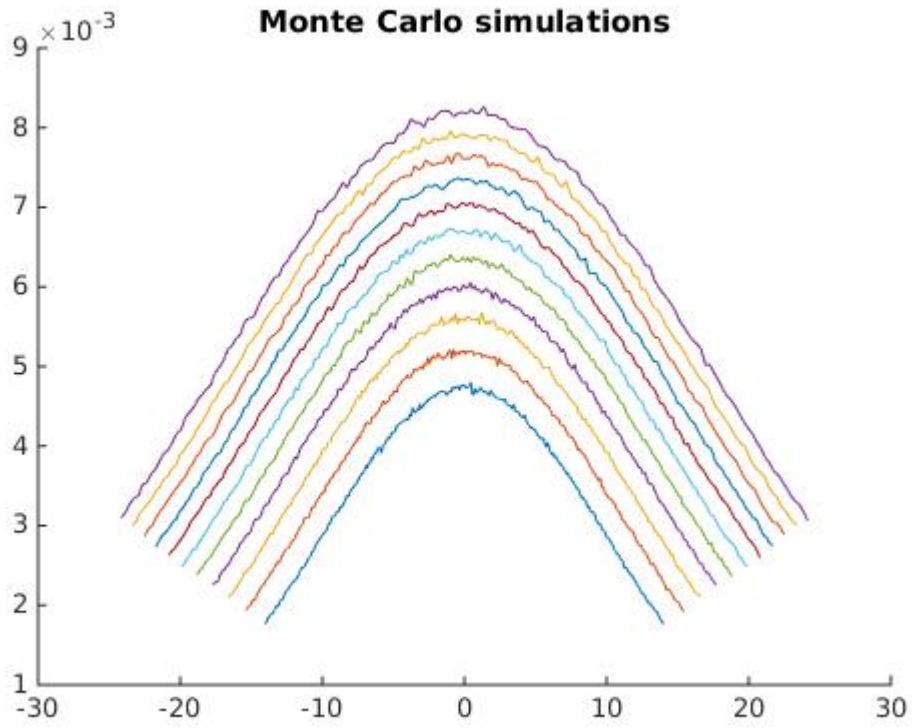

Figure 2. MC simulation results of probability distribution under different temperatures.