

# Metropolis Monte-Carlo Algorithm for two particles connected by a spring

Let's assume a system comprising of two beads connected by a spring. The initial positions of the two particles are  $x_1$  and  $x_2$ , the temperature  $T$ , spring constant  $k$ . The energy function  $E(x_1, x_2) = \frac{1}{2}k(|x_2 - x_1| - l_0)^2$ , where  $l_0$  is the equilibrium spring length.

Repeat the following steps for a number of iterations:

1. **Propose a random move:** For each particle  $i = 1, 2$ , propose a new position  $x'_i = x_i + \Delta x$ , where  $\Delta x$  is sampled from a Gaussian distribution.
2. **Compute the change in energy:**

$$\Delta E = E(x'_1, x'_2) - E(x_1, x_2).$$

3. **Accept or reject the move:**

- Accept the move if  $\Delta E$  is negative, indicating that the new state corresponds to the lower energy.
- In case  $\Delta E$  is positive, accept the move with a probability of  $\exp(-\Delta E/k_B T)$ .

This can be achieved by generating a uniform random number  $u \sim \mathcal{U}(0, 1)$  and checking  $u \leq \exp(-\Delta E/k_B T)$ , accept the move:

$$x_1 = x'_1, \quad x_2 = x'_2.$$

- Else, reject the move and keep  $x_1$  and  $x_2$  unchanged.