Jarzynski Equality and Monte Carlo

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1. Write a Monte Carlo program to sample the configurations of a particle in 1D subject to a harmonic potential at temperature $k_B T = 1$

$$U_\lambda(q) = \frac{1}{2} k(\lambda) \left(q - c(\lambda)\right)^2$$

   (Hint: start from what you did for assignment 2) Notice that both stiffness k and center c are function of a parameter λ. Write the program in such a way that you can change the functional form of $k(\lambda)$ and $c(\lambda)$ a posteriori. It should be also possible to change λ with time.

2. Now use $k(\lambda) = 1$ (constant) and $c(\lambda) = \lambda q_1$ so that the center will move from 0 to q_1 at constant speed in N MC steps. Choose $\lambda = i/N$ where i is the number of the MC step. Use the Jarzynski equality to compute the free-energy difference between the system with $\lambda = 0$ and the system with $\lambda = 1$. Which is the result you expect? How many independent trajectories do you need? How does this number depends on N (total number of steps for each trajectory)? How does it depend on the stepsize Δ used for the Metropolis update? *(Hint: to compute the work, accumulate the energy change due to changes in the value of λ).*

3. Repeat the previous point using $k(\lambda) = 1 + \lambda$ and $c(\lambda) = 0$, so that the stiffness will change from 1 to 2 in N MC steps.

4. Repeat the previous point using the backward schedule ($\lambda = 1 - i/N$, where N is the length of the trajectory and i is the number of the MC step). Draw a histogram for both forward and backward work and verify Crooks theorem.