Problem Set 6

1. *Detailed Balance*

   In class we discussed the Metropolis criterion, which says that we accept a proposal move (sometimes called a "trial move") using the following probability:

   $$p_{\text{acc}}(\boldsymbol{x} \to \boldsymbol{x}') = \min\left[1, e^{-\beta\Delta E(\boldsymbol{x},\boldsymbol{x}')}\right]. \tag{1}$$

   There are other criteria that could be employed—the condition that is necessary is that the acceptance probability leads to a dynamics that satisfies *detailed balance*,

   $$\rho(\boldsymbol{x})p(\boldsymbol{x} \to \boldsymbol{x}') = \rho(\boldsymbol{x}')p(\boldsymbol{x}' \to \boldsymbol{x}) \tag{2}$$

   a condition that ensures that generated configurations are sampled in proportion to their probabilities under the distribution ρ. Show that for $\rho(\boldsymbol{x}) = Z^{-1}(\beta)e^{-\beta E(\boldsymbol{x})}$ and any symmetric generation move (i.e., such that $p_{\text{gen}}(\boldsymbol{x} \to \boldsymbol{x}') = p_{\text{gen}}(\boldsymbol{x}' \to \boldsymbol{x})$) the Metropolis criterion preserves detailed balance.

2. *Ising Monte Carlo*

   Using the template provided, you will add a few functions to complete a Monte Carlo simulation of the Ising model. Then, using this simulation, you will extract some information about the system.

   (a) After each trial move, we need to accept or reject the configuration in order to ensure that we sample the Boltzmann distribution. In input cell 5 of the provided template, write code to compute the energy difference. In input cell 6, find the 'TODO' and implement the Metropolis acceptance criterion we discussed in class.

   (b) The updates we use are local in space (they operate on one spin at a time). Explain why it makes sense to treat N attempted moves (sometimes called a Monte Carlo sweep) as a unit of time.

   (c) Write a function to compute $\langle M \rangle = \frac{1}{N}\sum_i \sigma_i$ and collect a trajectory of 1000 MC sweeps and compute the running average of the magnetization as a function of trajectory time. Now, throw out the first 100 sweeps and repeat. Which result looks better? Why?

   (d) Plot $\langle M \rangle$ as a function of h at $T = 2.0$ for h in the range $[-0.5, 0.5]$ using 10 points. Explain why it is important to start the simulation with a random initial condition for each measurement.

   (e) Set $h = 0$. Compute the average energy as a function of T for $T \in [1, 4]$ using 10 points and plot it.

   (f) We know that $\frac{dE}{dT}$ tells us about the heat capacity at constant volume for canonically distributed samples. However, one of the profound consequences of the statistical point of view was that we were able to derive a fluctuation response relation. Compute $\langle E^2 \rangle - \langle E \rangle^2$ as a function a function T over the same range as above. Using the relation between the heat capacity and the variance, use this data to plot C_v as a function of T. Where is the function maximal? Why?