PH 4433/6433 HW 7, due Monday Oct. 30

1) Volume of a unit hypersphere (50 pts): see Exercise 10.7, page 471

A unit hypersphere in d dimensions is the region of space defined by points $\vec{r}$ such that $\sum_i r_i^2 \leq 1$. For $d = 2$ this is a circle, with area π; for $d = 3$ a sphere with volume $\frac{4}{3}\pi$. For general d the volume is

$$V_d = \frac{\pi^{d/2}}{\Gamma(d/2+1)},$$

where $\Gamma(z)$ is the gamma function, available in Python as the function `gamma` in `scipy.special`.

(a) Write a program to calculate the volume of a d dimensional unit hypersphere using "dart-throwing" Monte Carlo as outlined in the text.

Compare the results of your program to the exact volume for d=10. Make a plot of the relative error of the estimate versus the number of samples N for N up to 1,000,000. I suggest calculating error for values of N in multiples of 10,000.

(b) Make a plot comparing the results of this Monte Carlo calculation for d=10, 12, 15.

2) Monte Carlo Data analysis (50 pts)

In a Markov chain Monte Carlo calculation the data are usually correlated. The result is that a simple calculation of the standard error will give an underestimate of the actual error. A simple way to correct for this is by blocking or binning the data. An example program for a Monte Carlo simulation of an ideal gas is given on pages 485-486 of the text. This code produces a plot of energy versus Monte Carlo step. The question is: for a plot like Fig 10.5, what is the average energy, and what is the standard error of that average?

(a) Modify the code to calculate the average energy. For the average to be accurate you need to ignore some initial number of steps before the simulation has reached equilibrium. For the parameters of Fig 10.5, ignoring the first 50,000 steps should be sufficient.

Using the parameters of Fig 10.5, calculate the average energy and its standard error.

(b) To better estimate the standard error, write a second version of the program to calculate the average energy and standard error, using block averages:

Divide the steps after the equilibration phase into 10 equal-length bins. Calculate the average energy within each bin. It is best to do this as the simulation runs to avoid having to store all the measurement results.

At the end of the simulation, calculate the average energy by taking the average of the 10 bins. You should get exactly the same numeric value (within round-off error) as in (a) assuming you start both calculations with the same random seed.

Also calculate the standard error from the 10 bins. You should find a different (larger) value from the standard error in (a). This is a more accurate estimate of the error of the average energy.

(c) Try running the code of (b) for higher temperatures. Show that as temperature increases, the average energy per particle approaches the value expected by the equipartition theorem, which is $\frac{3}{2}kT$. Be sure to check if your assumptions about the equilibration time are valid when T changes.