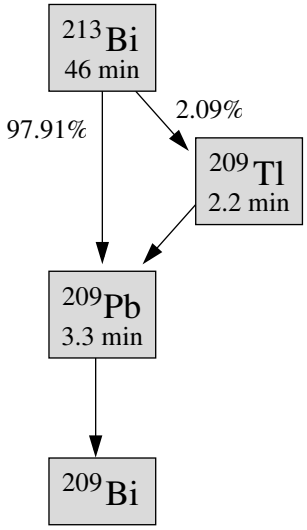
RANDOM PROCESSES AND MONTE CARLO METHODS

Homework 6: DUE ON MONDAY DECEMBER 5TH AT 12:30 PM

Problem 1: Radioactive decay chain

The isotope ^{213}Bi decays to stable ^{209}Bi via one of two different routes, with probabilities and half-lives given in this diagram:



(Technically, ^{209}Bi isn't really stable, but it has a half-life of more than 10^{19} years, a billion times the age of the universe, so it might as well be.)

Starting with a sample consisting of 10 000 atoms of ^{213}Bi, simulate the decay of the atoms by dividing time into slices of length $\delta t = 1$ s each and on each step doing the following:

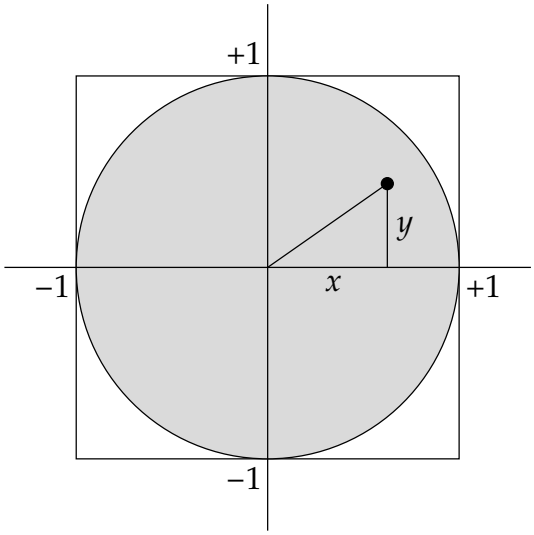
1. For each atom of ^{209}Pb in turn, decide at random, with the appropriate probability, whether it decays or not. (The probability can be calculated from Newman's Eq. 10.3). Count the total number that decay, subtract it from the number of ^{209}Pb atoms, and add it to the number of ^{209}Bi atoms.
2. Now do the same for ^{209}Tl, except that decaying atoms are subtracted from the total for ^{209}Tl and added to the total for ^{209}Pb.
3. For ^{213}Bi the situation is more complicated: when a ^{213}Bi atom decays you have to decide at random with the appropriate probability the route by which it decays. Count the numbers that decay by each route and add and subtract accordingly.

Note that you have to work up the chain from the bottom like this, not down from the top, to avoid inadvertently making the same atom decay twice on a single step.

Keep track of the number of atoms of each of the four isotopes at all times for 20 000 seconds and make a single graph showing the four numbers as a function of time on the same axes.

Problem 2: Volume of a hypersphere

This exercise asks you to estimate the volume of a sphere of unit radius in ten dimensions using a Monte Carlo method. Consider the equivalent problem in two dimensions, the area of a circle of unit radius:



The area of the circle, the shaded area above, is given by the integral

$$I = \iint_{-1}^{+1} f(x,y)\,\mathrm{d}x\,\mathrm{d}y,$$

where $f(x,y) = 1$ everywhere inside the circle and zero everywhere outside. In other words,

$$f(x,y) = \begin{cases} 1 & \text{if } x^2 + y^2 \le 1, \\ 0 & \text{otherwise.} \end{cases}$$

So if we didn't already know the area of the circle, we could calculate it by Monte Carlo integration. We would generate a set of N random points (x,y), where both x and y are in the range from -1 to 1. Then the Monte Carlo integral for this calculation would be

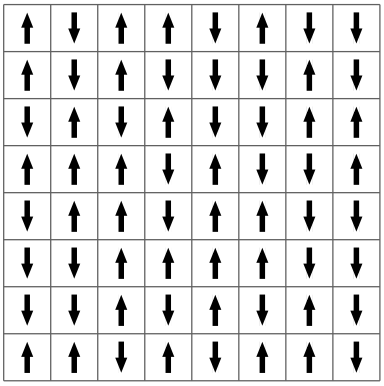
$$I \simeq \frac{4}{N} \sum_{i=1}^{N} f(x_i, y_i).$$

Generalize this method to the ten-dimensional case and write a program to perform a Monte Carlo calculation of the volume of a sphere of unit radius in ten dimensions.

If we had to do a ten-dimensional integral the traditional way, it would take a very long time. Even with only 100 points along each axis (which wouldn't give a very accurate result) we'd still have $100^{10} = 10^{20}$ points to sample, which is impossible on any computer. But using the Monte Carlo method we can get a pretty good result with a million points or so.

Problem 3: The Ising model

The Ising model is a theoretical model of a magnet. The magnetization of a magnetic material is made up of the combination of many small magnetic dipoles spread throughout the material. If these dipoles point in random directions then the overall magnetization of the system will be close to zero, but if they line up so that all or most of them point in the same direction then the system can acquire a macroscopic magnetic moment—it becomes magnetized. The Ising model is a model of this process in which the individual moments are represented by dipoles or "spins" arranged on a grid or lattice:



In this case we are using a square lattice in two dimensions, although the model can be defined in principle for any lattice in any number of dimensions.

The spins themselves, in this simple model, are restricted to point in only two directions, up and down. Mathematically the spins are represented by variables $s_i = \pm 1$ on the points of the lattice, $+1$ for up-pointing spins and -1 for down-pointing ones. Dipoles in real magnets can typically point in any spatial direction, not just up or down, but the Ising model, with its restriction to just the two directions, captures a lot of the important physics while being significantly simpler to understand.

Another important feature of many magnetic materials is that the individual dipoles in the material may interact magnetically in such a way that it is energetically favorable for them to line up in the same direction. The magnetic potential energy due to the interaction of two dipoles is proportional to their dot product, but in the Ising model this simplifies to just the product $s_i s_j$ for spins on sites i and j of the lattice, since the spins are one-dimensional scalars, not vectors. Then the actual energy of interaction is $-J s_i s_j$, where J is a positive interaction constant. The minus sign ensures that the interactions are *ferromagnetic*, meaning the energy is lower when dipoles are lined up. A ferromagnetic interaction implies that the material will magnetize if given the chance. (In some materials the interaction has the opposite sign so that the dipoles prefer to be antialigned. Such a material is said to be *antiferromagnetic*, but we will not look at the antiferromagnetic case here.)

Normally it is assumed that spins interact only with those that are immediately adjacent to them on the lattice, which gives a total energy for the entire system equal to

$$E = -J \sum_{\langle ij \rangle} s_i s_j \,,$$

where the notation $\langle ij \rangle$ indicates a sum over pairs i, j that are adjacent on the lattice. On the square lattice we use in this exercise each spin has four adjacent neighbors with which it interacts.

Write a program to perform a Markov chain Monte Carlo simulation of the Ising model on the square lattice for a system of 20×20 spins. You will need to set up variables to hold the value ± 1 of the spin on each lattice site, probably using a two-dimensional integer array, and then take the following steps.

1. First write a function to calculate the total energy of the system, as given by the equation above. That is, for a given array of values of the spins, go through every pair of adjacent spins and add up the contributions $s_i s_j$ from all of them, then multiply by $-J$. Hint 1:

Each unique pair of adjacent spins crops up only once in the sum. Thus there is a term $-Js_1s_2$ if spins 1 and 2 are adjacent to one another, but you do not also need a term $-Js_2s_1$. Hint 2: To make your final program to run in a reasonable amount of time, you will find it helpful if you can work out a way to calculate the energy using Python's ability to do arithmetic with entire arrays at once. If you do the calculation step by step, your program will be significantly slower.

2. Now use your function as the basis for a Metropolis-style simulation of the Ising model with $J = 1$ and temperature $T = 1$ in units where the Boltzmann constant k_B is also 1. Initially set the spin variables randomly to ± 1, so that on average about a half of them are up and a half down, giving a total magnetization of roughly zero. Then choose a spin at random, flip it, and calculate the new energy after it is flipped, and hence also the change in energy as a result of the flip. Then decide whether to accept the flip using the Metropolis acceptance formula, Newman's Eq. 10.60. If the move is rejected you will have to flip the spin back to where it was. Otherwise you keep the flipped spin. Now repeat this process for many moves.

3. Make a plot of the total magnetization $M = \sum_i s_i$ of the system as a function of time for a million Monte Carlo steps. You should see that the system develops a "spontaneous magnetization," a nonzero value of the overall magnetization. Hint: While you are working on your program, do shorter runs, of maybe ten thousand steps at a time. Once you have it working properly, do a longer run of a million steps to get the final results.

4. Run your program several times and observe the sign of the magnetization that develops, positive or negative. Describe what you find and give a brief explanation of what is happening. Then run it two further times at temperatures $T = 2$ and $T = 3$. Explain briefly what you see. How does the behavior of the system change as temperature is increased?