PY3C01: Assignment

IMPORTANT: Please read carefully through all of the following before you start! Send your solution via email to archert@tcd.ie before 9:00 am on the 15th of January.
IMPORTANT: NO SUBMISSIONS WILL BE ACCEPTED AFTER THAT TIME

Please note the following:

- You have to work on this assignment on your own, and submit your own genuine solution. You are not allowed to share your solution with other students. If I have any doubts on this, or if some other things in your code require clarification, we will arrange for a short (5-10 minutes) meeting where you will explain your solution to me.
- Even an incomplete solution or buggy code might earn you points particularly if you describe why your solution does not work.
- Use comments and proper indentation within your source code in order to make your code as clear and self-explaining as possible. Include appropriate error handling where necessary. Remember that good code is elegant and easy to understand. There are extra points to be gained for good programming style!
- The report should be submitted in pdf form. Wrod, Openoffice and Latax can all export at pdf.
- Your code should be developed using a version control system and submitted for assessment by providing a web link or invitation.

What will you be assessed on:

You are expected to create a scientific paper (4 sides long) in which you describe your investigation of the Ising model using numerical techniques.

The paper should have:

- Abstract - Describe the paper briefly including the main conclusion.
- Introduction - Give a background on the problem you investigate.
- Methods - Describe the algorithms used.
- Results - Show and describe your main results.
- Conclusion - Review your main findings, link this back to the introduction.
- References

Code should be provided in a git repository not as part of your submitted report. You should document and comment your code within the repository.

You must demonstrate in the report that you have:

- understood the algorithm you are implementing (a flow chart is recommended).
- Demonstrate the ability to used both Python and shell scripting.
- Implemented the Ising model as describe below for the Metropolis algorithm.
- Perform a scientific investigation of your choice using your implementation.
- To obtain the higher grades you must demonstrate original thinking.

Background - the Ising model

As physicists we try to interpret the world around us by fitting it to models. Many of the concepts of magnetism can be understood though the Ising model, this and similar models are active fields of research to help understand the properties of magnetic materials.

The model consists of a lattice of spins, for this project we will consider this to be a 2D lattice of collinear spins as shown in figure 1.

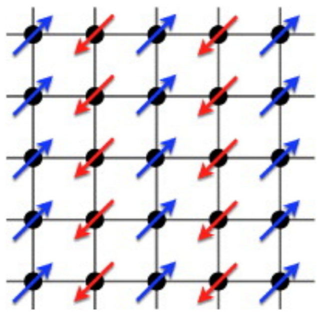

Figure 1: 2D collinear lattice of spins.

The Hamiltonian of the Ising model can be written as:

$$H = -J \sum_{<ij>} S_i.S_j - h \sum_i S_i$$

where the first sum is over pairs of adjacent spins (every pair is counted once). <ij> indicates that sites i and j are nearest neighbors. The second term represents the influence of an external magnetic field h. The spin vectors S are collinear and therefore may only take the values +1 or −1.

Statistical mechanics

The evolution of such a system can be evaluated from statistical mechanics. The configuration probability of state ν is given as:

$$p_\nu = e^{-\beta E_\nu}/Z$$

where $\beta = 1/K_B T$ and the partition function $Z = \sum_\nu e^{-\beta E_\nu}$.

Metropolis algorithm

Consider a single spin on the 2D lattice interacting with its nearest neighbours, the partition function is summed over all possible configurations so it can be considered constant. The probability that the spin will flip can be written as:

$$
\begin{aligned}
P_x/P_y &= \frac{e^{-\beta E_x}/Z}{e^{-\beta E_y}/Z} \\
&= e^{-\beta E_x}/e^{-\beta E_y} \\
&= e^{-\beta(E_x - E_y)} \\
P_{flip} &= e^{-\beta \delta E}
\end{aligned}
$$

Knowing the probability that any spin will flip allows us to cast the problem in terms of a metropolis algorithm:

- Set the desired temperature and magnetic field h.
- Choose a starting configuration for the spins on the lattice.
- Sweep through each lattice site calculate P_{flip} for each site.

  if the change in energy $\delta E < 0$ we accept the change.

  if the change in energy $\delta E > 0$, we accept the change with the probability P_{flip}. This can be done by comparing P_{flip} to a random number.
- run several sweeps though the lattice to reach equilibrium.
- allow to evolve to collect statistical information e.g. net magnetization, domain size magnetic susceptibility.

What to investigate with the Ising model

The Ising model was designed to describe magnetic systems and is still actively used in research to identify magnetic ordering temperatures, and to identify the ground state magnetic phase.

Once you have constructed your implementation of the 2D Ising model you should use it to do a scientific investigation. Whatever the investigation you chose to do you need to discuss the numerical accuracy of your simulation. For example when you first initialize you system you are not in thermodynamic equilibrium, the system needs to be evolved until equilibrium is reached, how many steps are appropriate? Statistics should be calculated over several steps after equilibrium has been reached, how many steps do you need to do to get a good statistical average?

Possible investigations

- Can you identify a phase transition with temperature? What happens physically through the phase transition?
- What is the effect of disorder on the system?
- How does the system size affect the results obtained?
- If the model is implemented in 1D, 2D or 3D does this change how the system behaves?
- Investigate the transition temperature in alternative lattice structures FCC, BCC, hexagonal, 2D layered systems. What aspects are required to obtain a high ordering temperature?
- Can you identify at what temperature a single domain can span the entire system, can you relate this to the bond-correlated percolation model?
- NiO is well described by a second nearest neighbor Ising model NiO has a rock salt structure, a 2D cut of the NiO structure is showing in figure 2. O carries no magnetic moment so you only need to model Ni, if J_1=2.3meV and J_2=-21meV what is the ordering temperature? How does this compare to experiment? What is the ground state phase?

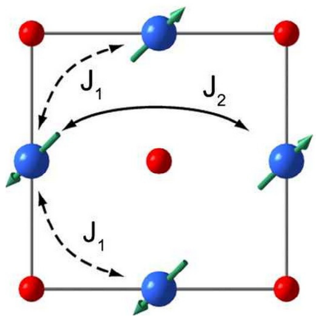

Figure 2: 2D J interactions in the NiO lattice.

- What is the ground state of a triangular lattice Ising model?
- The Ising model can be implemented using non-collinear spins. The dot product in the $S_i.S_j$ term allows spins to point in any direction. Implement the 2D triangular lattice for a non-collinear spin, what is the ground state?

$$H = -J \sum_{<ij>} S_i.S_j - h \sum_i S_i$$

- For many systems the ground state spin structure is difficult to find using the Metropolis algorithm. Other algorithms, for example genetic algorithms provide a route to find the system ground state. Using a genetic algorithm find the ground state of the 2D non-collinear Ising model on the triangular lattice.

Remember that more is not necessary better with scientific investigations, an in depth study of one aspect will provide more insight than a cursory look at everything. You are therefore not expected to complete every investigation below this is simply a list of possible directions you may wish to take your investigation.