5CCP211C — Introduction to Numerical Modelling
Physics Department — King's College London

Metropolis Monte Carlo

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Group 2

1 Background and Theory

Metropolis Monte Carlo The Monte Carlo approach uses random numbers to sample data and estimate such quantities and probabilities and areas which are representative of the original data. In this report a Metropolis Monte Carlo approach is used to study a Maxwell-Boltzmann distribution. A Maxwell-Boltzmann distribution is a probability distribution. In this report we will use Metropolis Monte Carlo(MMC) which uses Markov Chains to model a probability distribution of the energy of gas molecules at equilibrium. Markov Chains are random walks where the sequence of possible future events only depends on the present state. In this case the probability of a difference between the two points on a random step will be compared to the Maxwell-Boltzmann distribution and if there is a positive difference between the probability o the two points the step will be accepted. The Maxwell Boltzmann distribution is given below:-

$$p(T) = e^{\beta \delta E} \tag{1}$$

Ising Model The Ising model is used to model the gas. This model is used to study the ferromagnetic properties of metallic lattices but can also be used to examine a gas, as it can be modelled as a regular two dimensional lattice. Interactions with the nearest neighbours are considered only. This is effective as it allows us to use Markov Chains and hence MMC, so there are 4 possible steps we can take from each gas molecule to the next. In the Ising model each individual molecule is allocated a spin. Firstly a random flip is selected and its flip is measured if the flip is less than 0 then the flip is executed on its own whereas if a flip is above zero it is executed with a probability corresponding

the the Boltzmann Distribution. A key sign that the model has reached equilibrium is the energy reaching a steady state. Another property of the lattice is magnetisation, which acts as an ordered parameter. This is the sum of the values for each lattice point. The magnetisation per site is the magnetisation divided by the number of lattice points. The energy per site is the sum of the products of the values' lattice sites multiplied by the interaction strength -J. If two neighboring spins are in the same direction then J or the interaction strength will be negative and anti-ferromagnetic otherwise the direction of the spin of the interacting pair are different then J is positive and the interaction is ferro magnetic. The formula for specific heat capacity is

$$c = \frac{< E^2 > - < E >^2}{(k_B T)^2 N} \tag{2}$$

2 Overview of Algorithms

Plan and description Firstly certain modules are imported for calculations and the presentation of the graphical solutions. A class for the MMC is created and the functions involved are defined with given variables. The model is equilibrated within the default estimate. A second class is introduced for the Ising Model. The same is done with this, general parameters are set and functions to be used later on are defined. An experimental result is determined for temperature, energy, magnetization and specific heat and compared to a theoretical solution; $Onsager's\ Solution$. Probability is calculated through manipulating the Boltzmann equation by making the subject the change in energy . The local field at each side of the lattices and the sub lattices are flipped using the $TrueFalseMatrix$. Both the experimental and the theoretical Onsager solution are illustrated graphically using code from lines 156 to 239. This plot can be seen in $Figure$1 below;

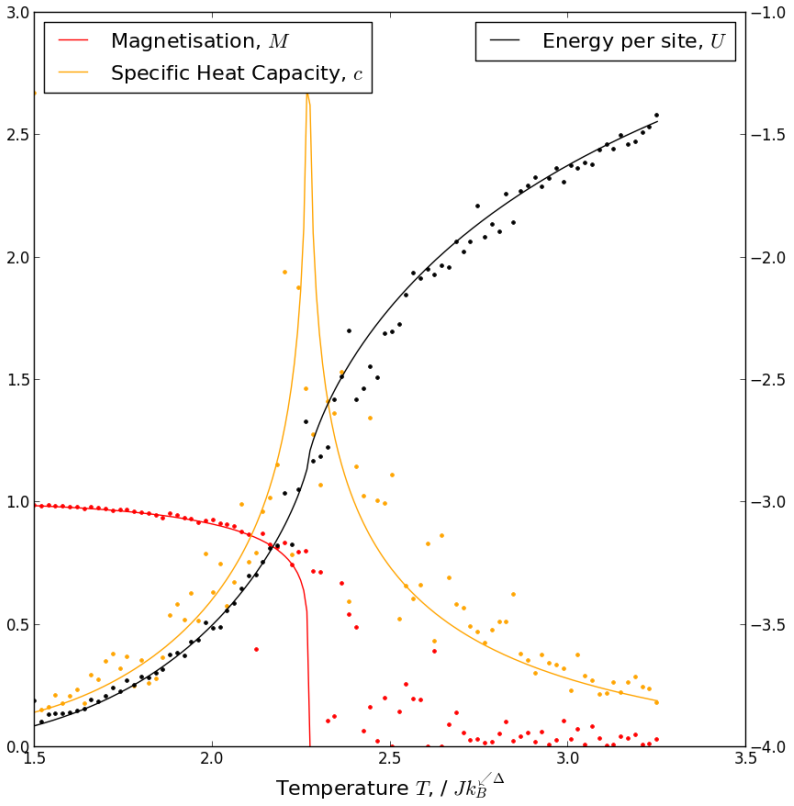

Figure 1

Metropolis Monte Carlo Class One of the functions assigned to the class, the *step* function performs parallel Metropolis-Hastings update on the model where it obtains a sequence of random samples from a probability distribution for which direct sampling is difficult. In this case, the Maxwell-Boltzmann distribution.

```
alpha = self.get_probability(state)

acceptance_mask = uniform(0,1,size=alpha.shape) < alpha
self.state[acceptance_mask] = state[acceptance_mask]
```

Here alpha plays the part of a *mask* which is small compact iteration producer. Equilibrate model is set within the default estimate of self.state.size iterations. Initially the system is not in a steady state, once the values stop

fluctuating and start oscillating around a fixed interval the system has reached thermal equilibrium. Part of the code it involves is seen below;

```
n_steps = n_steps if n_steps is not None else self.state.size
    for _ in xrange(n_steps) :
        self.step()
```

The sample model attributes given current equilibrated state.

Ising Model Class In this model, the *self interaction kernel* interacts with the matrix of its direct neighbours at a distance of a from its centre. The two dimensional model with spins (-1,1) defaults to nearest neighbour under certain periodic boundaries conditions. The interaction kernel gives the value of the field around the central spin by summing the *up* and *down* spins of its 4 neighbours. (above,below,left and right).

```
if interaction_kernel is None:
    self.interaction_kernel = array([[0,1,0],[1,0,1],[0,1,0]])
else :
    self.interaction_kernel = interaction_kernel
```

Where the matrices in the array describe the positions of the neighbours involved. A chequerboard sub lattice is introduced to help illustrate *random walk*. This random walk starts from an arbitrary point but makes it way and ends up fluctuating around an equilibrium point. It uses a matrix to flip the spins randomly while producing a specific probability of it being accepted. Another function is defined where energy is calculated by the following equation;

$$E = -J/2N \sum_{k=0}^{N} S_k n n_k \tag{3}$$

Here the two ns represent the direction of spin or self state and S represents the $field$ at that certain event point. The division by 2 is there as the interaction of the pair is only needed from a single side in this calculation. This iterable manipulation is done to the other functions and their parameters. Specific Heat, magnetization and temperature are all found using equations (1) and (2). These values are all experimental and the theoretical counterparts are calculated using Onsager's exact solution for two dimensional lattices. The acceptance probability of the flipped sub lattices is also calculated using equation (1). An assumption is made that the spin can only take place in two directions; up and down. These two directions are given the values; +1 and -1. The theory behind this neighbour interaction is that at low temperatures the spins are aligned and the magnetization is high while at high temperatures the spin fluctuates and magnetization averages 0. Energy changes between U' and U state are only considered.

$$H^{spin} == -J \sum_{k=0}^{N} s_i s_j \tag{4}$$

The command *evolve* is used to return but not overwrite a flipped chequerboard lattice. The original lattice is only overwritten until Monte Carlo allows it. S_i spin is selected arbitrarily if the change in energy between the states U' and U is less than 0 then the spin is flipped else the spin is flipped at probability calculated using equation 1 where *beta* (reduced temperature) is equal to inverse of k_bT.

Calculations An important point to note is that the Kinetic element of energy is ignored due to the fact *random walk* does not give trajectory as at each step, a new event is created. The only requirement is the equilibrium state energy. Once the thermal energy reaches equilibrium, the code no longer accepts flipped sub lattices as their probability of acceptance nears 0. The number of lattice spins is kept high at 2^8 spins to maximise efficient Monte Carlo counting.

3 Results and Discussion of Data

Specific Heat Capacity Figure 1 is the final plot illustrating specific heat capacities at different reduced temperatures. On the right hand axis we have the values of energy which range from 4.0 to 1.0 and on the left there is specific heat and magnetization. Each of the solid yellow line represents Onsager's theoretical solution to the Ising model. All of the coloured plot points follow the trend of their respective coloured line. There is a positive correlation between energy per site and temperature and the rate of change of energy per site is highest at critical temperature. It is clearly visible that the experimental values follow the trend of Onsager's solution, indicating that the code successfully models Onsager's solution and the Maxwell-Boltzmann Distribution as a whole. The critical temperature at which the graph is at its maximum is in the vicinity of the literature value given to be 2.276 at which thermal equilibrium takes place.