

2D_Ising_Notes

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1 2D Ising Model

In this exercise, you will simulate a 2D Ising model on a square lattice. The Ising model is a simple model to demonstrate ferromagnetism. It consists classical spins arranged in a lattice with nearest-neighbor interactions. The model can also be extended to higher dimensions.

2 Hamiltonian:

$$2.0.1 \quad H = J \sum_{\langle ij \rangle} \sigma_i^z \cdot \sigma_j^z - h \sum_i \sigma_i^z$$

where $\langle ij \rangle$ = nearest neighbor couplings. For simplicity assume that $\sigma = \pm 1$. J is the coupling strength ($J < 0$ for ferromagnetic interactions and $J > 0$ for antiferromagnetic interactions). h is the magnetic field. Set it to zero unless otherwise mentioned.

The spin lattice can be realized using a 2d (Integer) matrix of size L , e.g., `lattice[1:L,1:L]`. You can choose $L = 20$ to start with. Of course you can increase L later on.

Choose periodic boundary conditions, such that the the spin corresponding to $[i,L+1] = [i,1]$ and $[L+1,j] = [1,j]$

Choose $|J| = 1$ such that your temperature scale is in terms of J . Also choose $k_B = 1$, such that $\beta = 1/T$.

2.0.2 Start from a (high temperature) configuration where the spins are randomly distributed i.e., choose $\sigma_i = \pm 1$ with a probability 1/2.

```
In [ ]: # for each site [i,j]
        n = rand();
        if(n > 0.5)
            lattice[x,y]=1;
        else
            lattice[x,y]=-1;
```

2.0.3 Cool the system down in steps of $tstep$. E.g., you can choose $t_{hi} = 5.0$ and $t_{low} = 0.0$ with $tstep = 0.5$, the number of temperature steps $nstep = \frac{t_{hi}-t_{lo}}{tstep}$

2.0.4 At each temperature, thermalize the system using the Metropolis algorithm as described below:

3 Metropolis Algorithm:

3.0.1 Markov-Chain realized through changing the configuration of a single spin

a) Choose a random site (i,j)

```
In [ ]: x=rand(1:L); y=rand(1:L)
```

b) Calculate ΔE , the energy cost of flipping a the spin at site [i,j]

```
In [ ]: de = 2*h*lattice[i,j]- 2*j1*lattice[i,j]*(lattice[i,j+1]+lattice[i,j-1]+lattice[i-1,j]
```

Be careful near the edge of the lattice, eg, if you choose a spin at [L,j] then the site [L+1,j] corresponds to [1,j] Hint: You can use the following form to find out the adjacent site (verify that it works!!)

```
In [ ]: i1 = mod(i+1-1,L)+1; i2 = mod(i-1-1,L)+1
```

c) Choose the new configuration if

→ $\Delta E < 0$, or

→ with probability $\exp(\beta\Delta E)$

```
In [ ]: r = rand()
        if (de<0.0 || r < exp(-de/temp)) # Choose new configuration with probability ~ exp(-bet
        # change the spin
        lattice[i,j]=-1*lattice[i,j];
        end
```

d) Repeat steps a) through c) for at least $\approx L^3$ iterations. Better to choose even more iterations e.g., $100L^2$.

3.1 Visualize the system for different temperatures. You can save a copy of the configuration at each temperature step and plot the lattice at the end of the run.

```
In [ ]: # Save a copy of the lattice in some other matrix. eg,
        Lattice_save[iteration,:,:] = lattice[:,:]
        # ...
        # ...
        # Later on, you can plot the lattice, the different iterations corresponds to differen
        imshow(Lattice_save[iteration,:,:], cmap="gray", interpolation="none")
```