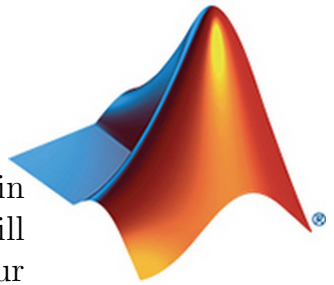


The Ising model

The ferromagnetic Ising chain is a model of interacting magnetic dipoles. Consider a chain made of N spins σ_i that each take the value 1 or -1 if the spin at site i is up or down. We will assume that the chain is *periodic*, therefore identifying $\sigma_{N+1} = \sigma_1$. The nearest-neighbour (n.n.) Ising model assumes that interactions only exists for adjacent spins; the energy of a particular configuration $\{\sigma_i\}_{i=1}^N$ is given by

$$E(\{\sigma\}) = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1}, \qquad J > 0, \tag{1}$$

and its magnetization is

$$M(\{\sigma\}) = \sum_{i=1}^{N} \sigma_i. \tag{2}$$

The model described by (1) can be solved exactly. As it turns out, the one-dimensional n.n. Ising chain does not feature a phase transition; it never goes from a disordered state ($\langle M \rangle = 0$) to an ordered state ($\langle M \rangle$ finite) as the temperature decreases.

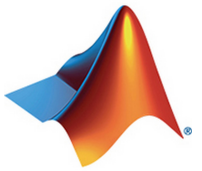
However, a phase transition may occur when spins are coupled beyond their nearest neighbours. The spin model

$$E(\{\sigma\}) = -\sum_{i \neq j} J_{ij} \sigma_i \sigma_j, \qquad J_{ij} = J|i-j|^{-a}, \qquad J > 0, \tag{3}$$

exhibits a phase transition from a disordered to a magnetized phase for a finite range of values a.

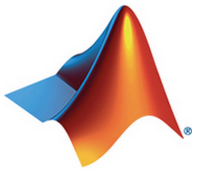
Rather than analytically looking for the existence or absence of an ordered phase at low enough temperatures, we will simulate the thermalization of the two Ising models above on a computer by using the Metropolis algorithm and observe whether the spin chains spontaneously magnetize or not.

The Metropolis algorithm



The Metropolis algorithm is a widely used Monte Carlo simulation that dynamically guides a given spin configuration towards thermal equilibrium. The steps needed to write the algorithm can be briefly outlined as follows:

1. Generate a random initial spin configuration $\{\sigma_i\}_{i=1}^{N}$ with energy E_0;
2. Flip a random spin ($\sigma_k \to -\sigma_k$) and calculate the energy E_t of this trial state;
3. Calculate the difference in energy generated by the spin flip, $\Delta E = E_t - E_0$, and the associated transition probability $p = \exp(-\beta \Delta E)$:
   - If $\Delta E \leq 0$, then we accept the spin flip because the trial spin configuration is energetically favoured over the initial state;
   - If $\Delta E > 0$, then we compare the transition probability p to a random number r. We accept the new configuration if $r \leq p$. Otherwise, we keep the spin unflipped.
4. Update the average energy, magnetization, etc.
5. Repeat steps (2) to (4) with the chosen spin configuration until thermal equilibrium has been reached.



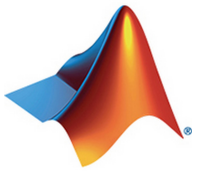
Question 1: Nearest-neighbours Ising model

A working version of the Metropolis algorithm for the n.n. Ising model can be found on the course web page at `http://www.phas.ubc.ca/~rozali/ising1D.m`. Be sure to understand the role of each line in the code. You should know:

- What does the function *circshift* do? Why do we use it?
- How is the change in energy ΔE computed?

Once you feel comfortable with the code, answer the following questions:

1. Run the simulation in the high temperature limit (use $N = 1000$, $T = 2$ and $J = 0.1$). How does the spin chain behave? How does that translate in the average energy per particle $\langle E \rangle / N$ and average magnetization per particle $\langle M \rangle / N$ over time?
2. Calculate the specific heat at constant volume $C_V = T^{-2} \langle (\Delta E)^2 \rangle$, where $\langle (\Delta E)^2 \rangle = \langle (E - \langle E \rangle)^2 \rangle = \langle E^2 \rangle - \langle E \rangle^2$.
3. Use the function *hist* to create a histogram of the energy per particle. Explain its shape, and how it is related to C_V. Is $\langle E \rangle = -NJ \tanh(J/T)$, as expected?
4. Run the simulation in the low temperature limit (use $N = 1000$, $T = 0.1$ and $J = 1$). Is the system spontaneously driven towards a magnetized phase? Plot the histogram of the net magnetisation (without the absolute value).
5. Create a histogram of the energy distribution at low temperatures. Why does the distribution look less continuous?



Question 2: Spatially coupled Ising chain

As you saw in Question 1, the one-dimensional n.n. Ising model does not spontaneously magnetize at some critical temperature. However, allowing the spins to interact with the ones beyond their nearest neighbours as in (3) deeply affects the behaviour of the Ising chain. Let's alter the existing Metropolis algorithm to see a phase transition emerge from a spatially dependent coupling. Only two things need to be modified:

- The energy of an initial random spin configuration needs to be computed according to (3). Be careful in your evaluation of the distance $|i - j|$ between two spins; because the chain is periodic, the distance between any two spins is *at most* floor$(N/2)$.
- The change in the energy ΔE after a random spin flip now gets influenced by all the other spins on the chain.

Once you have implemented these changes in your Metropolis algorithm, answer the following questions (with $a = 2$):

1. Run the simulation in the high temperature limit (use $N = 1000$, $T = 2$ and $J = 0.1$). How does the spin chain behave? How does that translate in the average energy and average magnetization over time?
2. Create a histogram of the energy distribution. Explain its shape.
3. Run the simulation in the low temperature limit (use $N = 1000$, $T = 0.1$ and $J = 1$). Is the system spontaneously driven towards a magnetized phase?