SET-UP

Hamiltonian and Gibbs measure

We use Monte-Carlo (M-C) to simulate our Ising model,

$$H = -\frac{J}{2N}\sum_{i=1}^{N} W_{ij} S_i S_j, \tag{1}$$

where factor $1/2$ is introduced to prevent overcounting (we assume that $W_{ij} = W_{ji}$). We want to understand how the spin configuration $\boldsymbol{S} = (S_1, \dots S_N)$ behaves for different temperatures. Our main object of interest is the average i-th spin value,

$$\langle S_i \rangle = \frac{1}{\mathcal{Z}} \sum_{\text{MS}} S_i e^{-\beta H(\boldsymbol{S})}, \tag{2}$$

where $\mathcal{Z}$ is the partition function and we know that the spins are distributed with the Boltzmann-Gibbs distribution with probability density

$$p(\boldsymbol{S}) = \frac{e^{-\beta H(\boldsymbol{S})}}{\mathcal{Z}}. \tag{3}$$

The notation $\sum_{\text{MS}}$ means the summation overall possible microstates of spins. The Boltzmann-Gibbs distribution arises as the *equilibrium* distribution, so it extremizes the free energy F.

Since the model is mean-field, we can derive the self-consistency equation for the local magnetization $m(x)$,

$$m(x) = \tanh\left\{\beta J \int_0^1 dy\, W(x,y) m(y)\right\}, \tag{4}$$

where we have taken $N \to \infty$ limit, have used graphon and now x is the continuous variable labeling the spins. Each solution of this self-consistency equation corresponds to the critical point of the free energy density f.

METROPOLIS-HASTINGS ALGORITHM

We start from the initial spin configuration $\boldsymbol{S}^{(0)}$. This configuration can be whatever we want. We cannot sum over all possible configurations, since for N spins we have 2^N configurations and we need the thermodynamic limit, $N \to \infty$. But we need the Boltzmann-Gibbs distribution to compute $\langle S_i \rangle$, so we need to *sample measure*. We cannot compute $\mathcal{Z}$, we would like to propose a method where computation of $\mathcal{Z}$ can be avoided. Our target distribution is known: it is the Boltzmann-Gibbs distribution $p(\boldsymbol{S})$.

Metropolis algorithm constructs the Markov chain of states, where each new state $\boldsymbol{S}^{(k+1)}$ is generated from the current state $\boldsymbol{S}^{(k)}$ by a simple rule. This rule is based on the so-called *proposal distribution* $g(\boldsymbol{S}'|\boldsymbol{S}^{(k)})$, where $\boldsymbol{S}'$ is the proposal for a new state and $\boldsymbol{S}^{(k)}$ is our current state. We accept this proposal state $\boldsymbol{S}'$ with acceptance probability,

$$A(\boldsymbol{S}^{(k)} \to \boldsymbol{S}') = \min\left(1, \frac{p(\boldsymbol{S}')}{p(\boldsymbol{S})} \frac{g(\boldsymbol{S}'|\boldsymbol{S}^{(k)})}{g(\boldsymbol{S}^{(k)}|\boldsymbol{S}')}\right) \tag{5}$$

Then, we generate a random number a from the uniform distribution on $[0,1]$. If $a \le A(\boldsymbol{S}^{(k)} \to \boldsymbol{S}')$, we accept our proposal state, i.e. $\boldsymbol{S}^{(k+1)} = \boldsymbol{S}'$. If $a > A(\boldsymbol{S}^{(k)} \to \boldsymbol{S}')$, we reject this change by keeping $\boldsymbol{S}^{(k+1)} = \boldsymbol{S}^{(k)}$. It is known (and proven, I assume) that after a large enough number of steps we will obtain the desired Boltzmann-Gibbs distribution that delivers the global minima for free energy.

This rule is as follows:

1. Pick i-th of N spins uniformly, i.e. $g(\boldsymbol{S}'|\boldsymbol{S}^{(k)}) = g(\boldsymbol{S}^{(k)}|\boldsymbol{S}') = N^{-1}$
2. Flip this spin, $S_i \mapsto -S_i$, all other spins are unchanged

Our acceptance probability becomes

$$A(\boldsymbol{S}^{(k)} \to \boldsymbol{S}') = \min\left(1, \frac{e^{-\beta H(\boldsymbol{S}')}}{e^{-\beta H(\boldsymbol{S}^{(k)})}}\right) = \\ = \min\left(1, e^{-\beta \Delta E}\right), \tag{6}$$

where $\Delta E = E' - E^{(k)}$ is the energy difference between state, where one spin is flipped and one spin is not flipped.

Some important features. If $\Delta > 0$ it means that it is "bad" spin flip: we want to decrease the energy, not increase. For large temperatures $\beta \ll 1$, we have $e^{-\beta \Delta E} \approx 1$, so we accept virtually always and continue to make spin flips. For small temperatures $\beta \gg 1$, we have $e^{-\beta \Delta E} \ll 1$, so unfavorable flips are rare, and we are trapped in the local energy minima.

Remark: there exist two realizations of M-C via the Metropolis-Hastings algorithm. The first one is *1-spin flip*, i.e. on each step we pick one spin randomly and flip it. The second one is *N-spin flip*, where we flip N spins.

OUR MODEL

General scheme

1. Prepare initial spin state $\boldsymbol{S}^{(0)}$, which corresponds to pattern of eigenvectors of the matrix W_{ij}, i.e. $\boldsymbol{S}^{(0)} = \text{sign}(\boldsymbol{v}_j)$, where $\boldsymbol{v}_j$ is the j-th eigenvector. Our eigenvalues are ordered, i.e. $\lambda_1 > \lambda_2 > \ldots$, so $\boldsymbol{v}_2$ corresponds to λ_2
2. Choose large N since all our results are applicable in $N \to \infty$ limit
3. Starting from the initial state, make `n_thermalization` steps.
4. Having reached the metastable state, make `n_measurements` steps and compute the average spin values: denoting `n_measurements` as L, we compute

$$\langle S_i \rangle = \frac{1}{L} \sum_{k=1}^{L} S_i^{(k)}. \tag{7}$$

AFM case: minimal eigenvalue

J	-1.0
T	$J\lambda_{-1} - 0.01 \approx 0.02$
N	5000
initial state	random uniform
`n_thermalization`	200000
`n_measurement`	100000

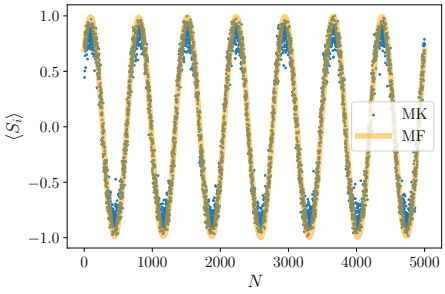

Fig. 1. AFM case: state that corresponds to λ_{-1}

J	1.0
T	$J\lambda_2 - 0.05 = 0.11$
N	10000
initial state	$\text{sign}(\boldsymbol{v}_2)$
`n_thermalization`	60000
`n_measurement`	40000

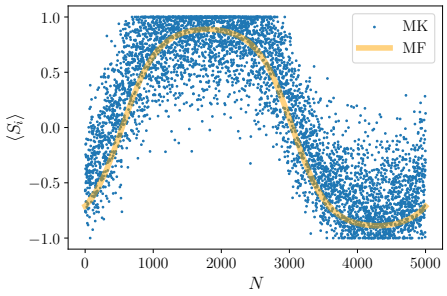

Fig. 2. FM case: transient state that corresponds to λ_2

FM case: second eigenvalue

FM case: third eigenvalue

J	1.0
T	$J\lambda_3 - 0.05 \approx 0.08$
N	5000
initial state	$\text{sign}(\boldsymbol{v}_3)$
`n_thermalization`	50000
`n_measurement`	50000

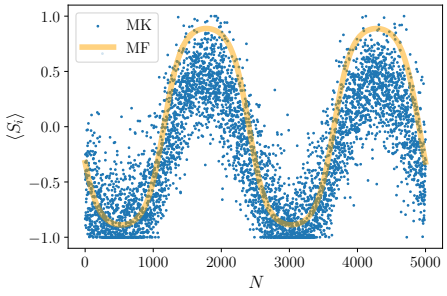

Fig. 3. FM case: transient state that corresponds to λ_3