Tutorial 4: Mean Field approach

TBD and Caterina De Bacco

Exercise 1: Curie-Weiss model again

The Hamiltonian of the Curie-Weiss model can be written as:

$$H(\mathbf{s}) = -\frac{J}{2N}\sum_{i,j} s_i s_j - h\sum_i s_i \,.$$

From the lecture, we know that the Mean Field free variational energy is:

$$F[Q] = -\frac{J}{2}m^2 - hm + \frac{1}{\beta}\left[\frac{1+m}{2}\log\left(\frac{1+m}{2}\right) + \frac{1-m}{2}\log\left(\frac{1-m}{2}\right)\right] \tag{1}$$

where m is the expected total magnetisation $\mathbb{E}_Q\left[\sum_i s_i/N\right]$.

(a) Plot the function $F[Q]$ as a function of m in the two following cases: (i) at $h = 0$ for different values of J larger and lower than 1 and (ii) at a value of J larger than 1 for different values (positive and negative) of h. Describe what you see in both cases.

(b) The minimizer m^* is also the solution of the "self-consistent equation":

$$m = \tanh\left[\frac{J}{2}m + h\right].$$

Compute the value of m^* in the three following cases:
(i) $h = 10^{-6}$ and J between 0 and 2;
(ii) $h = -10^{-6}$ and J between 0 and 2; and
(iii) $J = 1.5$ and h between -1 and 1.

(c) Focusing on the case $J = 1.5$. With $h = 0.1, 0.2$, how many solutions to the self-consistency equations are there? Which one is the correct one?
Plot the function $F[Q]$ to answer to these questions.

Solution.

(a) The plot of function $F_m(\beta, h, m)$ under $h = 0$ and $J = 0.9, 1, 1.2, 1.5$ are shown in Fig. (1).
At small couplings ($J < 1$), the curve has only one minimum at zero. At high couplings ($J > 1$), the curve has two local minimums symmetric around zero. There is a phase transition at $J = 1$.

The plot of function $F[Q]$ under $J = 1.2$ and $h = -0.1, -0.05, 0, 0.03, 0.07$ is shown in Fig. (2). Since $J > 1$, the minimum will drift away from zero. The number of local minima can be one or two depending on h. If $h < 0$, the global minimum will be closer to -1, if $h > 0$, the global minimum will be closer to 1. When h moves pass zero, the global minimum changes sharply to another value with opposite sign.

(b) The plot of function $m^*(\beta, h)$ under $h = \pm 10^{-6}$ and $J \in (0, 2]$ is shown in Fig. (3).
The plot of function $m^*(\beta, h)$ under $J = 1.5$ and $h \in [-1, 1]$ is shown in Fig. (4).

Figure 1: Gibbs free energy Curie-Weiss for varying parameters.

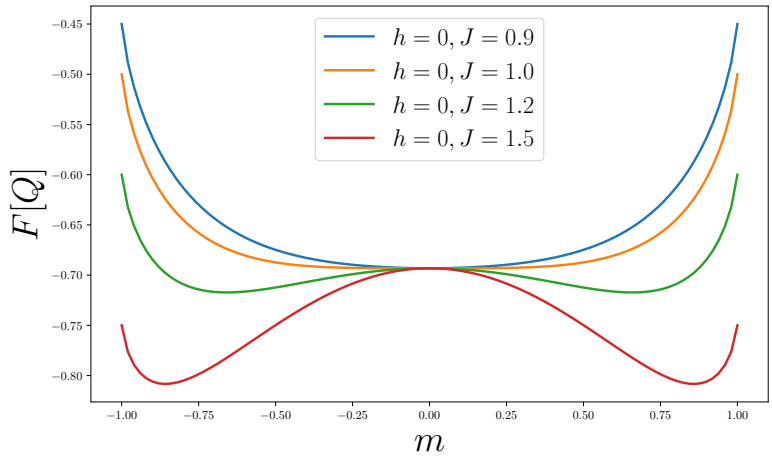
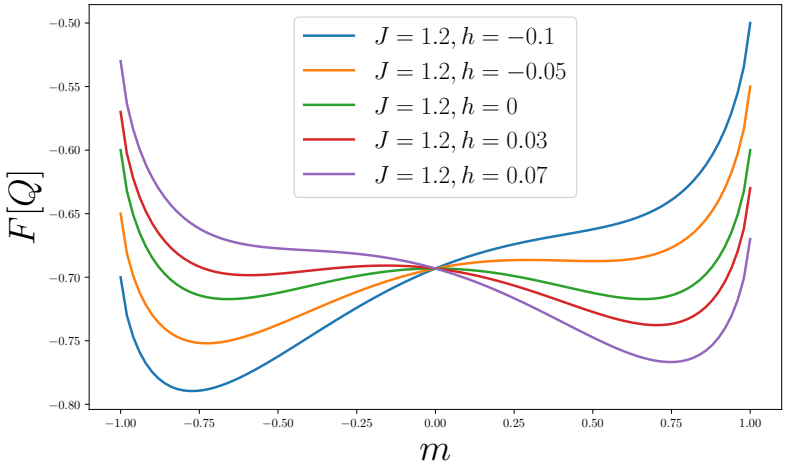


Figure 2: Gibbs free energy Curie-Weiss for varying external field.



(c) The plot of function $F[Q]$ under $J = 1.5$ and $h = 0.1, 0.2$ is shown in Fig. (5).
For $h = 0.1$, there are two solutions, the right one has lower function value thus it is the correct one. For $h = 0.2$, there is only one solution, so it is the correct one.

□

Figure 3: Magnetization Curie-Weiss for varying couplings.

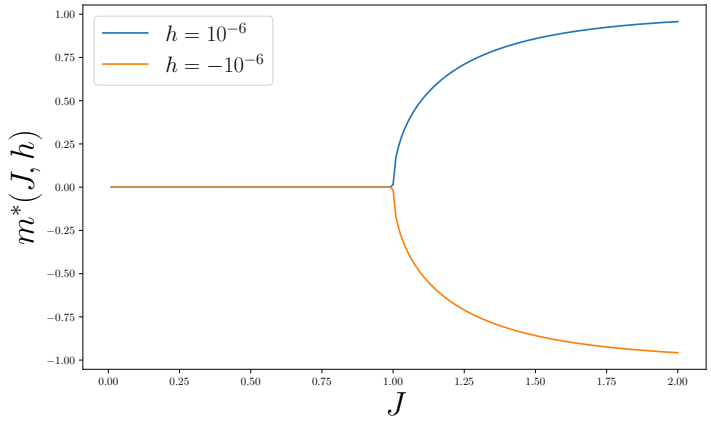
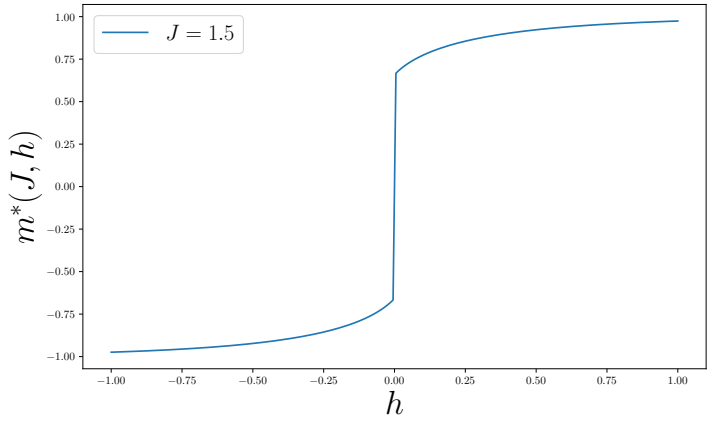


Figure 4: Magnetization Curie-Weiss for varying external field.



Exercise 2: sampling from the Curie-Weiss model

Consider again the Hamiltonian of the Curie-Weiss model.
A practical way to sample configurations of N spins from the Gibbs probability distribution:

$$P(\mathbf{s}) = \frac{e^{-\beta H(\mathbf{s})}}{Z} \quad ,$$

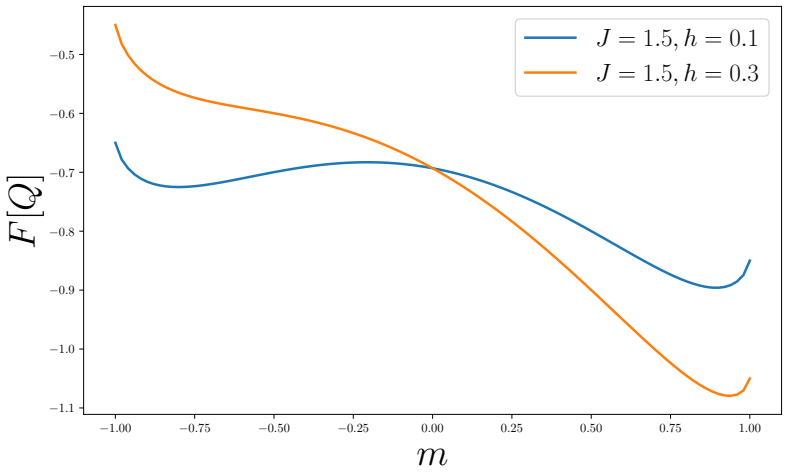
with

$$H(\mathbf{s}) = -\frac{J}{2N}\sum_{i,j} s_i s_j - h\sum_i s_i \,,$$

is the Monte-Carlo-Markov-Chain (MCMC) method, and in particular the Metropolis-Hastings algorithm.
It works as follows:

1. Choose a starting configuration for the N spins values $s_i = \pm 1$ for $i = 1, \ldots, N$.
2. Choose a spin i at random. Compute the current value of the energy H_{now} and the value of the energy H_{flip} if the spins i is flipped (that is if $s_i^{\text{new}} = -s_i^{\text{old}}$).
3. Sample a number r uniformly in $[0,1]$ and, if $r < e^{\beta(H_{\text{now}} - H_{\text{flip}})}$ perform the flip (i.e. $s_i^{\text{new}} = -s_i^{\text{old}}$) otherwise leave it as it is.
4. Goto step 2.

Figure 5: Gibbs free energy Curie-Weiss for varying external field.



If one is performing this program long enough, it is guarantied that the final configuration ($\mathbf{s}$) will have been chosen with the correct probability.

(a) Write a code to perform the MCMC dynamics, and start by a configuration where all spins are equal to 1. Take $h = 0$, $J = 1$, $\beta = 1.2$ and try your dynamics for a long enough time (say, with $t_{\max} = 100N$ attempts to flips spins) and monitor the value of the magnetization per spin $m = \sum_i s_i/N$ as a function of time. Make a plot for $N = 10, 50, 100, 200, 1000$ spins. Compare with the exact solution at $N = \infty$. Comment.

(b) Start by a configuration where all spins are equal to 1 and take $h = -0.1$, $J = 1$, $\beta = 1.2$. Monitor again the value of the magnetization per spin $m = \sum_i s_i/N$ as a function of time. Make a plot for $N = 10, 50, 100, 200, 1000$ spins. Compare with the exact solution at $N = \infty$. Comment.

Solution. We first need an expression for $H_{now} - H_{old}$ for a single-variable flip. Since we may try different β, h, N ($J = 1$ is fixed), to avoid confusion it is better to write them explicitly. For any $k \in 1, \ldots, N$, we can split the Hamiltonian as:

$$H(\mathbf{s}) = -\frac{J}{N}\sum_{i<j} s_i s_j - h\sum_{i=1}^{N} s_i \tag{2}$$

$$= \underbrace{-\frac{J}{N}\sum_{\substack{i>j \\ i\neq k, j\neq k}} s_i s_j - h\sum_{i\neq k} s_i}_{\text{do not contain } s_k} \underbrace{-\frac{J}{N} s_k \sum_{i\neq k} s_i - h s_k}_{\text{contains } s_k} \tag{3}$$

Suppose we flip the k-th spin; then the only difference is $s_k^{\text{new}} = -s_k^{\text{old}}$, yielding:

$$H_{\text{now}} - H_{\text{flip}} = H(\mathbf{s}_{old}) - H(\mathbf{s}_{new}) \tag{4}$$

$$= \left[-\frac{J}{N} s_k^{\text{old}} \sum_{i\neq k} s_i^{\text{old}} - h s_k^{\text{old}}\right] - \left[-\frac{J}{N} s_k^{\text{new}} \sum_{i\neq k} s_i^{\text{new}} - h s_k^{\text{new}}\right] \tag{5}$$

$$= \left[-\frac{J}{N} s_k^{\text{old}} \sum_{i\neq k} s_i^{\text{old}} - h s_k^{\text{old}}\right] - \left[\frac{J}{N} s_k^{\text{old}} \sum_{i\neq k} s_i^{\text{old}} + h s_k^{\text{old}}\right] \tag{6}$$

$$= -2 s_k^{\text{old}} \left[\frac{J}{N}\sum_{i\neq k} s_i^{\text{old}} + h\right] \tag{7}$$

Secondly, when $N \to \infty$, the Boltzmann distribution is dominated by configurations whose magnetization equals m^*, the minimum of the Hamiltonian. So if we can run a simulation with infinite N, the plot of m will start with a warm-up stage to reach m^*, once m^* is reached, the plot will get stuck there.

(a) Since $h = 0$, there the two local minimizers have same function value so either one can achieve the global minimum. However, we start our MCMC chain at all-one configuration, which is closer to the positive minimizer. It is possible that the random walk will reach the negative minimizer. Actually in the long run, the chain will first walk to the positive minimizer and stay for a while, then walk to the negative minimizer and stay for a while, and do this back and forth. The larger N is, the longer the chain stay at the minimizers, and the less fluctuation the chain will deviated from the minimizer.

(b) In this case we have similar behavior as part (a), the only difference is $h = -0.1$ breaks down the balance between two local minimizers. As discussed in Problem 2 (c), the negative minimizer is the correct one. So the trace plot will start with a warm-up stage to reach m^*, once m^* is reached, the trace plot will get stuck at there. The larger N is, the less fluctuation the chain will deviated from m^*.

□

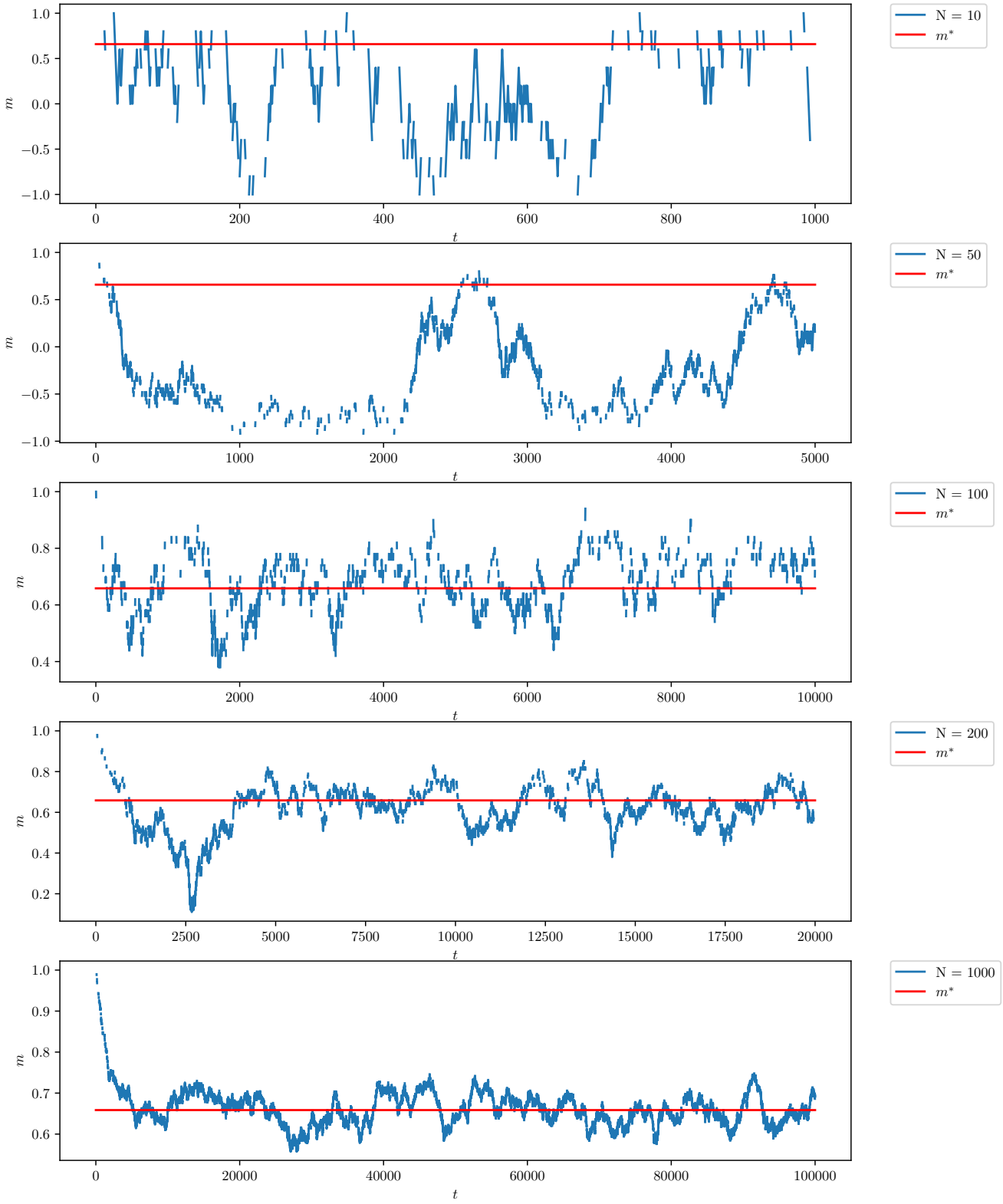


Figure 6: Instantaneous magnetization for $\beta = 1.2, h = 0$ and $N = 10, 50, 100, 200, 1000$

Figure 7: Instantaneous magnetization for $\beta = 1.2, h = -0.1$ and $N = 10, 50, 100, 200, 1000$