Advanced Probabilistic Machine Learning and Applications

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1 Tutorial 8: TAP approach

Exercise 1: planted SK model

We consider a model similar to the SK model, with the difference that the J_{ij} are generated from a particular realization, called "planted". Specifically, we start from the following generative model for the $P(\mathbf{s}, \mathbf{J})$:

$$s_i \sim \frac{1}{2}\delta(s_i - 1) + \frac{1}{2}\delta(s_i + 1) \quad , \quad i = 1, \dots, N \tag{1}$$

$$J_{ij} \,|\, s_i, s_j \sim \mathcal{N}\left(\frac{s_i s_j}{\sqrt{N}}, \sigma^2\right) \quad , \quad (i,j) \in N^2 \tag{2}$$

Goal: estimate the planted $\mathbf{s}$ given the $\mathbf{J}$.

(a) Use Bayes' theorem to write the posterior distribution $P(\mathbf{s}|\mathbf{J})$.

(b) Rewrite it as a Boltzmann distribution similar to the SK model with $\beta := \frac{1}{\sigma^2}$.

(c) We would like to estimate the mean of $P(\mathbf{s}|\mathbf{J})$. However, this is not tractable analytically. We will instead use the approximation introduced in the class.
Write in a *jupyter* notebook a function to *sample* an instance of $(\mathbf{s}, \mathbf{J})$.

(d) In the same notebook, write a function that implements the TAP equation to approximate the mean $\hat{\mathbf{s}}$ of $P(\mathbf{s}|\mathbf{J})$. This is an iteration that, if it converges, gives a very good approximation for $\hat{\mathbf{s}}$ as $N \to \infty$.

For numerical reasons implement the fixed point iterations as follows:

$$m_i^{(t+1)} = \tanh\left(\frac{1}{\sigma^2\sqrt{N}}\sum_j J_{ij}\, m_j^{(t)}\right) \qquad \text{Mean Field}$$

$$m_i^{(t+1)} = \tanh\left(\frac{1}{\sigma^2\sqrt{N}}\sum_j J_{ij}\, m_j^{(t)} - m_i^{(t-1)}\frac{1}{N\sigma^4}\sum_j J_{ij}^2\left(1 - (m_j^{(t)})^2\right)\right) \qquad \text{TAP}$$

(e) Run some experiments ($N_{real} \in [10, 100]$ re-samplings of J, s at your choice) for $N = 10, 100, 1000, 5000$ and fixed $\sigma^2 = 0.1$ and check that the overlap[1] with ground-truth improves with the iterations.

[1] The overlap is defined as: $overlap(\mathbf{m}, \mathbf{s}_0) := |\frac{\mathbf{m} \cdot \mathbf{s}_0}{N}|$

(f) i) Run sum experiments ($N_{real} \in [10, 100]$ re-samplings of J, s at your choice) for $N = 10, 100, 1000, 5000$ and varying $\sigma^2 \in [0.1, 2]$.
ii) Repeat the same experiments but using the MF approximation instead.
iii) Plot the performance metrics values at convergence for TAP and MF as a function of the noise σ^2 for various N.
Comment on what you observe.

[Solution]

(a) The posterior distribution is:

$$
\begin{aligned}
P(\mathbf{s}|\mathbf{J}) &= \frac{P(\mathbf{J}, \mathbf{s})}{P(\mathbf{J})} && (3)\\
&\propto \prod_{ij} \mathcal{N}\left(J_{ij}; \frac{s_i s_j}{\sqrt{N}}, \sigma^2\right) \prod_i p_0(s_i) && (4)\\
p_0(s_i) &= \frac{1}{2}\delta(s_i - 1) + \frac{1}{2}\delta(s_i + 1) && (5)
\end{aligned}
$$

(b) It can be rewritten as:

$$
P(\mathbf{s}|\mathbf{J}) \propto e^{\frac{\beta}{\sqrt{N}} \sum_{ij} J_{ij} s_i s_j} \quad (6)
$$

(c), (d), (e) see code in Jupyter notebook.

(f) The overlap score at different values of noise is presented in Figure 1. Recall that TAP differs from mean field only for taking into account fluctuations around the mean value. At low levels of noise these fluctuations are small, in which case the mean approximation is very close to exact, and corrections are not substantial. With the increase of σ^2 however, taking them into account improves the quality of the approximation. For this reason the TAP achieves higher overlap score.

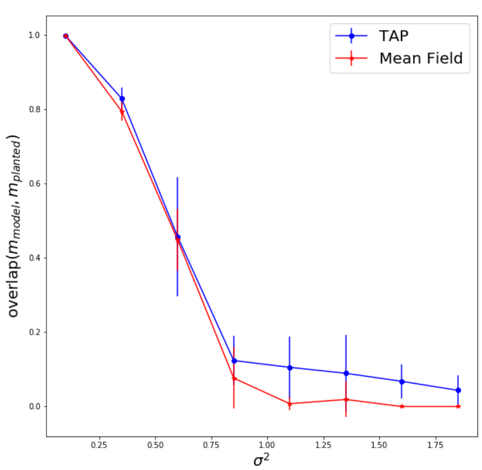

Figure 1: Overlap score for the Mean Field and TAP approximations in the planted spin glass model for $N = 500$. Overlap is computed between real and approximate average magnetization. Error bars are std over 10 samples.

Exercise 2: sampling from the SK model

Consider again the Hamiltonian of the SK model:

$$H(\mathbf{s}) = -\sum_{i\neq j} J_{ij} s_i s_j \quad . \tag{7}$$

We now want to *sample* configurations of N variables from the corresponding Boltzmann distribution for a particular realization of the couplings and comparing the empirical mean of the magnetizations with the one inferred using TAP and MF.
For sampling, we use the Monte-Carlo-Markov-Chain (MCMC) Metropolis-Hastings algorithm as we learned for the Curie Weiss model in tutorial 7.

(a) Write a code to perform the MCMC dynamics, and start by configurations extracted uniformly at random.
i) Sample a particular realization of $\mathbf{J} \sim \mathcal{N}(0, \sigma^2/\sqrt{N})$, for $\sigma^2 = 1$ and $\beta = 1.1$.
ii) Run your dynamics for a long enough time (say, with $t_{\max} = 10^3 N$ attempts to flips spins) and monitor the value of the magnetization $m = \sum_i s_i / N$ as a function of time. Make a plot for $N = 10, 100, 1000$ spins.

(b) Iterate MF and TAP equations and compare the values obtained from the ground truth MCMC sampler. To do so, draw a scatter plot of the single values m_i obtained from the MCMC sampler and the approximations (one plot per approximation, for a total of 2 plots).
Comment. Similarly to before, implement the consistency equations as

$$m_i^{(t+1)} = \tanh\left(\beta \sum_j J_{ij}\, m_j^{(t)}\right) \qquad \text{Mean Field}$$

$$m_i^{(t+1)} = \tanh\left(\beta \sum_j J_{ij}\, m_j^{(t)} - \beta^2 m_i^{(t-1)} \sum_j J_{ij}^2 (1 - (m_j^{(t)})^2)\right) \qquad \text{TAP}$$

[Solution]

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

$$H(\mathbf{s}) = -\sum_{i<j} J_{ij} s_i s_j \tag{8}$$

$$= -\underbrace{\sum_{\substack{i>j \\ i\neq k, j\neq k}} J_{ij} s_i s_j}_{\text{do not contain } s_k} - \underbrace{s_k \sum_{i\neq k} J_{ki} s_i}_{\text{contains } s_k} \tag{9}$$

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

$$H_{\text{now}} - H_{\text{flip}} = H(\mathbf{s}_{old}) - H(\mathbf{s}_{new}) \tag{10}$$

$$= \left[-s_k^{old} \sum_{i\neq k} J_{ki} s_i^{old}\right] - \left[-s_k^{new} \sum_{i\neq k} J_{ki} s_i^{old}\right] \tag{11}$$

$$= \left[-s_k^{old} \sum_{i\neq k} J_{ki} s_i^{old}\right] - \left[s_k^{old} \sum_{i\neq k} J_{ki} s_i^{old}\right] \tag{12}$$

$$= -2 s_k^{\text{old}} \sum_{i\neq k} J_{ki} s_i^{old} \tag{13}$$

A plot of the average magnetization resulting from MCMC samples is presented in Figure 2.

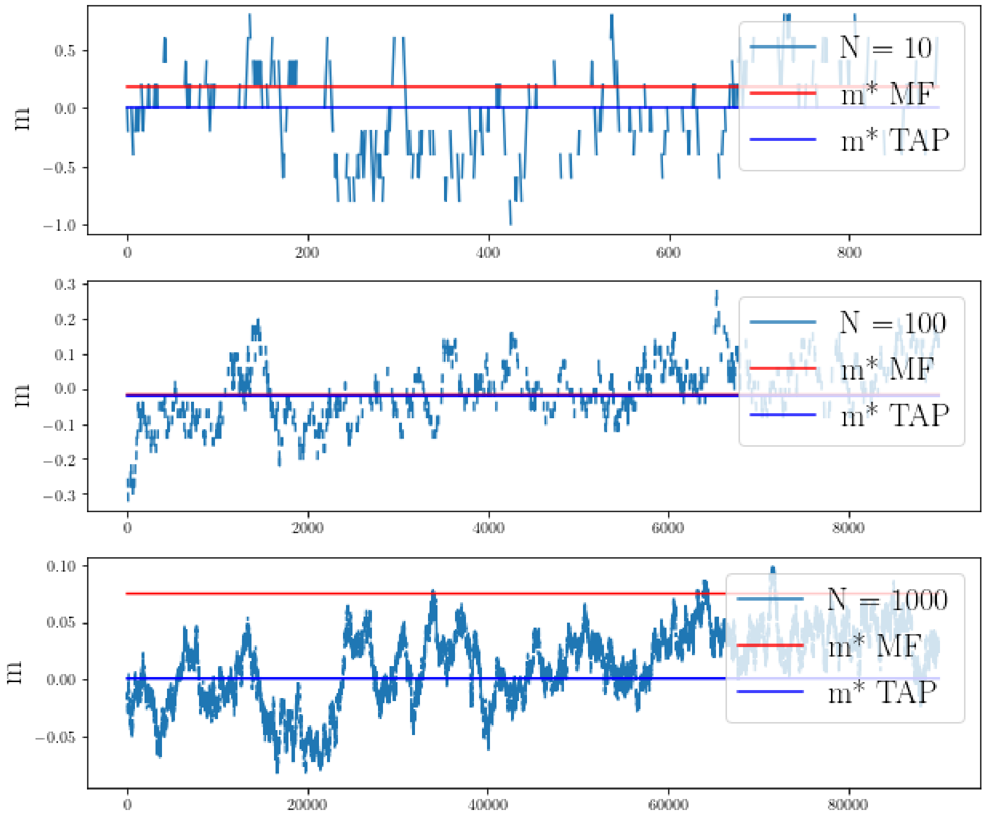

Figure 2: Empirical average magnetization obtained from MCMC sampling. Horizontal lines represent the average magnetization obtained via Mean Field and TAP approximations.

(b) A plot of the scatter plot of $m_i \, \forall i = 1, \ldots, N$ for MCMC and the approximations is presented in Figure 3. As we can see, TAP succeeds in obtaining values that are closer to the ones obtained from MCMC. Notice that MCMC has theoretical guarantees of sampling from the true Boltzmann distribution, and is therefore to be considered as a ground truth sampling. Plot closer to the $y = x$ line indicate better approximation.

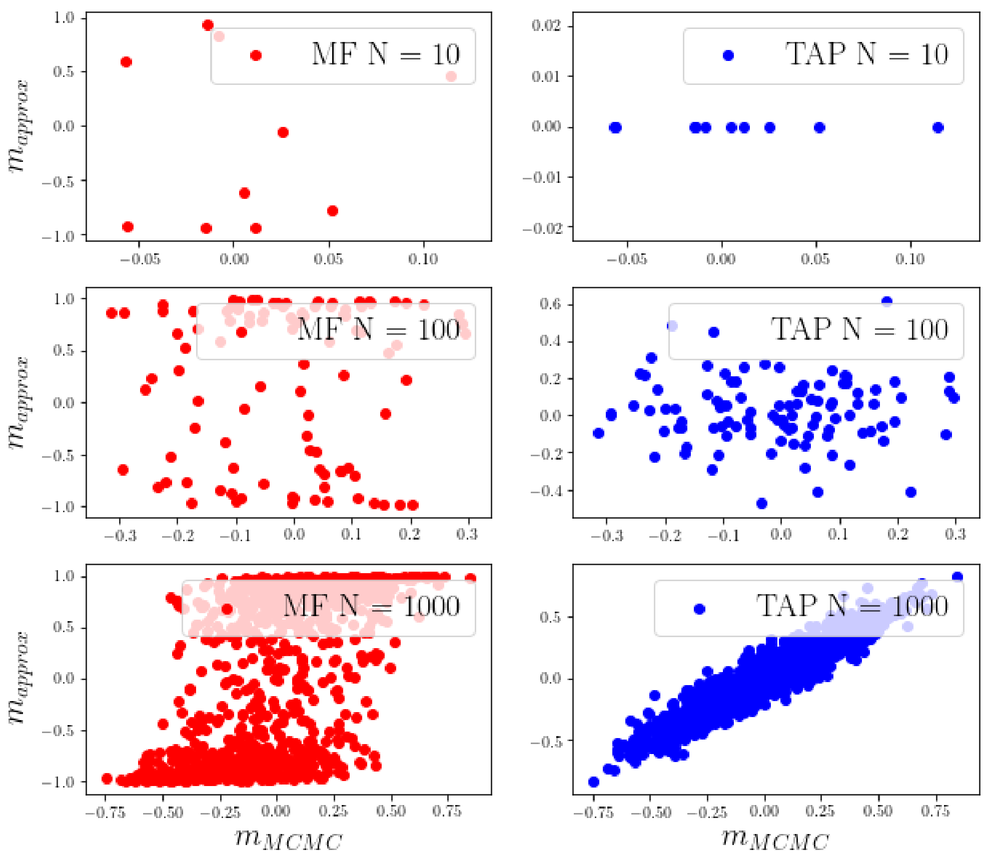

Figure 3: Scatter plot between the single entries of the average magnetization for TAP and Mean Field using the ground truth extracted via MCMC.