Advanced Probabilistic Machine Learning and Applications

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Tutorial 5: TAP approach

Exercise 1: Sampling from the SK model

Consider the Hamiltonian of the SK model with $h = 0$:

$$H(\mathbf{s}) = -\sum_{i \neq j} J_{ij} s_i s_j \quad . \tag{1}$$

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) algorithm as we learned for the Curie-Weiss model in a previous tutorial.

Perform the following tasks.

(a) Write a code to perform the MCMC dynamics:

- (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.) Start by configurations of spins extracted uniformly at random. Run your dynamics for a long enough time (say, with $t_{\max} = 10^2 N$ 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.
For numerical reasons implement the fixed point iterations as follows:

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

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

Exercise 2: 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 $P(\mathbf{s}, \mathbf{J})$:

$$\begin{aligned} s_i &\sim \frac{1}{2}\delta\left(s_i - 1\right) + \frac{1}{2}\delta\left(s_i + 1\right), \quad \forall i = 1, \dots, N && (2) \\ J_{ij} \,|\, s_i, s_j &\sim \mathcal{N}\left(\frac{s_i s_j}{\sqrt{N}}, \sigma^2\right), \quad \forall (i,j) \in N^2 && (3) \end{aligned}$$

Perform the following tasks.

(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 a function to *sample* an instance of $(\mathbf{s}, \mathbf{J})$.

(d) 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 $N = 10, 100, 1000$ and varying $\sigma^2 \in [0.1, 2]$. Plot the overlap ov $:= |\sum_i s_i m_i|/N$ (where s_i are the sampled spins, and m_i the magnetization at convergence) for TAP and MF as a function of the noise σ^2 for various N.
Comment on what you observe.