Chapter 3

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3.1 Belief propagation

Question: Use belief propagation to compute the C_{ij} of the Sherrington-Kirkpatrick(SK) model.

Answer: The Hamiltonlian of SK model within external field can be written as:

$$H = \sum_{i<j} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i \tag{1}$$

For simplification, we let $\beta = 1$. With similar calculation, eqs (2.31) and (2.32) turn out to be:

$$\begin{aligned}
u_{a\to i} &= \operatorname{artanh}\left[\tanh\left(J_a\right)\prod_{j\in\partial a\backslash i}\tanh\left(h_{j\to a}\right)\right] = \operatorname{artanh}\left[\tanh\left(J_a\right) m_{j\to a}\right] \\
m_{i\to a} &= \tanh\left(\sum_{b\in\partial i\backslash a} u_{b\to i} + h_i\right) \\
m_i &= \tanh\left(\sum_{b\in\partial i} u_{b\to i} + h_i\right)
\end{aligned} \tag{2}$$

Thus, the correlation can be obtained by:

$$\begin{aligned}
C_{ij} &= \frac{\partial m_i}{\partial h_j} \\
&= \left(1 - m_i^2\right)\left(\sum_{b\in\partial i}\frac{\partial u_{b\to i}}{\partial h_j} + \delta_{ij}\right)
\end{aligned} \tag{3}$$

In SK model, every factor node has only two neighbourhood variable nodes and we let $k = \partial b\backslash i$ be the another connected variable node except node i and J_b becomes J_{ik}. Thus:

$$\begin{aligned}
\frac{\partial u_{b\to i}}{\partial h_j} &= \frac{1}{1 - \left(\tanh\left(J_{ik}\right) m_{k\to b}\right)^2}\frac{\partial m_{k\to b}}{\partial h_j} \\
&= \frac{1}{1 - \left(\tanh\left(J_{ik}\right) m_{k\to b}\right)^2}\left(1 - m_{k\to b}\right)^2\left(\sum_{c\in\partial k\backslash b}\frac{\partial u_{c\to k}}{\partial h_j} + \delta_{kj}\right)
\end{aligned} \tag{4}$$

The above equation is self-consistant and we define $g_{b\to i,j} = \frac{\partial u_{b\to i}}{\partial h_j}$, which yield:

$$g_{b\to i,j} = \frac{\left(1 - m_{k\to b}\right)^2}{1 - \left(\tanh\left(J_{ik}\right) m_{k\to b}\right)^2}\left(\sum_{c\in\partial k\backslash b} g_{c\to k,j} + \delta_{kj}\right) \tag{5}$$

And finally we get:

$$C_{ij} = \left(1 - m_i^2\right)\left(\sum_{b\in\partial i} g_{b\to i,j} + \delta_{ij}\right) \tag{6}$$

3.2 Inverse Ising model

Question: Derive the Bethe solution of this inverse Ising problem.

Answer: Starting from the Bethe solution of the self-consistent equation eq (3.52) of m_i, we add external field h_i and yield:

$$m_i = \tanh\left(\sum_{j\in\partial i} \operatorname{artanh}\left(f\left(m_j, m_i, \tanh\beta J_{ij}\right)\tanh\left(\beta J_{ij}\right)\right) + h_i\right) \tag{7}$$

We can rewrite it as follows:

$$h_i = \operatorname{artanh}\left(m_i\right) - \sum_{j\in\partial i} \operatorname{artanh}\left(f\left(m_j, m_i, \tanh\beta J_{ij}\right)\tanh\left(\beta J_{ij}\right)\right) \tag{8}$$

And then we calculate the inverse of correlation C_{ij}^{-1}:

$$\begin{aligned} C_{ij}^{-1} =& \frac{\partial h_j}{\partial m_i} \\ =& \left(\frac{1}{1-m_i^2}\right)\delta_{ij} - \sum_{k\neq j} \frac{\tanh\beta J_{jk}\left(f_{1,jk}\cdot\delta_{ki} + f_{2,jk}\cdot\delta_{ij}\right)}{1-\tanh^2\left(\beta J_{jk}\right) f_{jk}^2} \\ =& \left[\frac{1}{1-m_i^2} - \sum_{k\neq j}\frac{t_{jk} f_{2,jk}}{1-t_{jk}^2 f_{jk}^2}\right]\delta_{ij} - \frac{t_{ij} f_{1,ij}}{1-t_{ij}^2 f_{ij}^2} \end{aligned} \tag{9}$$

where we use abbreviations $t_{ij} = \tanh\left(\beta J_{ij}\right)$, $f_{ij} = f\left(m_j, m_i, \tanh\beta J_{ij}\right)$, $f_1 = \frac{\partial f(a,b,t)}{\partial a}$, $f_2 = \frac{\partial f(a,b,t)}{\partial b}$.

For all $J_{ii} = 0$ and thus $t_{ii} = 0$, the freedom degree of weight matrix is $\frac{n(n-1)}{2}$. Therefore we only consider the non-diagonal $i \neq j$ correction:

$$C_{ij}^{-1} = -\frac{t_{ij} f_{1,ij}}{1-t_{ij}^2 f_{ij}^2} \tag{10}$$

Now we need to derive the weight J_{ij} or t_{ij}, which can be solve the above quartic equation and the result is:

$$t_{ij} = a_{ij}^{-} \pm \sqrt{a_{ij}^{-2} - 1} \quad \text{or} \quad t_{ij} = a_{ij}^{+} \pm \sqrt{a_{ij}^{+2} - 1} \tag{11}$$

where

$$a_{ij}^{\pm} = m_i m_j \pm \frac{1}{2\left(C_{ij}^{-1}\right)^2}\sqrt{4\left(C_{ij}^{-1}\right)^2\left(1-m_i^2\right)\left(1-m_j^2\right)+1} \tag{12}$$

However, not all the range of value $a^{\pm}$ are physical, which has two constraints. One is that $\left(a^{\pm}\right)^2 \geq 1$ and another one is that $t = \tanh\left(\beta J\right) \in (-1, 1)$. Here we plot sketch of the relation between $a^{\pm}$ and t:

As shown in fig. 1, only the blue part is valid and usually we take negative branch, i.e.

$$t_{ij} = a_{ij}^{-} + \sqrt{a_{ij}^{-2} - 1} \tag{13}$$

and finally

$$J_{ij} = \frac{1}{\beta}\operatorname{artanh}\left(a_{ij}^{-} + \sqrt{a_{ij}^{-2} - 1}\right) \tag{14}$$

Github code: https://github.com/Qjbtiger/SMNN-exercise/tree/main/Chapter%203

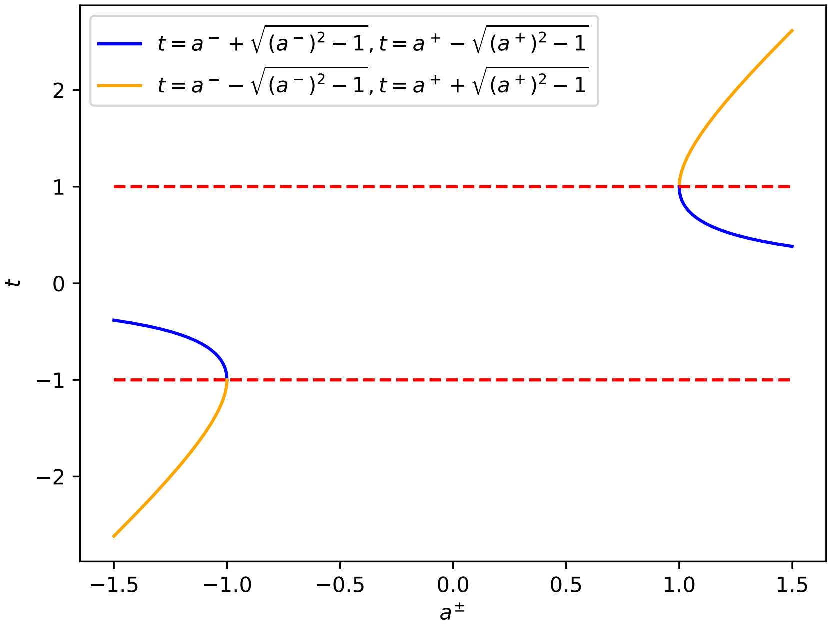

Figure 1: The sketch of the relation between $a^\pm$ and t