

Cavity Method for the Sherrington-Kirkpatrick Model

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This is an assignment on the course *Statistical Mechanics of Neural Networks* at the School of Physics, Sun Yat-sen University in the fall of 2024. We reviewed several theoretical solutions of the Sherrington-Kirkpatrick model in history. Through numerical calculations, we recover the phase diagram in the level of the replica symmetric solution. We obtain the free energy calculated by the replica symmetric solution and the cavity iteration equations on sparse graphs and compare these with the result from calculating the partition function by enumeration method for $N = 10$.

I. INTRODUCTION

The Hamiltonian of the Sherrington-Kirkpatrick model reads [1]

$$H = - \sum_{i < j} J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i, \quad (1)$$

where $\sigma_i \in \{1, -1\}$ are Ising spins, the interaction J_{ij} between any two spins is a quenched variable with the Gaussian distribution $J_{ij} \sim \mathcal{N}(J_0/N, J^2/N)$. The mean and variance of this distribution are both proportional to $1/N$:

$$\langle J_{ij} \rangle = \frac{J_0}{N}, \quad \langle J_{ij}^2 \rangle = \frac{J_0^2}{N^2} + \frac{J^2}{N}. \quad (2)$$

In some literature, the SK model without an external field is used, which can be obtained by setting $h = 0$ in any step of this article.

The probability of each configuration is given by the Gibbs-Boltzmann distribution $P(\boldsymbol{\sigma}) = \frac{1}{Z} e^{-\beta H(\boldsymbol{\sigma})}$, where Z is the partition function. We denote the expectation value with respect to the Boltzmann measure by $\langle\langle \cdot \rangle\rangle$, and the configuration average over the distribution of J_{ij} by $\langle \cdot \rangle$. The free energy after the quenched average is calculated as $\langle F \rangle = -\frac{1}{\beta} \langle \ln Z \rangle$. The Boltzmann average value of the spin, called the local magnetization, is $m_i = \langle\langle \sigma_i \rangle\rangle$, and the magnetization of the system is $m = \langle m_i \rangle$.

Due to the frustrated phenomenon, the spin in the SK model is frozen at low temperature, yet remains highly disordered, with the order parameter $m = 0$. This is a phase distinct from the paramagnetic phase and is called the spin glass phase. In order to distinguish between the two phases, it is necessary to introduce the so-called Edwards-Anderson parameter [2], defined as $q = \langle\langle \sigma_i \rangle\rangle^2$.

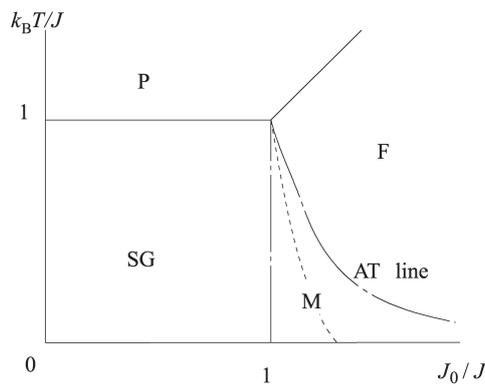


FIG. 1: Phase diagram of the Sherrington-Kirkpatrick model. [3]

Based on the different values of the order parameters m and q , the SK model can be divided into three different phases. The magnetization m distinguishes between the paramagnetic phase ($m = 0$) and the ferromagnetic phase ($m \neq 0$), while the EA order parameter q distinguishes between the paramagnetic phase ($q = 0$) and the spin glass phase ($q \neq 0$).

II. MAIN THEORETICAL SOLUTIONS

The first solution to the SK model was obtained by Sherrington and Kirkpatrick in 1975 when they first propose the model. [1] This solution is known as the replica symmetric solution, introduced by Edwards and Anderson [2]. The order parameters m and q are the fixed points of the following equations:

$$m = \int Dz \tanh \beta \tilde{H}(z), \quad (3)$$

$$q = \int Dz \tanh^2 \beta \tilde{H}(z), \quad (4)$$

where $Dz \equiv dz e^{-z^2/2}/\sqrt{2\pi}$ and $\tilde{H}(z) \equiv J\sqrt{q}z + J_0m + h$. The free energy is calculated as

$$f_{\text{RS}} = -\frac{1}{4}\beta J^2(1-q)^2 + \frac{1}{2}J_0m^2 - \frac{1}{\beta} \int Dz \log \left(2 \cosh \beta \tilde{H}(z) \right). \quad (5)$$

However, this solution was found to have the negative value $-\frac{1}{2}\pi$ of the ground state entropy for $J_0 = h = 0$. In 1978, de Almeida and Thouless analyzed the stability of the replica symmetric solution [4] and found that it is stable only if

$$\left(\frac{T}{J}\right)^2 > \int Dz \operatorname{sech}^4(\beta J\sqrt{q}z + \beta J_0m) \quad \text{for } h = 0, \quad \left(\frac{T}{J}\right)^2 > \int Dz \operatorname{sech}^4(\beta J\sqrt{q}z + \beta h) \quad \text{for } J_0 = 0, \quad (6)$$

which corresponds to the high-temperature regime. Eq. (6) describes the boundary of the stability region, which is known as the dAT line.

In 1977, Thouless, Anderson, and Palmer proposed the TAP equation [5], trying to solve the negative entropy crisis. This is a high-temperature expansion solution for the SK model. Given the random interactions $\{J_{ij}\}$, the local magnetization satisfies

$$m_i = \tanh \beta \left(\sum_j J_{ij}m_j + h - \beta \sum_j J_{ij}^2(1-m_j^2)m_i \right). \quad (7)$$

The third term is called the reaction field of Onsager and is added to remove the effects of self-response. The free energy is calculated as

$$f_{\text{TAP}} = -\frac{1}{2} \sum_{i \neq j} J_{ij}m_i m_j - \sum_i h_i m_i - \frac{\beta}{4} \sum_{i \neq j} J_{ij}^2(1-m_i^2)(1-m_j^2) + \frac{1}{2\beta} \sum_i \left\{ (1+m_i) \log \frac{1+m_i}{2} + (1-m_i) \log \frac{1-m_i}{2} \right\}. \quad (8)$$

The validity of the TAP equations for high temperature has been proved by Talagrand [6, 7], Chatterjee [8] and Bolthausen [9], while there is no rigorous proof at low temperature.

In 1979, Parisi proposed the replica symmetry breaking solution [10–15], which is believed to be the only exact solution so far. The free energy of the RSB solution is given by

$$f_{\text{RSB}} = -\frac{1}{4}\beta J^2 \left\{ 1 + \int_0^1 q(x)^2 dx - 2q(1) \right\} - \frac{1}{\beta} \int Du f_0(0, \sqrt{q(0)}u), \quad (9)$$

where f_0 satisfies the following Parisi equation:

$$\frac{\partial f_0(x, h)}{\partial x} = -\frac{J^2}{2} \frac{dq}{dx} \left\{ \frac{\partial^2 f_0}{\partial h^2} + x \left(\frac{\partial f_0}{\partial h^2} \right) \right\}. \quad (10)$$

In 1987, Mézard, Parisi and Virasoro introduced a new method, which does not use replicas, but can recover all the results of the replica symmetry-breaking solution of the SK model.[16] They titled their work *The Replica Solution without Replicas*, which later is known as the cavity method. The vanilla cavity method can directly derive the TAP equations (7), and through a more rough approximation, it can back to the RS solution (3)(4). Later, this method was found to be powerful in dealing with optimization problems [17], such as the K-satisfiability problem [18]. More importantly, it is equivalent to belief propagation, also known as sum-product message passing, which is an efficient algorithm applied to sparse graph models [19], as discussed in Chapter 2 in SMNN book [20]. Although the SK model considers fully connected interactions, which is a dense graph rather than a sparse one, we can still do approximate calculation by the cavity iteration equation as following

$$h_{i \rightarrow ij} = \frac{1}{\beta} \left(\sum_{k(\neq i, j)} \beta u_{ik \rightarrow i} \right), \quad (11)$$

$$u_{ij \rightarrow i} = \frac{1}{\beta} \tanh^{-1} \left[\tanh(\beta J_{ij}) \tanh(\beta h_{j \rightarrow ij}) \right]. \quad (12)$$

By iteratively solving for $u_{ij \rightarrow i}$, we can then solve for m_i using

$$m_i = \tanh \left(\sum_{j(\neq i)} \beta u_{ij \rightarrow i} \right), \quad (13)$$

and then we can calculate the free energy by $F = \sum_i \Delta F_i - \sum_{\langle ij \rangle} \Delta F_{ij}$, where

$$\Delta F_{ij} = \ln \left[\cosh(\beta J_{ij}) \left(1 + \tanh(\beta J_{ij}) m_{i \rightarrow ij} m_{j \rightarrow ij} \right) \right], \quad (14)$$

$$\Delta F_i = \ln \left(\prod_{j \neq i} \Lambda_{ij \rightarrow i}^+ + \prod_{j \neq i} \Lambda_{ij \rightarrow i}^- \right), \quad (15)$$

and

$$\Lambda_{ij \rightarrow i}^\pm = \cosh(\beta J_{ij}) \left[1 \pm \tanh(\beta J_{ij}) m_{ij \rightarrow i} \right]. \quad (16)$$

Equations (11)~(16) can converge to the RS solution in the limit $N \rightarrow \infty$.

In this paper, we primarily focus on the cavity iteration equations for finite N and the RS solution in the limit $N \rightarrow \infty$. The TAP equations will be discussed in detail in Chapter 5 of the SMNN book, while the RSB solution is beyond the scope of this paper.

III. MAIN RESULTS

A. the order parameters

We calculated the magnetization m and the EA parameter q for the RS solution and the cavity iteration solution in the ranges $T/J \in [0, 2]$ and $J_0/J \in [0, 2]$ using a grid-based approach, and recorded the number of iteration steps. In all numerical calculations, we set $J = 1$. The results of the RS solution (first row of Fig. 2) recover the phase diagram in the book [3] as shown in Fig. 1. However, near the three phase transition critical lines, Eqs. (3) and (4) are difficult to converge, as shown in Fig. 2(a). The convergence of the cavity iteration equations is significantly worse, as shown in Fig. 2. In particular, in the spin glass phase, the cavity method fails to converge correctly, as shown in Fig. 2(d).

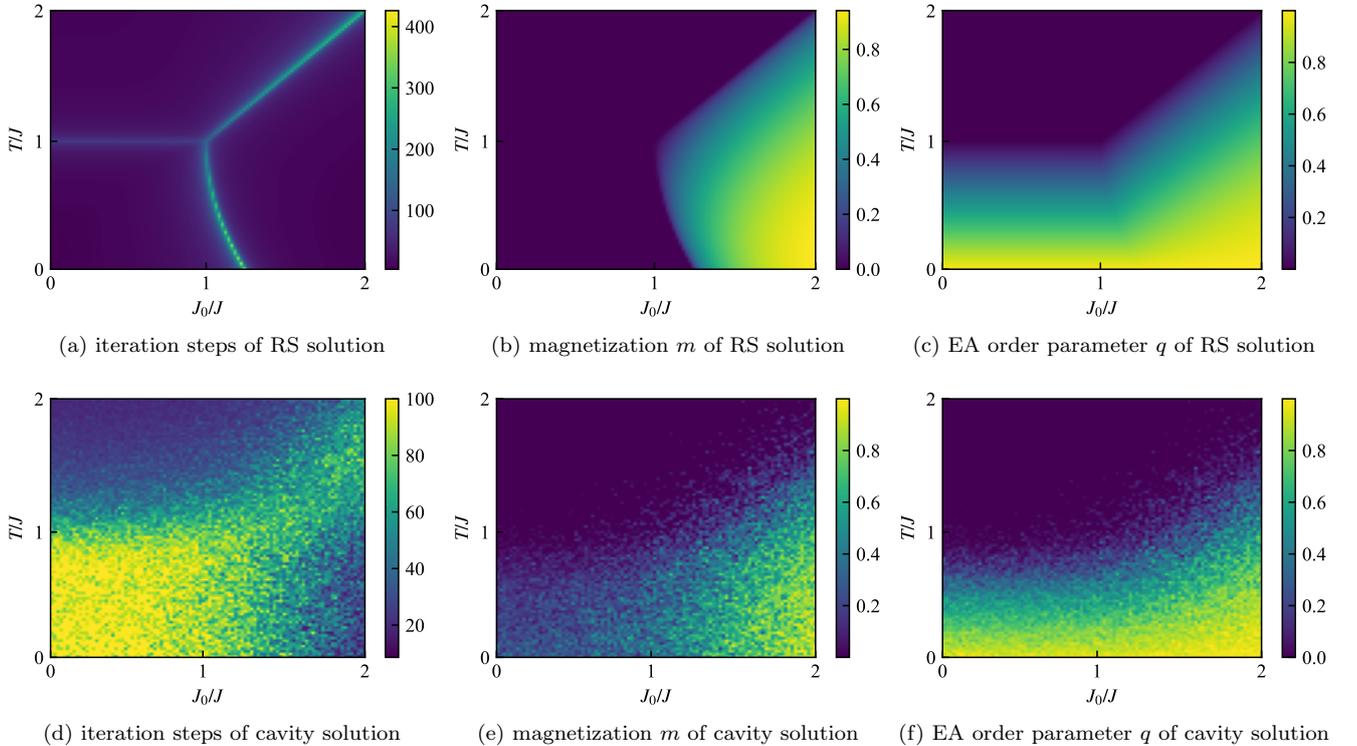


FIG. 2: Phase diagrams of the order parameters m and q and the number of iteration steps for the SK model.

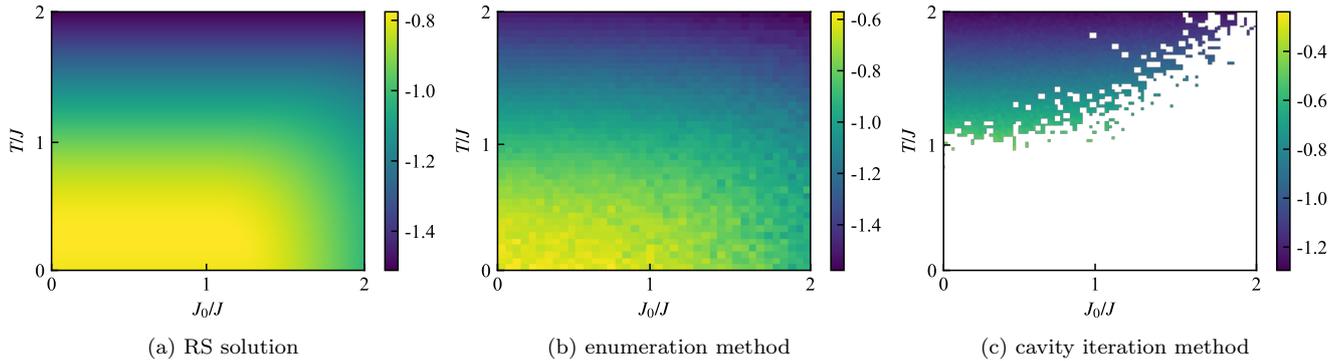


FIG. 3: Phase diagrams of the free energy density for the SK model.

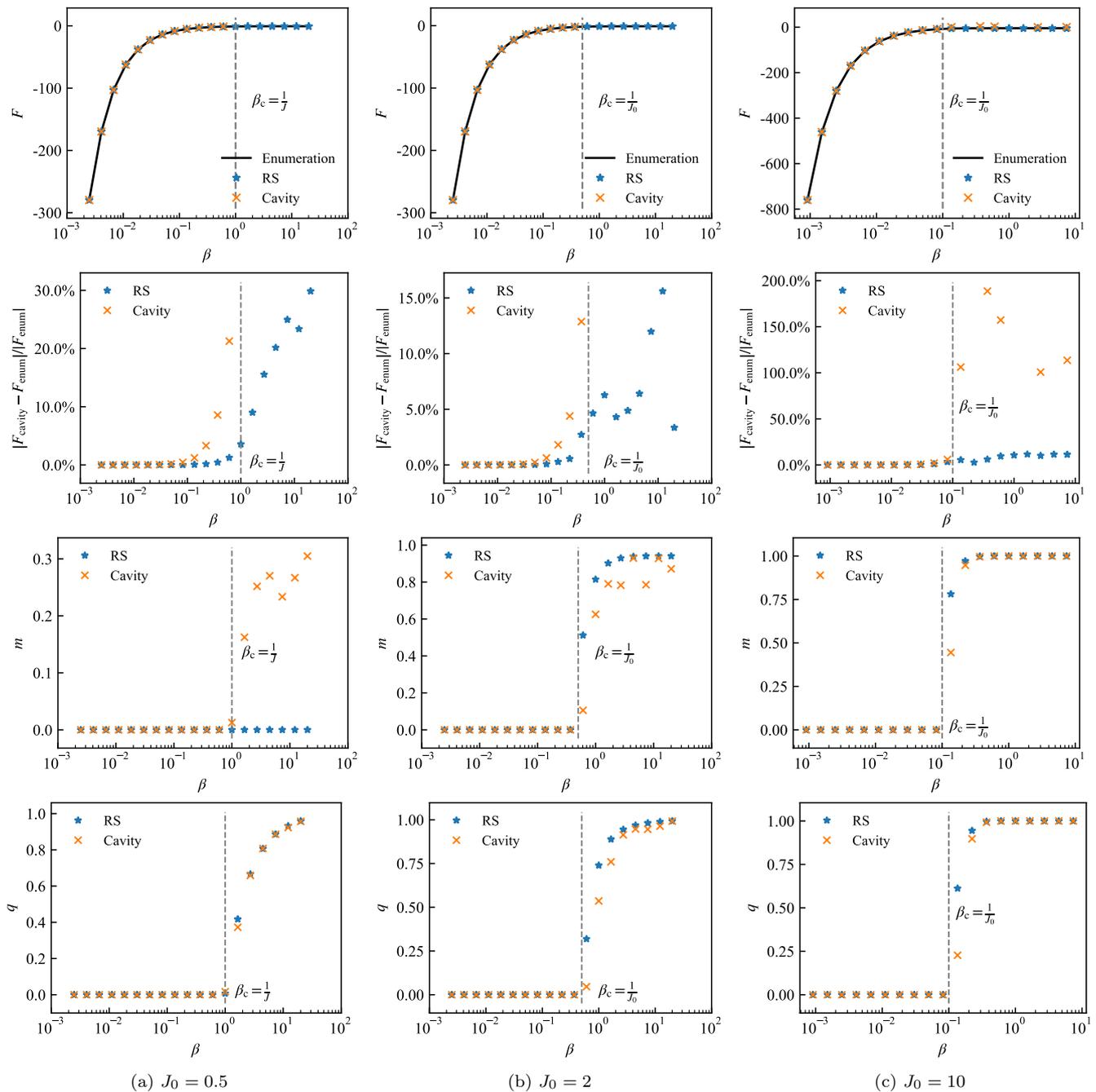


FIG. 4: Comparison of free energy density and order parameters obtained by different methods for various values of J_0 .

B. the free energy

We calculated the free energy density of the RS solution, which is shown in Fig. 3(a) in the same phase diagram format. Similarly, we calculated the free energy for $N = 10$ using the enumeration method (Fig. 3(b)) and the cavity method (Fig. 3(c)), averaging over 20 trials and dividing by N to obtain the free energy density. The results from the enumeration method are in complete agreement with the RS solution, while the cavity method only yields results for the paramagnetic phase.

In more detail, we take $J_0 = 0.5, 2, 10$, corresponding to the paramagnetic – spin glass phase transition, the paramagnetic – ferromagnetic phase transition near the spin glass phase, and the paramagnetic – ferromagnetic phase transition far from the spin glass phase, respectively. We compare the free energy density, error, and order parameters obtained by different methods, as shown in Fig. 4.

The first column of Fig. 4 corresponds to the case of $J_0 = 0.5$, where the critical temperature for the paramagnetic – spin glass phase transition is $T/J = 1$, i.e., $\beta_c = 1/J$. The second and third columns of Fig. 4 correspond to the cases of $J_0 = 2$ and $J_0 = 10$, respectively, where the critical temperature for the paramagnetic – ferromagnetic phase transition is $T/J = J_0/J$, i.e., $\beta_c = 1/J_0$.

The second row of Fig. 4 shows the relative error of the free energy obtained by the RS solution and the cavity solution compared to the enumeration method. At high temperatures, the free energies obtained by the three methods are essentially consistent. As the temperature decreases to the critical temperature, the error of the cavity solution begins to increase. Beyond the critical temperature, the cavity solution either fails to converge or, in cases where J_0 is large, sometimes converges but with an error exceeding 100%. In contrast, the error of the RS solution increases below the critical temperature but remains acceptable.

Moreover, the results indicate that the RS solution fetches all the order parameters in all cases, as referenced in [1]. While the cavity method only yields the correct m in the paramagnetic phase and the ferromagnetic phase when J_0 is large. Although it can obtain the correct q in all phases, but all the results of the cavity method near the phase transition points are not sufficiently accurate.

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