Minimal dominating set problem studied by simulated annealing and cavity method: analytics and population dynamics

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Abstract. The minimal dominating set (MDS) problem is a prototypical hard combinatorial optimization problem. We recently studied this problem using the cavity method. Although we obtained a solution for a given graph that gives a very good estimation of the minimal dominating size, we do not know whether there is a ground state solution or how many solutions exist in the ground state. We have therefore continued to develop a one-step replica symmetry breaking theory to investigate the ground state energy of the MDS problem. First, we find that the solution space for the MDS problem exhibits both condensation transition and cluster transition on regular random graphs, and prove this using a simulated annealing dynamical process. Second, we develop a zero-temperature survey propagation algorithm on Erdős–Rényi random graphs to estimate the ground state energy, and obtain a survey propagation decimation algorithm that achieves results as good as the belief propagation decimation algorithm.

Keywords: cavity and replica method, message-passing algorithms, random graphs, networks, spin glasses
1. Introduction

The statistical physics of spin glass systems has been widely applied to optimization problems, such as the minimal vertex cover problem [1, 2], the minimum feedback vertex set problem [3, 4] and the minimal dominating set (MDS) problem, and to satisfiability problems, such as K-SAT [5–7] and XOR-SAT [8, 9]. Many combinatorial optimization problems in computer science can be mapped to an appropriate random spin glass model. The cavity method is often used to estimate the occupancy probability of each node, and to construct a solution for the given graph under this probability. If the graph does not contain any shortest cycles or has a tree-like local structure, then we can find a stable point from the iterative cavity equations.

At present, our research on spin glass systems is concentrated on replica symmetry and the one-step replica symmetry breaking (1RSB) level. Much of the research into combinatorial optimization problems focuses on the following questions. First, can we find the smallest set that satisfies the problem for a given graph. Second, how many configurations (or solutions) of the given graph satisfy the problem. Third, for a given real number $x_c(0 < x_c < 1)$, can we decide whether there exists a solution with size not exceeding $x_cN$, where $N$ represents the number of nodes in the given graph.

We have previously tried to answer the first question for the MDS problem using the cavity method and obtained good results [10, 11]. In this paper, we focus on the
last question for the MDS problem, again using the cavity method [12]. The following are the known bounds on $\gamma(G)$, the size of an MDS (Haynes, Hedetniemi and Slater 1998a, section 2) [13]. Because each vertex can dominate at most $\Delta$ other vertices, $\gamma(G) \geq N/(1 + \Delta)$. Therefore, $x_c = 1/(1 + \Delta)$, and for a large regular random graph we find a sharp threshold value of $x_c \geq 1/(1 + \Delta)$, which is closely related to the computational complexity. For $x > x_c$, we can construct an MDS of size $\geq xN$ for a given graph, but not for $x < x_c$. When $x > x_c$, the simulated annealing (SA) algorithm finds such an MDS relatively easily; however, when $x$ is close to $x_c$, the search complexity increases dramatically, and tends to infinity at $x = x_c$. Thus it cannot give a solution in finite computational time. At a temperature of zero, we use survey propagation (SP) to find the threshold value $x_c$ for Erdős–Rényi (ER) random graphs.

A (vertex) minimal dominating set [13] of a graph $G$ is a set of vertices $D$ such that every vertex of $G$ is either in $D$ or has at least one neighbor in $D$. Having been widely studied by mathematicians and physicists from both a theoretical and an algorithmic point of view, MDSs are an important branch of graph theory that plays important role in computer science and artificial intelligence. It is widely applied in complex network systems [14–21].

The MDS problem has been studied since the 1950s, with increased research on the problem since the mid-1970s. More than 400 papers related to the MDS problem have appeared, most of which address the following three factors: (1) the diversity of applications to both real-world and other mathematical ‘covering’ or ‘location’ problems; (2) the wide range of domination parameters that can be defined; (3) the NP-completeness of the basic domination problem, its close relationships to other NP-complete problems, and the subsequent interest in finding polynomial-time solutions to domination problems for special classes of graphs [22]. The MDS problem is a nondeterministic polynomial-complete (NP-complete) optimization problem [13], so finding an exact solution is extremely difficult in general. It is also hard to find an approximate MDS solution for a given graph. Some heuristic algorithms [14–16, 18, 23, 24] and statistical physics algorithm [10, 11] have been used to solve the MDS problem, but only a small portion of this research relates to solution space structure, bounds on the threshold value $x_c$ and the size of an MDS.

In this paper, we use 1RSB theory from statistical physics to study the solution space for the MDS problem. The paper is organized as follows. In section 2, we recall replica symmetry theory for spin glass models before explaining replica symmetry breaking theory and presenting the belief propagation (BP) equation and some thermodynamic quantities. In section 3, we introduce 1RSB theory and some thermodynamic quantities. In the second part of this section, we derive 1RSB theory and thermodynamic quantities at $y = \beta$, where $y$ is the Parisi parameter and $\beta$ is the inverse temperature, and then introduce a dynamic SA process for MDSs. In the third part, we introduce the population dynamics for this case in detail. In section 4, we derive warning propagation, SP and survey propagation decimation (SPD) algorithms. In section 5, we conclude and summarize our results.
2. Replica symmetry

To estimate the MDS for a given graph using mean field theory, we must have a partition function for the graph. The partition function $Z$ is defined as

$$Z = \sum_{\xi} \prod_{i \in W} e^{-\beta c_i} \left[ 1 - (1 - c_i) \prod_{k \in \partial i} (1 - c_k) \right],$$

where $\xi \equiv (c_1, c_2, \ldots, c_N)$ denotes one of the $2^N$ possible configurations, with $c_i = +1$ if node $i$ is occupied and $c_i = 0$ otherwise, $\beta$ is the inverse temperature, and $\partial i$ denotes the neighbors of node $i$. The partition function therefore only takes into account the dominating sets.

We use replica symmetry mean field theory, such as the Bethe–Peierls approximation [25] or partition function expansion [26, 27], to solve the above spin glass model. We apply the cavity message $p_{i \rightarrow j}^{(c_i, c_j)}$ to every edge, where these messages must satisfy following equation:

$$p_{i \rightarrow j}^{(c_i, c_j)} = A_{i \rightarrow j} \left[ p_{\partial i \upharpoonright j} \right] = \frac{e^{-\beta c_i} \prod_{k \in \partial i} \sum_{c_k} p_{k \rightarrow i}^{(c_k, c_i)} - \delta_{c_i} \delta_{c_j} \prod_{k \in \partial i} p_{k \rightarrow i}^{(0,0)}}{\sum_{\hat{c}_i, \hat{c}_j} e^{-\beta \hat{c}_i} \prod_{k \in \partial i} \sum_{\hat{c}_k} p_{k \rightarrow i}^{(\hat{c}_k, \hat{c}_i)} - \prod_{k \in \partial i} p_{k \rightarrow i}^{(0,0)}}. \tag{2}$$

This equation is called the BP equation. The Kronecker symbol satisfies $\delta_{m,n} = 1$ if $m = n$ and $\delta_{m,n} = 0$ otherwise. The cavity message $p_{i \rightarrow j}^{(c_i, c_j)}$ represents the joint probability that node $i$ is in occupation state $c_i$ and the adjacent node $j$ is in occupation state $c_j$ when constraints on node $j$ are not considered. The marginal probability $p_i^c$ of node $i$ can be expressed as

$$p_i^c = \frac{e^{-\beta c_i} \prod_{j \in \partial i} \sum_{c_j} p_{j \rightarrow i}^{(c_j)} - \delta_{c_i} \prod_{j \in \partial i} p_{j \rightarrow i}^{(0,0)}}{\sum_{c_i} e^{-\beta c_i} \prod_{j \in \partial i} \sum_{c_j} p_{j \rightarrow i}^{(c_j)} - \prod_{j \in \partial i} p_{j \rightarrow i}^{(0,0)}}. \tag{3}$$

Finally, the free energy can be calculated using mean field theory:

$$F_0 = \sum_{i=1}^N F_i - \sum_{(i,j)=1}^M F_{(i,j)}, \tag{4}$$

where

$$F_i = -\frac{1}{\beta} \ln \left[ \sum_{c_i} e^{-\beta c_i} \prod_{j \in \partial i} \sum_{c_j} p_{j \rightarrow i}^{(c_j, c_i)} - \prod_{j \in \partial i} p_{j \rightarrow i}^{(0,0)} \right], \tag{5}$$

$$F_{(i,j)} = -\frac{1}{\beta} \ln \left[ \sum_{c_i, c_j} p_{i \rightarrow j}^{(c_i, c_j)} p_{j \rightarrow i}^{(c_j, c_i)} \right]. \tag{6}$$

The term $F_i$ denotes the free energy of node $i$, and $F_{(i,j)}$ denotes the free energy of the edge $(i,j)$. We iterate the BP equation until it converges to a stable point, and then

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calculate the mean free energy \( f \equiv F/N \) and the energy density \( \omega = 1/N \sum_i p_i^+ \) using equations (3) and (4). The entropy density is calculated as \( s = \beta(\omega - f) \).

### 3. One-step replica symmetry breaking theory

In this section, we introduce 1RSB theory for spin glass models by the graph expansion method. We first introduce the generalized partition function, grand free energy and SP for the general case. To increase the simulation speed, we must simplify the equations. We therefore derive simplified equations for \( y = \beta \) for the MDS problem, and then introduce the numerical simulation process using population dynamics.

#### 3.1. General one-step replica symmetry breaking theory

At higher temperatures, the thermodynamic microscopic state that consists of a higher energy configuration decides the statistical physics properties of the given system, and a subspace of this microscopic state is ergodic. However, at lower temperatures the microscopic state is not ergodic, but can be divided into several subspaces where the contributions of these subspaces to the equilibrium property are not identical. If we select the energy function as the order parameter, then we do not know the properties of these subspaces or how they evolve. Thus we select the free energy function as the order parameter to develop 1RSB theory. We define the generalized partition function \( \Xi \) as

\[
\Xi(y; \beta) = \sum_\alpha e^{-yF_0^\alpha(\beta)},
\]

where \( \alpha \) denotes the macroscopic states, and \( F_0^\alpha \) has the form

\[
F_0^{\alpha} = \sum_i f_i - \sum_{(i,j)} f_{(i,j)}.
\]

Four cavity messages \( p_{i \rightarrow j} \equiv (p_{i \rightarrow j}^0, p_{i \rightarrow j}^1) \) are defined on edges \((i, j)\) of the given graph, and the cavity messages \( p_{i \rightarrow j} \) averaged on solution clusters is denoted by \( P_{i \rightarrow j}(p_{i \rightarrow j}) \). The iteration equation for \( P_{i \rightarrow j}(p_{i \rightarrow j}) \) is

\[
P_{i \rightarrow j}(p) = \prod_{k \in \partial i \setminus j} \int Dp_k P_k \delta(p_{i \rightarrow j} - \int Dp_{i \rightarrow k} P_{i \rightarrow k}(p)e^{-yf_{i \rightarrow j}}),
\]

where \( A_{i \rightarrow j}[p_{\partial i \setminus j}] \) abbreviates the notation in the message updating equations in equation (2). The generalized free energy density \( g_0 \) is

\[
g_0 \equiv G_0 = \frac{1}{N} \sum_i g_i - \sum_{(i,j)} g_{(i,j)} \frac{1}{N},
\]

where
and the conditional message \( p_{i \to j} \), when we
\[
\ln \prod \mathcal{D} p_{i \to j} P_{i \to j}(p) e^{-yf_i},
\]

We further have the mean free energy density
\[
\langle f \rangle \equiv \frac{F}{N} = \frac{\sum_i \langle f_i \rangle - \sum_{(i,j)} \langle f_{(i,j)} \rangle}{N},
\]
where
\[
\langle f_i \rangle = \prod_{j \in \partial i} \int \mathcal{D} p_{i \to j} P_{i \to j}(p) e^{-yf_i f_i},
\]

\[
\langle f_{(i,j)} \rangle = \frac{\int \mathcal{D} p_{i \to j} \mathcal{D} p_{j \to i} P_{i \to j}(p) P_{j \to i}(p) e^{-yf_{(i,j)} f_{(i,j)}}}{\int \mathcal{D} p_{i \to j} \mathcal{D} p_{j \to i} P_{i \to j}(p) P_{j \to i}(p) e^{-yf_{(i,j)}}}.
\]

Finally, we combine the mean free energy \( \langle f \rangle \) and the generalized free energy \( g \) to derive the complexity as \( \Sigma(y) = y(\langle f \rangle - g) \).

### 3.2. Dynamical and condensation transitions at \( y = \beta \)

We consider the case \( y = \beta \) to determine the clustering transition and condensation transition. To simplify the formula for replica symmetry breaking theory and to increase the simulation speed, we define two kinds of message. We define the average message \( \bar{p}_{i \to j}^{(c_{i}, c_{j})} \) and the conditional message \( P_{i \to j}^{(c_{i}, c_{j})} \) by
\[
\bar{p}_{i \to j}^{(c_{i}, c_{j})} = \int \mathcal{D} p P_{i \to j}(p) p_{i \to j}^{(c_{i}, c_{j})},
\]

\[
P_{i \to j}^{(c_{i}, c_{j})} \left( p_{i \to j}^{(c_{i}, c_{j})} | p_{i \to j}^{(c_{i}, c_{j})} \right) = \frac{p_{i \to j}^{(c_{i}, c_{j})} P_{i \to j} \left[ p_{i \to j}^{(c_{i}, c_{j})} \right]}{p_{i \to j}^{(c_{i}, c_{j})}},
\]
where the conditional message \( P_{i \to j}^{(c_{i}, c_{j})} \) represents the macroscopic conditional probability of the cavity probabilistic distribution function \( \bar{p}_{i \to j}^{(c_{i}, c_{j})} \) when we investigate the pair node \( (i, j) \) in the state \( (c_{i}, c_{j}) \). From these two equations and the BP equations we can derive the new update rules for these two messages:
\[
\bar{p}_{i \to j}^{(c_{i}, c_{j})} = \frac{e^{-\beta c_{i}} \prod_{k \in \partial i \setminus j} \sum_{c_{k}} p_{k \to i}^{(c_{k}, c_{i})} - \delta_{c_{i} c_{j}} \prod_{k \in \partial i \setminus j} \bar{p}_{k \to i}^{(0,0)}}{\sum_{c_{i}, c_{j}} e^{-\beta c_{i}} \prod_{k \in \partial i \setminus j} \sum_{c_{k}} p_{k \to i}^{(c_{k}, c_{i})} - \prod_{k \in \partial i \setminus j} \bar{p}_{k \to i}^{(0,0)}},
\]

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where $A_{i\rightarrow j}[p_{\partial i\setminus j}]$ abbreviates the notation in the message updating equations in equation (2), and

$$\omega^{(c_i,c_j)}_{i\rightarrow j} = \frac{e^{-\beta c_i} \prod_{k \in \partial i \setminus j} p^{(c_k,c_i)}_{k \rightarrow i} - \delta^{c_i}_0 \delta^{c_j}_0 \prod_{k \in \partial i \setminus j} \bar{p}^{(0,0)}_{k \rightarrow i}}{\sum_{c_{i,j}} e^{-\beta c_i} \prod_{k \in \partial i \setminus j} \sum_{c_j} p^{(c_j,c_i)}_{j \rightarrow i} - \prod_{k \in \partial i \setminus j} \bar{p}^{(0,0)}_{j \rightarrow i}},$$

(20)

denotes the sampling joint probability. This can be calculated from the average messages to obtain one configuration sample for $\partial i \setminus j \equiv \{c_k : k \in \partial i \setminus j\}$. We then update the conditional messages using this configuration sample. Although this SP looks complicated and more difficult to implement than the original SP equation, these equations converge more easily. The thermodynamic quantities can be derived in the same way, and the total free energy can be expressed as

$$F = \sum_i \langle f_i \rangle - \sum_{i,j} \langle f_{i,j} \rangle,$$

(21)

where $\langle f_i \rangle$ denotes the mean free energy of node $i$. This can be expressed as

$$\langle f_i \rangle = -\frac{1}{\beta} \sum_{c_i} \omega^c_i \prod_{j \in \partial i} \int Dp_{j \rightarrow i} p^{(c_j,c_i)}_{j \rightarrow i} (p^{(c_j,c_i)}_{j \rightarrow i} | p^{(0,0)}_{j \rightarrow i})$$

$$\times \ln \{ \sum_{c_j} e^{-\beta c_i} \prod_{j \in \partial i} p^{(c_j,c_i)}_{j \rightarrow i} - \prod_{j \in \partial i} p^{(0,0)}_{j \rightarrow i} \},$$

(22)

where $\omega^c_i$ denotes the sampling probability:

$$\omega^c_i = \frac{e^{-\beta c_i} \prod_{j \in \partial i} \bar{p}^{(c_j,c_i)}_{j \rightarrow i} - \delta^{c_i}_0 \delta^{0}_0 \prod_{j \in \partial i} \bar{p}^{(0,0)}_{j \rightarrow i}}{\sum_{c_j} e^{-\beta c_i} \prod_{j \in \partial i \setminus c_j} \bar{p}^{(c_j,c_i)}_{j \rightarrow i} - \prod_{j \in \partial i \setminus c_j} \bar{p}^{(0,0)}_{j \rightarrow i}},$$

(23)

To obtain good results, effective sampling of the conditional message is important. This is the core problem in our numerical simulation. According to the above equation and appendix, we determine the state of the selected variables one at a time to obtain a single configuration. We select the conditional message from this configuration to calculate the mean free energy of node $i$. In the same way, we can calculate the free energy of edge $(i,j)$ as

$$\langle f_{i,j} \rangle = -\frac{1}{\beta} \sum_{c_i,c_j} \omega^{(c_i,c_j)}_{i \rightarrow j} \int Dp_{i \rightarrow j} p^{(c_i,c_j)}_{i \rightarrow j} (p^{(c_i,c_j)}_{i \rightarrow j} | p^{(0,0)}_{i \rightarrow j})$$

$$\times \ln \{ \sum_{c_i,c_j} p^{(c_i,c_j)}_{i \rightarrow j} \bar{p}^{(c_j,c_i)}_{j \rightarrow i} \},$$

(24)

where
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\[ \omega_{i \rightarrow j}^{(c_i, c_j)} = \frac{P_{i \rightarrow j}^{(c_i, c_j)} P_{j \rightarrow i}^{(c_j, c_i)}}{\sum_{c_i, c_j} P_{i \rightarrow j}^{(c_i, c_j)} P_{j \rightarrow i}^{(c_j, c_i)}} \] (25)

and the grand free energy of edge \((i, j)\) and node \(i\) as

\[ g_{(i,j)} = -\frac{1}{\beta} \ln \{ \sum_{c_i, c_j} P_{i \rightarrow j}^{(c_i, c_j)} P_{j \rightarrow i}^{(c_j, c_i)} \} \] (26)

\[ g_i = -\frac{1}{\beta} \ln \left[ \sum_{c_i} e^{-\beta c_i} \prod_{j \in \partial i} P_{j \rightarrow i}^{(c_j, c_i)} - \prod_{j \in \partial i} P_{j \rightarrow i}^{(0,0)} \right]. \] (27)

The total mean free energy, the total mean grand free energy and the complexity are then calculated as follows:

\[ g_0 = \frac{G_0}{N} = \frac{1}{N} \sum_{i=1}^{N} g_i - \frac{M}{N} \sum_{(i,j)=1}^{M} g_{(i,j)}, \] (28)

\[ f_0 = \frac{F_0}{N} = \frac{1}{N} \sum_{i=1}^{N} \langle f_i \rangle - \frac{M}{N} \sum_{(i,j)=1}^{M} \langle f_{(i,j)} \rangle, \] (29)

\[ \Sigma = g(f_0 - g_0), \] (30)

where \(f_0\) denotes the mean free energy density and \(g_0\) denotes the grand free energy density.

We now discuss the influence of cluster transitions on the dynamical properties of a regular random graph with mean degree \(C = 5\). Figure 1(a) indicates the relationship between complexity and inverse temperature \(\beta\) when \(y = \beta\). The complexity becomes positive when \(\beta \approx 7.90\), and then decreases as \(\beta\) increases, finally reaching zero when \(\beta \approx 8.19\). We find that figure 1 is similar to a three-body interaction spin glass system [28–30]. We calculate the condensation transition and cluster transition using the population dynamics, and the procedure of the population dynamics is very important to get the good results, so we introduce this procedure in the whole next part of this section in detail.

Figure 2 indicates the evolution of energy density with \(\beta\) in the SA process. In this process, we first carry out enough single spin heat bath dynamical process at \(\beta = 1\) to obtain an equilibrium microscopic configuration sample. Starting from this configuration, we increase \(\beta\) at a specified step-size \(\delta \beta = 0.001\). For each new value of \(\beta\), we first carry out \(\omega\) steps (at every step, we try on average to flip every spin of the system), and then record the energy density of the configuration. We average over 96 independent paths to obtain the average energy density.

Figure 2 shows that, if the rate of increase of \(\beta\) is very fast (or if the waiting time is very small), then the energy density deviates from the value predicted by mean field theory for small \(\beta\). If we slow down the rate of increase of \(\beta\), then the energy density deviates from the predicted value when \(\beta\) is larger. The reason for this difference between SA and mean field theory is that the characteristic relaxation time lengthens as \(\beta\) increases. If the characteristic relaxation time exceeds the average SA waiting time,
then the configuration obtained by the SA process is not an equilibrium configuration, and the energy is higher than the average equilibrium energy.

Furthermore, as $\omega \to \infty$, the average energy density cannot equal the equilibrium energy density when $\beta > \beta_d$. We can correctly compute the equilibrium mean energy density using the BP equation when $\beta_d < \beta < \beta_c$. From figure 2, we see that there is an obvious difference between the SA mean energy density and the equilibrium mean energy density in the range $\beta_d < \beta < \beta_c$.

The intrinsic reason for this difference is that the microscopic equilibrium configuration space appears to be ergodicity-breaking. In SA, when $\beta$ increases to $\beta_d$, the configuration obtained by the SA process is not an equilibrium configuration, and the energy is higher than the average equilibrium energy.

### Figure 1.
The horizontal-axis denotes the inverse temperature, the vertical-axis denotes the complexity of a regular random graph with variable degree $C = 5$ in the left panel (a) and $C = 6$ in the right panel (b). When $C = 5$, the complexity has a condensation transition at $\beta = 7.90$ and has a cluster transition at $\beta = 8.19$.

### Figure 2.
The horizontal-axis denotes the inverse temperature, and the vertical-axis denotes the energy density of the regular random graph. The mean connectivity is $C = 5$ and includes 1000 variables. The value of $\omega$ is the number of iterations at every step.
the microscopic configuration of the system can be captured by the thermodynamic macroscopic state $\alpha$, and even when the waiting time $\omega$ is very long, the system cannot escape from this thermodynamic macroscopic state. Therefore, the system remains in the microscopic configuration subspace of the thermodynamic macroscopic state $\alpha$ as $\beta$ increases further. Thus the SA mean energy density is the energy density of the thermodynamic macroscopic state $\alpha$ for this value of $\beta$. This mean energy density is higher than the equilibrium energy density because, when the inverse temperature $\beta$ exceeds $\beta_d$, another thermodynamic macroscopic state with smaller energy density determines the equilibrium statistical properties of the system.

When $\beta$ is close to $\beta_d$, the ergodicity of the microscopic configuration begins to fail and the dynamical relaxation time increases, and diverges to infinity as $\beta = \beta_d$, so the system remains in a non-equilibrium state. To compute the characteristic relaxation time, we start from a randomly obtained equilibrium microscopic configuration, perform two completely independent single-spin heat bath dynamical processes, and record the overlap $q_t$ between the microscopic configurations for the two processes at time $t$. Figure 3 shows the three evolution curves for the overlap obtained by starting from three different equilibrium microscopic configurations against time $t$. These curves are obtained from a regular random graph with $N = 1000$ variable nodes and variable degree $C = 5$, and where $\beta = 7.5$ is less than cluster transition point $\beta_d = 7.9$.

The overlap is $q_0 = 1$ when $t = 0$. When the evolution time is long enough, the system totally forgets the original state, and so $q_t \rightarrow q^*$. We record the time that the overlap first time decreases to less than $q^* = 0.6$ as the characteristic relaxation time $\tau$. 

Figure 3. We implement a single-spin heat bath dynamical process on a regular random network for the MDS problem at $\beta = 7.5$. The mean connectivity is $C = 5$ and includes 1000 variables. The horizontal-axis denotes the evolution log time, and the vertical-axis denotes the overlap. The graph indicates that the overlap between two microscopic configurations for two independent heat bath dynamical processes evolves over time. The three curves originate at three distinct microscopic configurations. The horizontal line indicates an overlap value of 0.6.
for a path. We can obtain the distribution of characteristic relaxation times by simulating many evolution paths, and from this distribution we can obtain the average value and median value of the characteristic relaxation time. Figure 4 indicates the changes in the average characteristic relaxation time and the median characteristic relaxation time against $\beta$. For the case $C = 5$, we find that the characteristic relaxation time of the system diverges when $\beta = 7.9$.

In the simulation process, we find that the overlap curve reaches a plateau very quickly for every value of $\beta$, and that the overlap value then varies over a very small interval. However, the overlap value for the plateau increases with the inverse temperature. For example the overlap is $q \approx 0.1$ when $\beta = 2.0$, and $q \approx 0.35$ when $\beta = 7.8$. When $\beta$ approaches $\beta_d$, the relaxation time does not follow a Gaussian distribution but has a long tail, and thus the average relaxation time does not represent a physical quantity. The reason for this phenomenon is that, although the equilibrium microscopic configuration is ergodic, the microscopic configuration forms several communities and different microscopic configuration communities have different characteristic relaxation times. The appearance of different microscopic configuration communities may explain why the overlap $q_t$ does not decrease exponentially, instead maintaining a plateau before declining very quickly. In logarithmic coordinates, the plateau in the overlap $q_t$ corresponds to the same community in the microscopic configuration space being explored by two different single-spin heat bath dynamical processes, and the subsequent rapid decrease in the overlap $q_t$ corresponds to at least one of the heat bath dynamical processes escaping from this microscopic configuration community.

**Figure 4.** For a regular random network with $N = 1000$ nodes, we obtain 1000 samples of the relaxation time using a heat bath dynamical simulation process, and then calculate the average $\tau_{\text{mean}}$ and median $\tau_{\text{median}}$ relaxation times for these 1000 relaxation time samples. The solid line is the curve that fits the average relaxation time $\tau_{\text{mean}} = a (\beta^* - \beta)^z$, where $a = (4.75668 \pm 0.005399) \times 10^5$, $\beta^* = 7.9004 \pm 0.446$, $z = 6.3125 \pm 1.273$. 

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When the difference between the relaxation times for different evolution paths is very large, figure 4 indicates that the mean value of the relaxation time is still a good statistical representation of the relaxation time.

3.3. Population dynamics for 1RSB at $y = \beta$

We next explain in detail the numerical procedure for deriving thermodynamic quantities such as mean free energy, grand free energy and the complexity $\Sigma(y)$ for a given value of $\beta$.

(1) Initialization: We construct an array $S_0, S_1, S_2, \cdots S_{N_0 - 1}$ with $N_0$ rows, where each row has two elements $(\tilde{p}_{i \rightarrow j}, P_{i \rightarrow j}(\rho|\beta))$. Each average message $\tilde{p}_{i \rightarrow j}$ contains four messages, namely $(\tilde{p}^{(0,0)}_{i \rightarrow j}, \tilde{p}^{(0,1)}_{i \rightarrow j}, \tilde{p}^{(1,0)}_{i \rightarrow j}, \tilde{p}^{(1,1)}_{i \rightarrow j})$. However, these four messages are not independent of each other, so we use only two messages $(\tilde{p}^{(0,0)}_{i \rightarrow j}, \tilde{p}^{(0,1)}_{i \rightarrow j})$ to describe the average message. For the conditional message, we define eight messages of four different types: 

- $\{1\}p_{i \rightarrow j}(0, 0), p_{i \rightarrow j}(0, 1), p_{i \rightarrow j}(0, 0), p_{i \rightarrow j}(0, 0)$;
- $\{2\}p_{i \rightarrow j}(0, 0), p_{i \rightarrow j}(0, 1), p_{i \rightarrow j}(0, 1), p_{i \rightarrow j}(0, 1)$;
- $\{3\}p_{i \rightarrow j}(0, 0), p_{i \rightarrow j}(0, 1), p_{i \rightarrow j}(0, 1), p_{i \rightarrow j}(0, 1)$;
- $\{4\}p_{i \rightarrow j}(0, 0), p_{i \rightarrow j}(0, 1), p_{i \rightarrow j}(0, 1), p_{i \rightarrow j}(0, 1)$,

where $p_{i \rightarrow j}(0, 0)$ represents the probability that node $i$ is in state 0 and node $j$ is in state 0 when we observe that node $i$ is in state 0 and node $j$ is in state 0. Initializing the messages is very important for obtaining correct results. We initialize the messages as $\{1\}p_{i \rightarrow j}(0, 0) = 0.5$, $p_{i \rightarrow j}(0, 1) = 0.5$, $p_{i \rightarrow j}(0, 0) = 0.0$, $p_{i \rightarrow j}(0, 1) = 1.0$; $\{2\}p_{i \rightarrow j}(0, 0) = 0.0$, $p_{i \rightarrow j}(0, 1) = 0.0$, $p_{i \rightarrow j}(0, 1) = 0.0$, $p_{i \rightarrow j}(0, 1) = 0.0$.

(2) Updating: There are several possible sampling schemes [31–33]. In this paper, we update the messages using the sampling scheme in appendix.

(2.1): At each iteration, we randomly choose $k - 1$ messages from the population, and then calculate the new average message using equation (18).

(2.2): We could obtain four different conditional messages using the equations in appendix.

(2.3): The type (1) and type (2) conditional messages are sampled by equations (A.3), (A.4), (A.7) and (A.8). The type (3) and type (4) conditional messages are sampled by equations (A.5), (A.6), (A.9) and (A.10). We generate a random number $\mathcal{R}$. If $\mathcal{R} < p_{i \rightarrow k\backslash j}^{(0, 0)}$ (which is calculated using equation (A.7)), then we select $p_{k \rightarrow i}(c_k, c_i|0, 0)$ as the insert message; otherwise, we select $p_{k \rightarrow i}(c_k, c_i|0, 1)$ as the insert message. We then generate another random number $\mathcal{R}$. If $\mathcal{R} < p_{i \rightarrow k\backslash j}^{(1, 0)}$ (which is calculated using equation (A.8)), then we select $p_{k \rightarrow i}(c_k, c_i|0, 0)$ as the insert message; otherwise, we select $p_{k \rightarrow i}(c_k, c_i|0, 1)$ as the insert message.

(3) Calculate thermodynamic quantity: We randomly select $k$ average messages from the population.
1. We generate a random number $R$. If $R < p_{i\to j}^{(0,0)}$ (which is calculated using equation (A.3)), then we select $p_{j\to i}(c_j, c_i|0, 0)$ as the insert message; otherwise, we select $p_{j\to i}(c_j, c_i|1, 0)$ as the insert message.

2. We generate another random number $R$. If $R < p_{i\to j}^{(1,0)}$ (which is calculated using equation (A.5)), then we select $p_{j\to i}(c_j, c_i|0, 1)$ as the insert message; otherwise, we select $p_{j\to i}(c_j, c_i|1, 1)$ as the insert message.

3. We determine the state of the variable $k$, using equations (A.7)–(A.10) to obtain the insert messages. In the same way, we determine the states of the remaining variables and insert messages. We calculate the mean free energy of node $i$ using equation (22) and the general free energy using equation (27).

4. We randomly choose two messages and calculate the general free energy $g_{i,j}$ of edge $(i, j)$ using equation (26), and select two conditional messages using equation (24) to calculate the mean free energy $\langle f_{i,j} \rangle$ of edge $(i, j)$.

5. Finally, we calculate the mean free energy density, the grand free energy density and the complexity using equations (28)–(30).

In the simulation, we update the population $M_I = 100 000$ times to reach a stable point in the population, and sample $M_S = 100 000$ times to obtain the condensation transition point for the regular random graph. We can reach a stable point in the population by using fewer updates when number of variables is large. Furthermore, we update the population $M_I = 5000$ times to reach a stable point in the population, and sample $M_S = 5000$ times to obtain the cluster transition point for the regular random graph. However, a cluster transition point is only correct within a range of $\nabla y = 0.05$. The population size is $N = 10 000$. Increasing the population size does not affect the simulation results. However if we increase the number of samples number when calculating the thermodynamic quantities, then the results improve. Within a range of $\nabla y = 0.05$, we can also obtain good results with a small number of updates. However, in the range $\nabla y = 0.01$ we need an increasing number of updates to obtain good results. In the table 1 we indicate the cluster transition and the condensation transition of the regular random graph.

4. Zero-temperature mean field theory

In this section, we introduce BP at $\beta = \infty$, which is called warning propagation. Even though warning propagation converges very quickly, it only converges for $C < 2.41$ on ER random networks. We must therefore consider 1RSB theory further. We also derive the SP and estimate the ground state energy. Finally, we predict the energy density using the SPD method. We find that the SP results fit with the SPD results, and that the SPD results are as good as the belief propagation decimation (BPD) results.
4.1. Warning propagation

To estimate the minimal energy of an MDS, we must consider the limiting property for \( \beta = \infty \). There are three cases to consider for a single node: (1) node \( i \) appears in every MDS, or \( p_i = 1 \); (2) node \( i \) does not appear in any MDS, or \( p_i = 0 \); (3) node \( i \) appears in some MDSs, or \( p_i = 0.5 \). Thus there are nine cases for a pair of nodes \((i, j)\). However, only four cavity messages are possible: (1) node \( i \) in the pair \((i, j)\) appears in every MDS, or \((p_i^{1,0}, p_{ij}^{1,1}) = (0.5, 0)\); (2) node \( i \) in the pair \((i, j)\) does not appear in any MDS and node \( j \) appears in some MDSs, or \((p_i^{0,0}, p_{ij}^{0,1}) = (0, 0.5)\); (3) node \( i \) in the pair \((i, j)\) does not appear in any MDS and node \( j \) appears in every MDS, or \((p_i^{1,0}, p_{ij}^{1,1}) = (0, 0)\); (4) node \( i \) in the pair \((i, j)\) appears in some MDSs and node \( j \) appears in some MDSs, or \((p_i^{1,0}, p_{ij}^{1,1}) = (0.5, 0.5)\).

There is one warning message, \( p_{ij}^{0,1} = 1 \), for a single node. However, there are two warning messages for a pair of nodes \((i, j)\), namely \((p_i^{0,1}, p_{ij}^{0,1}) = (1, 0.5)\).

\[
\begin{align*}
  p_i^{0,1} & = \begin{cases} 
    0.0 & \sum_{k \in \partial i} \delta_{0,1}^{1,0} p_k^{0,1} \geq 2 \\
    0.25 & \sum_{k \in \partial i} \delta_{0,1}^{1,0} p_k^{0,1} = 1 \\
    0.5 & \sum_{k \in \partial i} \delta_{0,1}^{1,0} p_k^{0,1} = 0 \quad \text{and} \quad \sum_{k \in \partial i} \delta_{0,1}^{0,5} p_k^{0,1} < k - 1 \\
    1.0 & \sum_{k \in \partial i} \delta_{0,1}^{1,0} p_k^{0,1} = 0 \quad \text{and} \quad \sum_{k \in \partial i} \delta_{0,1}^{0,5} p_k^{0,1} = k - 1.
  \end{cases}
\end{align*}
\]

(31)

Equation (31) is called the warning propagation equation. If we find a stable point in the warning propagation equation, then we can calculate the coarse-grained state of every node as

\[
\begin{align*}
  p_i^{1} & = \begin{cases} 
    0.0 & \sum_{j \in \partial i} \delta_{0,1}^{1,0} p_{j-i}^{0,1} = 0 \\
    0.5 & \sum_{j \in \partial i} \delta_{0,1}^{1,0} p_{j-i}^{0,1} = 1 \\
    1.0 & \sum_{j \in \partial i} \delta_{0,1}^{1,0} p_{j-i}^{0,1} \geq 2,
  \end{cases}
\end{align*}
\]

(32)

and the free energy in the general case is then

\[
\begin{align*}
  F_i = -\frac{1}{\beta} \ln \left( \prod_{j \in \partial i} (p_{j-i}^{0,0} + p_{j-i}^{1,0}) \right) \\
  & + e^{-\beta} \prod_{j \in \partial i} (p_{j-i}^{0,1} + p_{j-i}^{1,1}) - \prod_{j \in \partial i} p_{j-i}^{0,0},
\end{align*}
\]

(33)

\[
\begin{align*}
  F_{ij} = -\frac{1}{\beta} \ln \left( p_{i-j}^{0,0} p_{j-i}^{0,0} + p_{i-j}^{0,1} p_{j-i}^{1,0} \\
  + p_{i-j}^{1,0} p_{j-i}^{0,1} + p_{i-j}^{1,1} p_{j-i}^{1,1} \right).
\end{align*}
\]

(34)

From the two equations above, we can express the free energy for \( \beta = \infty \) as
\[ E_{\text{min}} = \lim_{\beta \to \infty} F_0 = \sum_{i=1}^{N} \Big[ \Theta \left( \sum_{j \in \partial_i} \delta_{P_{j \to i}}^{1,0} - 1 \right) + \delta \left( \sum_{j \in \partial_i} \delta_{P_{j \to i}}^{0.5}, k \right) \Big] \]

\[ - \sum_{(i,j) \in w} \left[ (\delta_{P_{i \to j}}^{1,0} + \delta_{P_{i \to j}}^{0.5} \delta_{P_{j \to i}}^{0.5} \delta_{P_{j \to i}}^{0.5} \delta_{P_{j \to i}}^{0.5} \delta_{P_{j \to i}}^{0.5} \delta_{P_{j \to i}}^{0.5} ) \right]. \]  

(35)

Warning propagation gives same results as replica symmetry theory. However, it does not converge on ER random graphs when the average degree is larger than 2.41.

4.2. Coarse-grained survey propagation

To obtain the SP, we need to know the form of the free energy, \( F_{i \to j} \), at a temperature of zero. From the general form

\[ F_{i \to j} = -\frac{1}{\beta} \ln \{ 2 \prod_{k \in \partial_i \setminus j} (p_{k \to i}^{(0,0)} + p_{k \to i}^{(1,0)}) \] 

\[ + 2e^{-\beta} \prod_{k \in \partial_i \setminus j} (p_{k \to i}^{(0,1)} + p_{k \to i}^{(1,1)}) - \prod_{k \in \partial_i \setminus j} p_{k \to i}^{(0,0)} \} \]  

we can derive the free energy \( F_{i \to j} \) as

\[ F_{i \to j} = \Theta \left( \sum_{k \in \partial_i \setminus j} \delta_{P_{k \to i}}^{0,1} - 1 \right). \]  

(37)

The SP for the general case is

\[ P_{i \to j}(p) = \prod_{k \in \partial_i \setminus j} \int Dp_{k \to i} P_{k \to i}(p)e^{-yf_{i \to j}} \delta(p_{i \to j} - I_{i \to j}[p_{\partial_i \setminus j}]) \]  

\[ \prod_{k \in \partial_i \setminus j} \int Dp_{k \to i} P_{k \to i}(p)e^{-yf_{i \to j}}. \]  

(38)

We can obtain the SP at a temperature of zero by using equations (37) and (38):

\[ P_{i \to j}(\delta_{P_{j \to i}}^{0,1}) = \prod_{k \in \partial_i \setminus j} [1 - P_{k \to i}(\delta_{P_{k \to i}}^{0,1})] + e^{-yP_{01}^i}, \]  

(39)

where \( P_{01}^i = 1 - \prod_{k \in \partial_i \setminus j} [1 - P_{k \to i}(\delta_{P_{k \to i}}^{0,1})] \), and

\[ P_{i \to j}(\delta_{P_{j \to i}}^{0.5}) = \prod_{k \in \partial_i \setminus j} [1 - P_{k \to i}(\delta_{P_{k \to i}}^{0.5})] - \prod_{k \in \partial_i \setminus j} P_{k \to i}(\delta_{P_{k \to i}}^{0.5}) \]  

\[ \prod_{k \in \partial_i \setminus j} [1 - P_{k \to i}(\delta_{P_{k \to i}}^{0.5})] + e^{-yP_{01}^i}. \]  

(40)

These two equations are the SP at a temperature of zero. In the same way, we can derive the free energy of node \( i \) and edge \((i, j)\) as

\[ f_i = \Theta \left( \sum_{j \in \partial_i} \delta_{P_{j \to i}}^{0,1} - 1 \right) + \delta \left( \sum_{j \in \partial_i} \delta_{P_{j \to i}}^{0.5}, k \right), \]  

(41)
Minimizing the free energy of the macroscopic state \( \alpha \) when \( \beta = \infty \) is equal to the ground state energy \( E_{\text{min}} \). The macroscopic average minimal energy \( \langle E_{\beta=\infty} \rangle \) is calculated using the following equation:

\[
\langle E_{\beta=\infty} \rangle = \frac{\partial (yG_0)}{\partial y} = \sum_{i=1}^{N} e^{-y} \left\{ \left[ \prod_{j \in \partial i} \left[ 1 - P_{j \rightarrow i}(\delta_{p_{j \rightarrow i}^{0.5}}) \right] \right] \times \frac{1}{N} \right\} - \sum_{(i,j) \in E} e^{-y} p_{i \rightarrow j}^{0.1}[nh].
\]

The ensemble average property for the MDS problem can be studied by applying population dynamics with equations (39)–(42), (45) and (46). In figure 5, we show the ensemble average 1RSB population dynamics results for the MDS problem on https://doi.org/10.1088/1742-5468/aa8c1e
an ER random graph with mean connectivity $C = 5$ and complexity $\Sigma = 0$ at $y = 0$. The complexity is not a monotonic function of $y$, but increase with $y$ to its maximum value when $y \approx 3.5$. The complexity then begins to decline and becomes negative when $y \approx 7.15$. From figure 5, we can see that there are two parts to the complexity graph as a function of energy. However, only the concave part represents a decreasing function of energy and therefore has a physical meaning. The grand free energy is also not a monotonic function of $y$, reaching a maximum when the complexity changes to negative at $y \approx 7.15$. Thus the corresponding energy density $u = 0.2068$ is the minimum energy density (or ground state energy) for $C = 5$.

We can calculate the some microscopic statistical quantities using equations (39) and (40)) the zero-temperature equations. For example, for the probability (statistical total weight of all macroscopic states) that a variable remains in the coarse-grained state, we use $p_i(0)$ to denote the probability that the variable remains in a totally not covered state, $p_i(1)$ to denote the probability that the variable remains in a totally covered state, and $p_i(\ast)$ to denote the probability that the variable remains in a not freezing (that is, covered in some microscopic state) state. We can derive representations of these three probabilities using 1RSB mean field theory:

\[\text{Figure 5. The SP results for the zero-temperature MDS problem on an ER random graph with mean connectivity } C = 5 \text{ using population dynamics. In the first three graphs, the horizontal-axis denotes the Parisi parameter } y, \text{ and the vertical-axis denotes the thermodynamic quantities. The complexity is equal to zero when the Parisi parameter } y \text{ is approximately 7.15. At this point, we select the corresponding energy as the ground state energy, which equals 0.2068. In the lower right graph, the horizontal-axis denotes the energy density and the vertical-axis denotes the complexity. In this case the SP equation does not converge when } y \geq 6.9, \text{ and the standard deviation is } \sigma \approx 10^{-5}.\]
Table 1. The cluster transition of the inverse temperature $\beta_d$ and the condensation transition of the inverse temperature $\beta_c$ for a regular random graph.

| C  | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|----|-----|-----|-----|-----|-----|-----|-----|-----|
| $\beta_d$ | 8.06 | 7.81 | 7.9 | 8.06 | 8.24 | 8.43 | 8.63 | 8.76 |
| $\beta_c$ | 8.25 | 8.04 | 8.19 | 8.41 | 8.65 | 8.88 | 9.11 | 9.33 |

We can apply the 1RSB population dynamics to different mean connectivities for ER random graphs, and obtain the minimal energy density for ER random networks. In Table 2, we list the theoretical computation results for different mean connectivities for ER random networks. In the simulation, we update the population $M_I = 5000$ times to reach a stable point in the population, and sample $M_S = 5000$ times to obtain $\Sigma = 0$ points and the corresponding ground energy values $E_{\text{min}}$ on the ER random graph. The cluster transition point is only correct within a range of $\forall y = 0.05$. However, the ground energy is correct within a range of $\forall E = 0.0001$. The population size is $N = 100,000$. Increasing the number of updates or the number of samples does not affect the simulation results. However, increasing the population size $N$ for calculating the thermodynamic quantities improves the results. Within a range of $\forall y = 0.05$, we can also obtain good results with fewer updates. However, in the range $\forall y = 0.01$, we need an increasing number of updates to obtain good results. The required numbers of updates and samples increases as the variable degree decreases.

4.3. Survey propagation decimation

We can still study the statistical properties of microscopic configurations on a single network system using the SP in equations (39) and (40). The SP makes finding a stable point for a given network easy when the Parisi parameter $y$ is small enough, and we can then calculate the thermodynamic quantities using equations (41), (42), (45)–(47). However, the SP does not converge when $y$ is too large. For example, our simulation results indicate that the SP does not converge when $y \geq 2.1$ for an ER random network when $C = 10$. The reason for this is that the coarse-grained assumption is no longer valid.
good for microscopic configuration spaces with energy close to the ground state energy, so a more detailed coarse-grained assumption is required. A more intrinsic reason is that 1RSB mean field theory is not good enough to describe microscopic configuration spaces with energy close to the ground state energy, and we should consider a higher-level expansion of the partition function. For further discussion of convergence of coarse-grained SP, see [34, 35].

It is possible to construct one or more solutions that are close to the optimal MDS for a given graph $W$ using 1RSB mean field theory. One very efficient algorithm is the SPD algorithm [6]. The core idea of this algorithm is to determine the probability of being frozen, and then select a small subset of variables that has the highest probability of been covered. We then set the covered probability for this subset of variables to $c_i = 1$, and simplify the network iteratively. If a node $i$ is unobserved (it is empty and has no adjacent occupied node), the output message $P_{i \rightarrow j}$ is updated according to equation (39) and (40). On the other hand, if node $i$ is empty but observed (it has at least one adjacent occupied node), this node then presents no restriction to the occupation states of all its unoccupied neighbors. For such a node $i$, the output message $P_{i \rightarrow j}$ is then updated according to the following equation:

$$P_{i \rightarrow j}(\delta_{P_{j \rightarrow i}}^{1,0}) = 0,$$

$$P_{i \rightarrow j}(\delta_{P_{j \rightarrow i}}^{0,1}) = \prod_{k \in \partial_i \setminus j} [1 - P_{k \rightarrow i}(\delta_{P_{k \rightarrow i}}^{1,0})] / \prod_{k \in \partial_i \setminus j} [1 - P_{k \rightarrow i}(\delta_{P_{k \rightarrow i}}^{1,0})] + e^{-y}P_{i \rightarrow j}^{0,1}.$$  \hspace{1cm} (54)

Similar to equations (53) and (54), the marginal probability distribution $P_i$ for an observed empty node $i$ is evaluated according to

$$P_i(0) = \frac{\prod_{j \in \partial i} [1 - P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{1,0})]}{(1 - e^{-y})\{\prod_{j \in \partial i} [1 - P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{1,0})]\} + e^{-y}},$$

$$P_i(*) = \frac{\sum_{j \in \partial i} P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{1,0}) \prod_{k \in \partial i \setminus j} [1 - P_{k \rightarrow i}(\delta_{P_{k \rightarrow i}}^{1,0})]}{(1 - e^{-y})\{\prod_{j \in \partial i} [1 - P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{1,0})]\} + e^{-y}},$$

$$P_i(1) = 1 - P_i(0) - P_i(*) .$$ \hspace{1cm} (57)

We now present the process of this algorithm in detail.

(1) Read in the network $W$, set the being covered probability of every vertex as uncertain, and define four coarse-grained messages, $P_{i \rightarrow j}(\delta_{P_{j \rightarrow i}}^{0,1})$, $P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{1,0})$, $P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{0,1})$, and $P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{1,0})$, on each edge of the given graph. Randomly initialize the messages in the interval $(0,1)$, ensuring that for every pair of messages $P_{i \rightarrow j}(\delta_{P_{j \rightarrow i}}^{0,1})$, $P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{1,0})$, the normalization condition $P_{i \rightarrow j}(\delta_{P_{j \rightarrow i}}^{1,0}) + P_{i \rightarrow j}(\delta_{P_{j \rightarrow i}}^{0,1}) + P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{1,0}) + P_{j \rightarrow i}(\delta_{P_{j \rightarrow i}}^{0,1}) = 1$.
is satisfied. An appropriate setting for the macroscopic inverse temperature $y$ is a value close to the threshold value. For example, if SP does not converge when $y \geq 3.01$, then we set $y = 3$.

(2) Iterate the coarse-grained SP equations, equations (39) and (40) or (53) and (54), for $L_0$ steps, aiming for convergence to a stable point. At each iteration, select one node $i$ and update all messages corresponding to node $i$. After updating the node messages $L_0$ times, calculate the coarse-grained probability $(P_i(1), P_i(*), P_i(0))$ using equations (50)–(52) or equations (55)–(57).

(3) Sort the variables that are not frozen in descending order according to the value of $P_i(1)$. Select the first $r$ percent to set the covering state $c_i = 1$, and add these variables to the MDS.

(4) Simplify the network by deleting all the edges between the observed nodes and deleting all the occupied variables. If the remaining network still contains one or more leaf nodes [11], then we apply the GLR process [10] until there are no leaf nodes in the network, and simplify the network again. This procedure is repeated (simplify-GLR-simplify) until the network contains no leaf nodes. If the network contains no nodes and no edges, then stop the program and output the MDS.

Figure 6. The solid line is the result of the SPD algorithm, and the line of crosses the result of the BPD algorithm. Our simulation was performed on an ER random graph containing $10^4$ variables.

Table 2. The cluster transition point inverse temperature $y_d$ for ER random graphs.

| C  | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  |
|----|-----|-----|-----|-----|-----|-----|-----|-----|
| $y^* \approx$ | 8.0 | 7.29| 7.15| 7.19| 7.31| 7.47| 7.64| 7.82|
| $u_{\text{min}}(1RSB)$ | 0.3176 | 0.2498 | 0.2068 | 0.178 | 0.1576 | 0.142 | 0.130 | 0.120 |
| $u_{\text{min}}(RS)$ | 0.3176 | 0.2495 | 0.2058 | 0.1769 | 0.1566 | 0.1415 | 0.1296 | 0.1199 |
(5) If the network still contains some nodes, then iterate equations (39), (40) or (53), (54)) for $L_1$ steps. Repeat steps (3)–(5).

Figure 6 shows the numerical results of the SPD algorithm on an ER random graph. We can see that the SPD results are very close to the BPD results, and thus the SPD algorithm finds an almost optimal solution. We perform the BPD algorithm as detailed in [10].

From the figure 6 we can see that the results of SPD and BPD are almost same each other. It is not surprising that the SPD and BPD algorithms have almost the same effect, because the ground state energy predicted by RS and 1RSB is slightly different (table 2).

5. Discussion

In this paper, we derived the 1RSB equations for the MDS problem at $y = \beta$, and found the condensation transition point and cluster transition point for regular random graphs. The corresponding energy of the cluster transition point $\beta_d$ is the ground state energy. The complexity graph for the MDS problem is similar to the three-body interaction spin glass model and the 4-SAT problem [32, 33]. However, the behavior of these transition points as the average degree changes is different from the three-body interaction spin glass model. In the three-body interaction spin glass model, these two transition points always decrease as the average degree increases, but they are not monotonic functions of degree for the MDS problem. We next derived the warning propagation and proved that the warning propagation equation only converges when the network does not contain a core [10]. There is only one warning for the vertex cover problem [12]. However, the MDS problem has two warnings. We then derived the SP function at a temperature of zero to find the ground state energy and the corresponding transition point for $Y$, and to determine the behavior of the transition point as with the vertex cover problem. The corresponding energy density of the transition point equals the threshold value $x_c$. Finally, we implemented the SPD algorithm at a temperature of zero to estimate the size of an MDS. The results were as good as those using the BPD algorithm.

Previously, we studied the MDS problem on undirected networks and directed networks using statistical physics, and we have now studied the undirected MDS problem using 1RSB mean field theory. We plan to extend this study to the directed MDS problem using 1RSB mean field theory, and to applying long-range frustration theory to the MDS problem.

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Appendix. Samples by probability function (18)

We use equation (18) to discuss the sampling scheme. Our problem is to give a spin value to the variables surrounding node $i$, where the joint probabilities of these spin values must satisfy equation (18). The direct sampling method is to calculate $2^k$ different spin value configuration probabilities using equation (18), to generate a random number in the interval (0, 1), and to select the spin value configuration corresponding to the random number. Using direct sampling, we need to calculate the probabilities for all configurations, which is not feasible when $k \gg 1$.

Another convenient sampling method is sequential sampling. We first determine the value $c_i$ for node $i$, then use this value to determine the value $c_j$ for node $j$, then use these values to determine the value $c_k$ for node $k$. This continues until the values for all nodes adjacent to node $i$ are known.

We use equation (18) to derive the marginal probability for node $i$ as

$$
p_i^{(0)} = \frac{\prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) - \prod_{j \in i} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)})}{\prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)})} - e^{-\beta} \prod_{j \in i} (\bar{p}_j^{(1,1)} + \bar{p}_j^{(0,1)}) - \prod_{j \in i} (\bar{p}_j^{(0,0)}),
$$

(A.1)

$$
p_i^{(1)} = \frac{\prod_{j \in i} (\bar{p}_j^{(1,1)} + \bar{p}_j^{(0,1)})}{\prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) + \prod_{j \in i} (\bar{p}_j^{(1,1)} + \bar{p}_j^{(0,1)}) - \prod_{j \in i} (\bar{p}_j^{(0,0)}).}
$$

(A.2)

From the above equations, we can determine the spin value for node $i$, and can then derive the conditional probabilities for node $j$ as

$$
p_{i-j}^{(0,0)} = \frac{\prod_{j \in i} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) - \prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)})}{\prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) + \prod_{j \in i} (\bar{p}_j^{(0,0)} + \bar{p}_j^{(1,0)}) + e^{-\beta} \prod_{j \in k} (\bar{p}_j^{(0,1)} + \bar{p}_j^{(1,1)})},
$$

(A.3)

$$
p_{i-j}^{(0,1)} = \frac{\prod_{j \in i} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) - \prod_{j \in i} (\bar{p}_j^{(0,0)} + \bar{p}_j^{(1,0)}) + e^{-\beta} \prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,1)})}{\prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) + \prod_{j \in i} (\bar{p}_j^{(0,0)} + \bar{p}_j^{(1,0)}) + e^{-\beta} \prod_{j \in k} (\bar{p}_j^{(0,1)} + \bar{p}_j^{(1,1)})},
$$

(A.4)

$$
p_{i-j}^{(1,0)} = \frac{\prod_{j \in i} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) - \prod_{j \in i} (\bar{p}_j^{(0,0)} + \bar{p}_j^{(1,0)}) + e^{-\beta} \prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,1)})}{\prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) + \prod_{j \in i} (\bar{p}_j^{(0,0)} + \bar{p}_j^{(1,0)}) + e^{-\beta} \prod_{j \in k} (\bar{p}_j^{(0,1)} + \bar{p}_j^{(1,1)})},
$$

(A.5)

$$
p_{i-j}^{(1,1)} = \frac{\prod_{j \in i} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) - \prod_{j \in i} (\bar{p}_j^{(0,0)} + \bar{p}_j^{(1,0)}) + e^{-\beta} \prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,1)})}{\prod_{j \in k} (\bar{p}_j^{(1,0)} + \bar{p}_j^{(0,0)}) + \prod_{j \in i} (\bar{p}_j^{(0,0)} + \bar{p}_j^{(1,0)}) + e^{-\beta} \prod_{j \in k} (\bar{p}_j^{(0,1)} + \bar{p}_j^{(1,1)})},
$$

(A.6)
The conditional probabilities \( p(k|i, j) \) for node \( k \) when the spin values for nodes \((i, j)\) are given can then be calculated:

\[
p_{i \rightarrow k \setminus j}^{(0,0)} = \frac{\tilde{p}_{k \rightarrow i}^{(0,0)} \times \prod_{l \in i \setminus j} (\tilde{p}_{l \rightarrow i}^{(0,1)} + \tilde{p}_{l \rightarrow i}^{(0,0)}) - \delta_{c_j} \prod_{l \in i \setminus j} \tilde{p}_{l \rightarrow i}^{(0,0)}}{\prod_{l \in i \setminus j} (\tilde{p}_{l \rightarrow i}^{(1,0)} + \tilde{p}_{l \rightarrow i}^{(0,0)}) - \delta_{c_j} \prod_{l \in i \setminus j} \tilde{p}_{l \rightarrow i}^{(0,0)}},
\]

(A.7)

\[
p_{i \rightarrow k \setminus j}^{(0,1)} = \frac{\tilde{p}_{k \rightarrow i}^{(1,0)} \times \prod_{l \in i \setminus j} (\tilde{p}_{l \rightarrow i}^{(1,1)} + \tilde{p}_{l \rightarrow i}^{(0,1)}) - \delta_{c_j} \prod_{l \in i \setminus j} \tilde{p}_{l \rightarrow i}^{(0,1)}}{\prod_{l \in i \setminus j} (\tilde{p}_{l \rightarrow i}^{(1,0)} + \tilde{p}_{l \rightarrow i}^{(0,0)}) - \delta_{c_j} \prod_{l \in i \setminus j} \tilde{p}_{l \rightarrow i}^{(0,0)}},
\]

(A.8)

\[
p_{i \rightarrow k \setminus j}^{(1,0)} = \frac{\tilde{p}_{k \rightarrow i}^{(1,0)} \times \prod_{l \in i \setminus j} (\tilde{p}_{l \rightarrow i}^{(0,1)} + \tilde{p}_{l \rightarrow i}^{(1,0)})}{\prod_{l \in i \setminus j} (\tilde{p}_{l \rightarrow i}^{(1,0)} + \tilde{p}_{l \rightarrow i}^{(0,1)})},
\]

(A.9)

\[
p_{i \rightarrow k \setminus j}^{(1,1)} = \frac{\tilde{p}_{k \rightarrow i}^{(1,1)} \times \prod_{l \in i \setminus j} (\tilde{p}_{l \rightarrow i}^{(0,1)} + \tilde{p}_{l \rightarrow i}^{(1,1)})}{\prod_{l \in i \setminus j} (\tilde{p}_{l \rightarrow i}^{(1,1)} + \tilde{p}_{l \rightarrow i}^{(0,1)})}.
\]

(A.10)

From these equations, we can determine the spin value for node \( k \). Repeating this procedure determine all spin values for one configuration.

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