Minimum vertex cover problems on random hypergraphs: replica symmetric solution and a leaf removal algorithm

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We study minimum vertex cover problems on random $\alpha$-uniform hypergraphs using two different approaches, a replica method in statistical mechanics of random systems and a leaf removal algorithm. It is found that there exists a phase transition at the critical average degree $\epsilon/(\alpha - 1)$. Below the critical degree, a replica symmetric ansatz in the statistical-mechanical method holds and the algorithm estimates a solution of the problem which coincides with that by the replica method. In contrast, above the critical degree, the replica symmetric solution becomes unstable and these methods fail to estimate the exact solution. These results strongly suggest a close relation between the replica symmetry and the performance of approximation algorithm.

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The more crucial part of everyday life computers bear, the more significance computer science and information theory seem to have. In particular, the computational complexity theory shows the difficulty, the limit of improving algorithms, to solve theoretical computational problems. It has revealed that the problems belong to several classes such as P and NP and there are many inclusion relations between these classes. For example, 2-satisfiability problems (2-SAT) belong to a class of P guaranteed to be solved in polynomial time. 3-SAT and the vertex cover problems belong to a class of NP-complete. These problems are deeply related to the well-known P versus NP problem plaguing the theoretical computer scientists, who have studied the worst-case performance to solve the computational problems. Among many types of combinatorial optimization problems, the minimum vertex cover problem (min-VC) belongs to a class of NP-hard. The approximation algorithm for the min-VC and its performance have been studied. The application of the problem is to search a file on a file storage and to improve the group testing.

In contrast to the worst-case analysis, an important alternative is the study of typical-case behavior on a class of random instances of the computational problems. Recently, statistical-mechanical methods of random spin systems have been applied to the problems such as K-SAT and constraint-satisfaction problems. These methods, developed in the spin-glass theory, enable us to study the typical properties of the randomized problems. For example, the statistical-mechanical approaches find a SAT/UNSAT transition of K-SAT, p-XOR-SAT, q-coloring and min-VCs on K-uniform regular random hypergraphs. It is also found that there exists a P/NP transition between 2-SAT and 3-SAT. Here we study the typical case of the size of the min-VC, explained later, on random $\alpha$-uniform hypergraphs and focus on the relation between the replica symmetry and the performance of an approximation algorithm called a leaf removal algorithm.

Let us suppose that an $\alpha$-uniform hypergraph $G = (HV, HE)$ consists of $N$ vertices $i \in HV = \{1, \ldots, N\}$ and (hyper)edges $(i_1, \ldots, i_\alpha) \in HE \subset HV^\alpha (i_1 < \cdots < i_\alpha)$. We define covered vertices as a subset $HV' \subset HV$.
and covered edges as a subset of edges connecting to at least a covered vertex. The vertex cover problem on the hypergraph $G$ is to find a set of the covered vertices $HV$ by which all edges are covered. We define the cover ratio on $G$ as $|HV|/|N|$ with $|HV|$ being the size of the vertex cover problem. The min-VC on $G$ is to search a set of the covered vertices with the minimum cover ratio. In the random $\alpha$-uniform hypergraph all the edges are set independently from all $\alpha$-tuples of vertices with probability $p$. The degree distribution of the graph converges to the Poisson distribution with the average degree $c$, which is given as $c = pN^{\alpha-1}/(\alpha - 1)!$ for large $N$. In this Letter, we focus on an average of the minimum cover ratio $x_c$ over the sparse random hypergraphs with the average degree $c$ being $O(1)$.

The vertex cover problems are mapped on the lattice gas model $[10, 11, 21]$ on the random hypergraphs. We define a variable $\nu_i$ on each vertex, representing the existence of a gas particle, which takes 0 if a vertex $i$ is covered and 1 if uncovered. An covered edge has at least a vertex with $\nu_i = 0$ in its connecting vertices. Thus, an indicator function for a given particle configuration $\xi = \{\nu_i\} = \{0, 1\}^N$ is defined as

$$\chi(\xi) = \prod_{(i_1, \ldots, i_\alpha) \in HE} (1 - \nu_{i_1} \cdots \nu_{i_\alpha}), \quad (1)$$

which takes 1 if $\xi$ is a solutions of the vertex cover problem on the hypergraph, and 0 otherwise. Using the indicator function, the grand canonical partition function of the model reads

$$\Xi = \sum_\xi \exp \left( \mu \sum_{i = 1}^N \nu_i \right) \chi(\xi), \quad (2)$$

where $\mu$ is a chemical potential and the sum is over all configurations of $\xi$. In this formulation, only the solutions of the vertex cover problem contribute the partition function and its ground states in a large $\mu$ limit are given by the solutions of the min-VC. To study the typical case of min-VCs we need to take the average over the random hypergraphs and the limit as $N \to \infty$. Then, the average minimum-cover ratio is represented as

$$x_c(c) = 1 - \lim_{\mu \to \infty} \lim_{N \to \infty} \frac{1}{N} E \left( \sum_i \nu_i \right), \quad (3)$$

where $\langle \cdots \rangle_\mu$ is the grand canonical average and $E$ is the average over the random hypergraph ensemble. Our aim is to obtain the theoretical estimate of the average minimum-cover ratio as a function of the average degree $c$.

The average minimum-cover ratio is derived from the averaged grand potential density $-\langle \mu N \rangle^{-1} E \ln \Xi$, which is obtained by using the replica method for finite connectivity graphs $[22]$. Following the standard procedure of the replica method, the original problem is reduced to solving a saddle-point equation of a replicated order parameter functional. To proceed the calculation, we assume the RS ansatz that the solution of the saddle-point equation has a replica symmetry. Introducing a local field on a vertex associated to the order parameter and its distribution function, we obtain the saddle-point equation of the distribution. Finally, under the RS ansatz, the average minimum-cover ratio is obtained as a function of the average degree $c$,

$$x_c(c) = 1 - \frac{W((\alpha - 1)c)}{(\alpha-1)c} \left( 1 + \frac{W((\alpha - 1)c)}{\alpha} \right), \quad (4)$$

where $W(x)$ is the Lambert W function defined as $W(x) \exp(W(x)) = x$. We call this estimate the RS solution of min-VCs. This solution is also obtained by an alternative cavity method $[12]$. Although the instability of the RS solution such as the de Almeida-Thouless instability $[23]$ must be examined to validate the solution, we here naively study an instability condition of the saddle-point equation against a perturbation of the local field distribution within the RS sector. The analysis leads to a critical value of the average degree $c_\alpha = e/(\alpha - 1)$ above which the RS solution becomes unstable. These results, $x_c$ and $c_\alpha$, include the case of $\alpha = 2$ $[10]$. The obtained $x_c$ gives a correct value below the critical average degree, while a RSB solution for $x_c$ is required above it.

Here we turn our attention to the estimate of $x_c$ by using an approximation algorithm. The leaf removal algorithm has been proposed as an approximation algorithm to solve a min-VC on a graph with $\alpha = 2$ $[24]$ and has also been applied to search for a $k$-core $[23]$ and a 3-XOR-SAT solution $[13]$. For a min-VC on a given graph, this algorithm consists of iterative steps, where vertices called a leaf, as well as the edges connecting to the leaves, are removed from the graph with covered vertices appropriately assigned to those vertices. This removal step makes new leaves and the algorithm continues in an iterative way until the leaf is empty. By this procedure, the minimum cover ratio is estimated correctly at least for the removed part of the graph. We consider the global leaf removal (GLR) algorithm $[14]$, which removes simultaneously all the leaves found in a recursive step. We focus on the expansion of this algorithm for the min-VC on a hypergraph with $\alpha = 3$, while it is straightforward to extend it to that on a hypergraph with $\alpha \geq 4$. A crucial point in our algorithm is in definition of leaf, where a leaf $\{i, j, k\} \in HV^3 (i < j < k)$ is defined as a $3$-tuple of vertices connecting to an edge $(i, j, k)$, at least two of which the degree is one. The definition of the GLR algorithm is as follows:

**Step 1:** The initial graph $G$ is named $G^{(0)}$. Set $k = 0$.

**Step 2:** Search all leaves from the graph $G^{(k)}$. If there is no leaf, go to **Step 6**.

**Step 3:** Remove a leaf from the graph $G^{(k)}$.

**Step 4:** Make new leaves by removing the part of the graph associated to the removed leaf.

**Step 5:** Set $k = k + 1$ and go to **Step 2**.
Step 3: Remove all the leaves except for the vertices which belong to more than two leaves, named bunch of leaves [14], and remove only one of leaves in each bunch.

Step 4: Assign covered vertices to the one with the maximal degree in each removed leaf from $\mathcal{G}^{(k)}$.

Step 5: The left graph is named $\mathcal{G}^{(k+1)}$, and return to Step 2 with $k$ increased by one.

Step 6: If there exist connected vertices in the left graph, assign all of them to covered vertices. Stop the algorithm.

It is proven that the result of the algorithm is independent of order of removal and a selection of a leaf out of a bunch of leaves in the removal process. When the recursive steps stop, the left graph consists of isolated vertices and a core, which is defined as a set of vertices connecting to edges without leaves. Vertices in a bunch of leaves which are not selected for the removal in Step 3 become isolated and the core of the order $O(N)$ exists in large $c$. We note that Step 4 can be omitted if one is interested only in the minimum cover ratio, not the covered vertices. Because the algorithm covers all vertices in the core without searching the solution of the min-VC as shown in Step 6, the existence of the core of the order $O(N)$ leads to overestimation of the average minimum-cover ratio. We study the core size at the end of the GLR algorithm by numerically performing the above-mentioned procedure for finite-size random hypergraphs with $\alpha=3$. While the computational time for the GLR algorithm is proportional to the number of vertices, it takes time of the order $O(N^{3/2})$ for generating a random graph. To avoid it, we use the microcanonical ensemble [14] with fixing the number of edges to the expectation number of edges $cN/3$, ignoring fluctuation of the average degree. We expect that such fluctuation is irrelevant in a large size $N$ limit. In Fig. 1 the core size density obtained by numerical simulations is presented as a function of the average degree $c$ up to the size $N=10^5$. The data averaged over $10^4$ random graphs converges well for large sizes and a giant core with $O(N)$ emerges above a certain value of $c$.

We discuss the asymptotic behavior of the recursive procedure in the GLR algorithm. We introduce the average fraction of the core $e_n$ and the isolated vertices $i_n$ over random hypergraphs after $n$-th step of the algorithm, and find

$$i_n = e_{2n+1} + 2e_{2n} + 2ce_{2n}e_{2n-1}^2 - 2,$$

$$e_n = e_{2n} - e_{2n+1} - 2ce_{2n}e_{2n-1}^2 + 2ce_{2n-1}^3,$$  \hfill (5)

where a parameter $\epsilon_n$ obeys a recursion relation $\epsilon_n = \exp(-ce_{n-1}^2)$ with the initial condition $\epsilon_{-1} = 0$. A detailed derivation of the formulas will be reported in a separate paper [24]. By definition, the average fraction of the removed vertices $r_n$ up to the $n$-th step is given by $r_n = 1 - i_n - e_n$. These fractions are governed by the sequence of $e_n$ and their values at the end of the algorithm are determined by the asymptotic behavior of the recursion relation of $\{e_n\}$. It is found that there exists a critical average degree $c_\ast = e/2$ for the recursion relation. Below the critical value, the sequence $\{e_n\}$ converges to the unique value $[W(2c)/(2c)]^{1/2}$ and consequently the core size $e_\infty$ is zero. Above the critical value, however, a bifurcation occurs in the recursion relation and the sequence has a cycle with period two. This type of the transition would occur above $\alpha = 3$ at the critical average degree $c_\ast = e/(\alpha - 1)$. Because $e_{-1} = 0$, an even term $e_{2n}$ is larger than that at one-step later, that is $e_{2n+1}$. We compute the limiting values $\lim_{n \to \infty} e_{2n+1}$ and $\lim_{n \to \infty} e_{2n}$ numerically as a function of $c$. The difference between them yields emergence of the core of the order of $O(N)$. We present the core size density obtained from the asymptotic analysis of the recursion relation by the solid line in Fig. 1 which coincides with the data by numerical simulations. Thus, we confirm that a core percolation occurs at the critical average degree in the GLR algorithm, which coincides with that of the RS instability. From the analysis near the critical degree, it is found that the size of the core emerges linearly near above the critical average degree. These findings, the bifurcation in the recursion relation and the core percolation, are common in the min-VCs on random graphs with $\alpha=2$.

As mentioned above, the GLR algorithm estimates the minimum cover ratio by the size of the removed part in the graph during the recursive procedure, which is given as $r_\infty = 1 - i_\infty - e_\infty$. Taking one-third of $r_\infty$ and adding

FIG. 1. (Color Online). The core size density in the GLR algorithm as a function of the average degree $c$. Open marks are the data obtained by the GLR algorithm with the vertex size $10^4$, $5 \times 10^4$, and $10^5$, which are taken an average over $10^4$ random hypergraphs. The solid line is the core size density predicted by our recursive analysis. The vertical dotted line represents the critical average degree $c_\ast = e/2$. 

Below the critical value, the sequence $\{e_n\}$ converges to the unique value $[W(2c)/(2c)]^{1/2}$ and consequently the core size $e_\infty$ is zero. Above the critical value, however, a bifurcation occurs in the recursion relation and the sequence has a cycle with period two. This type of the transition would occur above $\alpha = 3$ at the critical average degree $c_\ast = e/(\alpha - 1)$. Because $e_{-1} = 0$, an even term $e_{2n}$ is larger than that at one-step later, that is $e_{2n+1}$. We compute the limiting values $\lim_{n \to \infty} e_{2n+1}$ and $\lim_{n \to \infty} e_{2n}$ numerically as a function of $c$. The difference between them yields emergence of the core of the order of $O(N)$. We present the core size density obtained from the asymptotic analysis of the recursion relation by the solid line in Fig. 1 which coincides with the data by numerical simulations. Thus, we confirm that a core percolation occurs at the critical average degree in the GLR algorithm, which coincides with that of the RS instability. From the analysis near the critical degree, it is found that the size of the core emerges linearly near above the critical average degree. These findings, the bifurcation in the recursion relation and the core percolation, are common in the min-VCs on random graphs with $\alpha=2$.

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\(c_\infty\) to the value, we obtain the estimate of the average minimum-cover ratio by the algorithm. Thus, we find that below the critical average degree \(c/2\) the estimate \(r_\infty/3\) coincides with the RS solution Eq. (4) estimated by the replica method. In contrast, the sequence \(\{c_n\}\) of the algorithm does not converge to a unique value above the critical value and the GLR algorithm could not give a precise estimate of \(x_c\) there.

In order to confirm whether these analyses estimate the average minimum-cover ratio \(x_c\) correctly, we also evaluate the min-VCs by the Markov chain Monte Carlo method. We use the replica exchange Monte Carlo method (EMC) \([27]\), for accelerating the dynamics of the system, with 50 replicas in the range of the critical potential from \(-2\) to \(-10\). In our Monte Carlo simulations, the smallest cover ratio found in typically \(2\times^{10^5}\) Monte Carlo steps is used as the estimate of \(x_c\) for each random graph, which is averaged over \(800\) hypergraphs randomly generated. The number of vertices of the graph is up to \(N = 512\). The average minimum-cover ratio is extrapolated from these numerical results for finite \(N\).

Fig. 2 shows the obtained minimum cover ratio as a function of the average degree \(c\). Below the critical average degree \(c/2\) where the RS solution is considered to be correct, we observe that the MC result is consistent with those by the two approaches, the replica method and the GLR algorithm. Above the critical value, on the other hand, the MC estimate stays slightly above that by the replica method and considerably deviates from that by the GLR algorithm. The former is due to the instability of the RS solution and the latter is the existence of the core of the order \(O(N)\).

To summarize, we consider the minimum vertex cover problems on random \(\alpha\)-uniform hypergraphs, and analyze them by the statistical-mechanical method and the approximation algorithm. The replica method estimates the average minimum-cover ratio \(x_c\) as a function of the average degree \(c\) under the replica symmetric assumption. We find that there is an RS/RSB phase transition at the critical average degree \(c_c = e/(\alpha - 1)\), which is well above a percolation threshold \(c = 1/(\alpha - 1)\) in the random graph. We also perform the global leaf removal algorithm and study the asymptotic behavior of the recursive procedure of the algorithm, particularly in the case of \(\alpha = 3\). If the average degree is below the critical value which coincides with that in the replica theory, there is a core of the order \(O(1)\) in the remaining part of the graph, which does not affect the estimate of the minimum cover ratio. In contrast, above the critical value, the core of the order \(O(N)\) emerges, leading to a wrong estimation of the minimum cover ratio. Comparing the results obtained by MC simulations, we confirm that these estimates are correct below the critical average degree, but this is not the case above the critical degree. These results strongly suggest that there is a close relation between the replica symmetry in statistical physics and the performance of the leaf removal algorithm even when the edge size \(\alpha\) is larger than two.

It is noted that this relation is not always true for all types of random graphs. For instance, the GLR algorithm removes no vertex on regular random graphs with \(c \geq 2\) because no leaf is found there while, from the point of the statistical-mechanical view, the min-VCs on regular random \(2\)-uniform graphs with degree 2 is described by the RS solution \([19]\). Thus, the relation depends on a type of random graphs and approximation algorithms. In addition to the leaf removal algorithm, a recent work for the min-VC problem with \(\alpha = 2\) \([16]\) suggests that linear programming algorithms, which are one of the most commonly used tools for solving optimization problems, have the relation discussed in the present work. Further study will need to establish the relation between the replica symmetry and the performance of numerous algorithms.

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