Statistics and algorithms on the organization and quantitative analysis of minimal vertex covers

Wei Wei*, Renquan Zhang, Baolong Niu, Binghui Guo, and Zhiming Zheng

LMIB and School of mathematics and systems sciences, Beihang University, 100191, Beijing, China
*weiw@buaa.edu.cn
(Dated: March 18, 2014)

Abstract

Counting the solution number of combinational optimization problems is an important topic in the study of computational complexity, especially research on the #P-complete complexity class can provide profound understanding of the hardness of the NP-complete complexity class. In this paper, we first investigate some topological structures of the unfrozen subgraph of Vertex-Cover unfrozen vertices based on its solution space expression, including the degree distribution and the relationship of their vertices with edges, which indicates that giant component of unfrozen vertices appears simultaneously with the leaf-removal core and reveals the organization of the further-step replica symmetry breaking phenomenon. Furthermore, a solution number counting algorithm of Vertex-Cover is proposed, which is exact when the graphs have no leaf-removal core and the unfrozen subgraphs are (almost) forests. To have a general view of the solution space of Vertex-Cover, the marginal probability distributions of the unfrozen vertices are investigated to recognize the efficiency of survey propagation algorithm. And, the algorithm is applied on the scale-free graphs to see different evolution characteristics of the solution space. Thus, detecting the graph expression of the solution space is an alternative and meaningful way to study the hardness of NP-complete and #P-complete problems, and appropriate algorithm design can help to achieve better approximations of solving combinational optimization problems and corresponding counting problems.
Vertex-Cover problem is one of the six basic NP-complete problems [1, 2] and has a large range of applications such as immunization strategies in networks [3], the prevention of denial-of-service attacks [4] and monitoring of internet traffic [5]. To solve Vertex-Cover instances efficiently and have better understanding of its typical solution space/ground states structures, is considered as a kernel way to probe the essence of computational complexity, which is highly concerned by many mathematicians, physicists and computer scientists.

An important result is obtained on the complexity phase transition for solving Vertex-Cover instances, that is, a random graph instance can be easily minimally covered by a leaf-removal algorithm [6] with high probability (w.h.p.) when its average degree $c < e$ and the algorithm fails when $c > e$ w.h.p. The complexity phase transition on Vertex-Cover is strongly correlated with the replica symmetry breaking phenomenon [7, 8], and when $c > e$ the ground states collapse into many different clusters. The evolution of the ground-state structures of Vertex-Cover is assumed to undergo replica symmetry and further-step replica symmetry breaking phases [9], which greatly differs from that of 3-SAT [10]. However, the organization of the ground states in further-step replica symmetry breaking phases is far from being clearly understood.

For the statistical characteristics of the solution space of Constraint Satisfaction Problems (CSPs), another basic and quite important one except the structure (but strongly correlated with the structure) is the solution number, which is also named entropy in statistical physics and investigated as #CSP [11]. #CSP problems, such as #SAT and #Graph Colorings [12, 13], belong to an important complexity class - the #P class, and solving the #Vertex-Cover is #P-complete [14] which is at least as hard as the NP-complete class. Evidently, counting all the answers of CSP problems is quite a difficult job, even for 2-SAT [14]. The methods of cavity and mean field can be used to calculate the entropy of the ground-state space [15], which has direct correspondence with the counting problems but is still an approximated one.

By the results in [16], we propose a description on the solution space structures, named reduced solution graph for Vertex-Cover. The reduced solution graph $S(G)$ based on the given graph $G$ can provide a detailed description on the status of each vertex in the solution space, that is, the covered backbones, the uncovered backbones and the unfrozen vertices with their connections. When the given graph has no leaf-removal core, the reduced solution graph can exactly express the solution space, and it can also be effective when there are no
FIG. 1. Left figure: the leaf-removal levels for the unfrozen subgraph. In each level, there are some mutual-determinations, and connections between different levels are retained by original edges. Vertices in higher levels will become new leaves when those in the lower levels are removed. Right figure: the local evolution of the solution number calculation.

odd-node-number cycles (cycles with $2k + 1$ unfrozen vertices and $k$ mutual-determinations, $k = 0, 1, 2, \cdots$) in the leaf-removal core. In fact, each mode of appropriately breaking the odd-node-number cycles could help to achieve an exact description of a cluster of solutions. Thus, the whole solution space possesses a direct correspondence to all the modes of breaking the odd-node-number cycles with minimum cost.

As the backbones on the graph make little contributions to the relationship among the vertices, what should be concerned is the unfrozen subgraph without frozen vertices on $S(G)$, i.e., the unfrozen vertices with their connections, on which the double edges are used to denote the mutual-determination relations and single edges are retained by the original ones among the mutual-determinations on graph $G$. Based on the leaf-removal process, we can define the leaf-removal levels for the unfrozen subgraph, shown in Fig.1. Evidently, the vertices in the top level can produce great influence on those in the lowest level.

To see topological structures of unfrozen subgraphs, we take advantage of mean field and cavity methods to understand the distribution and organization of mutual-determinations. For convenience, we use symbols $q_0, q_+, q_-$ to represent the ratios of unfrozen vertices, positive backbones and negative backbones on the reduced solution graph, and $q_0 + q_+ + q_- = 1$. Using the analysis in [16, 17], one unfrozen vertex connects other $k$ unfrozen ones only
when it has only one positive neighbor and \( k - 1 \) unfrozen neighbors with the rest negative backbones, so its probability for random graphs can be obtained by

\[
F_r(k) = \sum_{i=k}^{\infty} P_r(i) \cdot C_i^1 \cdot q_+ \cdot C_{i-1}^{k-1} \cdot q_0^{k-1} \cdot q_-^{i-k},
\]

where \( P_r(i) = \frac{e^{-ci}}{i!} \) is the degree distribution of random graphs. In the insets of Fig.2, theoretical results of \( F_r(k) \) with numerical ones are provided to show the validity of equation (1). By the average \( q_{\text{edg}} = \sum_{k=1}^{\infty} k \cdot F_r(k)/2 \), the ratio of free edges \( q_{\text{edg}} \) (edges connecting free vertices) can be obtained, and the comparison of free edges with unfrozen vertices \( q_0 \) is given in Fig.2, which shows that the number of free edges increases over \( q_0 \) at \( c = e \).

For the organization of unfrozen subgraph, the double edges connect vertices of mutual-determinations and original edges connect different mutual-determinations. Then, it is indicated that \( q_{\text{edg}} \) free edges involve \( q_0/2 \) double edges and \( q_{\text{edg}} - \frac{q_0}{2} \) original edges. Thus, for each unfrozen vertex, there are other \( 2 \cdot (q_{\text{edg}} - \frac{q_0}{2})/q_0 \) neighbors in average except the mutual-determination. For \( c < e \), the unfrozen subgraph must have almost tree structure to avoid giant component, otherwise long-rang correlations should exist \[17\]. At \( c \geq e \), we have \( q_{\text{edg}} \geq q_0 \), which implies the unfrozen subgraph can not keep the tree structures and a large quantity of cycles emerge. Thus, by the theory of random graphs, there must be some giant component on the unfrozen subgraph which has local tree-like structure. This phenomenon reveals that the emergence of the long-range correlations \[17, 18\] is due to formation of unfrozen giant component, and by the increase of \( q_{\text{edg}} - \frac{q_0}{2} \) inter edges among mutual-determinations, the unfrozen subgraph involves more and more cycles.

The giant component on the unfrozen subgraph emerges at \( c = e \), which accords with the easily-solving phase transition point \[8\]. By the viewpoint of leaf-removal, the leaf-removal core exists only after the emergence of the unfrozen giant component, and all the status of removed leaves can be easily determined. But for the vertices in the leaf-removal core, proper selection of some covered backbones can lead to a consistent structure without odd-node-number cycles, which can also be expressed as reduced solution graph. When \( c \geq e \), there are different selections of the covered backbones, and each effective selection corresponds to the expression of a solution sub-space. As unfrozen giant component exists in one such expression, long-range correlations also exist, which implies that the replica symmetry breaking performs and the solution sub-space has many different macroscopic states. Besides, the whole solution space still has great complexity in finding different selections, i.e.,
different solution sub-space. Therefore, combing the complicated organization of the selections and the replica symmetry breaking in each selection, we think it may be the essence of the further-step replica symmetry breaking phenomena \cite{9} in Vertex-Cover.

Next, we concern on the solution number counting of Vertex-Cover. For a random graph $G$ with $n$ vertices, its unfrozen subgraph is also of local tree-like structure and can only have cycles of at least $O(\log(n))$ scale. For $c < e$, there is no giant unfrozen component with high probability, so almost no cycles on the unfrozen subgraph can exist. When the unfrozen subgraph is a tree, the accurate solution number of Vertex-cover can be achieved using the cavity method. By adding vertices from the leaves to the root of the tree hierarchically, a sub-tree is obtained after adding a new vertex $i$ in each step. We can define $S(i)$ as the solution number of the current sub-tree, and $S^+(i), S^-(i)$ are the solution numbers of the current sub-tree when vertex $i$ takes $+1$ (uncovered) or $-1$ (covered). Then by the right figure of Fig.1, we have in case (a)

$$S^+(i) = \prod_{j=1}^{h} S^-(k_j), S^-(i) = \prod_{j=1}^{h} S(k_j), S(k_j) = S^+(k_j) + S^-(k_j), \quad (2)$$
and in case (b)

\[ S^+(i) = S^-(k) \cdot \prod_{j=1}^{h} S^-(k_j), \quad S^-(i) = S^+(k) \cdot \prod_{j=1}^{h} S(k_j), \quad S^+(k) = S^+(k_j) + S^-(k_j). \]  

(3)

Iterating the formula from the leaves to the root on the unfrozen subgraph, the total number of solutions can be obtained as \( S(\text{root}) \). When the unfrozen subgraph is a forest \( T \) of trees \( T_1, \cdots, T_s \), Equations (2-3) also work for each connected component, and the total number of solutions can be expressed as

\[ S(T) = \prod_{k=1}^{s} S(T_k), \]  

(4)

where \( S(T_k) \) is the solution number of \( T_k \) and \( S(T) \) is the total solution number of forest \( T \).

Here, the whole time consumption of the algorithm is \( O(n) \).

If the unfrozen subgraph has cycles, the above method will not be an accurate one, and a modified kind of exhaustive method should be used. For those with fewer cycles on the unfrozen subgraph which can become a forest or a tree after deleting \( k \) (no more than \( O(\log n) \)) vertices, simply having an exhaustion on the status of these vertices will produce \( 2^k \) subproblems with tree structure, and the whole time consumption is polynomial.

In the frame of our leaf-removal levels in Fig.1, having the exhaustion on the status of the mutual-determination vertices in the top level, a great number of unfrozen vertices (nearly a half in probability) should be fixed by the requirement of Vertex-Cover and mutual-determination relations for each exhaustive assignments of the top-level vertices. Supposing there are \( n_k \) mutual-determinations in the top level \( k \), the exhaustive number of this level is \( 2^{n_k} \), each of which will cause about a half unfrozen vertices to be frozen and the unfrozen subgraph greatly contracted. Thus, defining \( C(n) \) as the complexity of counting the solution number of an unfrozen subgraph with \( n \) vertices, we have \( C(n) = 2^{n_k}C(n/2) \) after exhausting the top level \( k \). Then, the original problem is reduced to sub-problems with size about \( n/2 \), and new top levels in each sub-problem can be located with a new round of exhaustion.

As a result, if the number of mutual-determinations in each exhaustive top level is of at most \( L = O(1) \), the total complexity \( C(n) \) will be polynomial \( (O(n^L)) \) in the worst case by recursive solving; if the number of mutual-determinations in each exhaustive top level is of at most \( O(\log(n)) \), the total complexity \( C(n) \) will be super-polynomial and sub-exponential \( (O([\log(n)]^{\log(n)})) \) in the worst case) by recursive solving, but if only \( O(1) \) exhaustive top levels have \( O(\log(n)) \) mutual-determinations and the others have \( O(1) \) mutual-determinations, the
total complexity is still polynomial; if there exists at least one exhaustive top level with $O(n)$ mutual-determinations, the complexity by this strategy will be exponential.

Furthermore, the above strategy can be revised to perform more efficiently. First, if the sub-problems after some exhaustion steps are with the form of a tree or a forest, the above algorithm on the tree should be performed; if the sub-problems are with the form of unconnected graphs, they can be handled with different unfrozen components separately and the complexity will greatly decrease. Then, as there are many even-node-number cycles (cycles with $2k$ unfrozen vertices and $k$ mutual-determinations, $k = 1, 2, \cdots$) on the unfrozen subgraph, all the vertices on each cycle can be viewed as an equivalent class, which means that the fixation of each vertex will cause fully fixation of all the other vertices on this cycle. Thus, treating vertices on one such even-node-number cycle as one unfrozen vertex can greatly reduce the size of the unfrozen subgraph. At last, the above exhaustive levels are actually the top levels in each (sub-)problem, however, for each specific instance, it is not necessary to only choose the top levels of each (sub-)problem as exhaustive levels, and the exhaustion on some next-top levels would produce the similar effects. Therefore, the strategy for counting the solutions can be modified by choosing exhaustive levels with relatively fewer mutual-determinations nearby the top levels.

For a random graph $G$, its unfrozen subgraph can be handled by the above strategies, and mean entropy density $s(c) = \ln S(G, c)/n$ is calculated for random graphs in Fig.3. In Fig.3, our algorithmic results (the red squares) fit very well with the simulations by [7] when $c \leq 3$, but have a big gap with the results of 1RSB cavity method and the simulations [7, 15] when $c > 3.5$. In fact, our algorithmic results are for the meta-stable states when $c > e$, the entropy of which should be much higher than that of ground states. In order to analyze the agreement of our algorithmic results with the simulations and 1RSB results, instances with higher entropies are neglected in our statistics (adjusted results by the red triangles in Fig.3): when $c = 4$, 50% instances with the lowest entropies are kept for the statistics of the mean entropy density; when $c = 5$, 10% instances are kept and when $6 \leq c \leq 10$ only 1% instances are kept. It suggests that even though the coverage by mutual-determinations has little error with the 1RSB and simulation results [16], the entropy still has great deviation with these results and only a small proportion of instances under our algorithm can have good performance especially when $c > 4$.

Furthermore, we will use the cavity method analysis to calculate the marginal probability
FIG. 3. The mean entropy density for random graphs with average degree $0 < c < 10$. The algorithmic and adjusted results are achieved by 10000 instances with $n = 1000$, which fit very well with those of simulations and the 1RSB cavity method when $c \leq 3$ [15]. When $c = 4, 5$ and $c \geq 6$, a data cut-off with 50%, 10%, 1% separately is performed to obtain the adjusted results. The replica symmetric results are also provided as a comparison [15].

distribution of Vertex-cover, which has a similar meaning of cavity field in statistical mechanics. When the unfrozen subgraph is almost of a forest or a tree, the marginal probability $P(x_r = +1) = P^+_r$ of vertex $r$ can be determined by the following steps:

Step 1: Choose vertex $r$ as a root of its connected component on the unfrozen subgraph, and initialize the marginal probability of the leaves by a probability $P^+(\text{leaf}_i) = 0$. If root $r$ is also a leaf, do not give it any initialized value.

Step 2: Iterate the following formulas similarly as those in equations (2-3) from the leaves to the root,

$$P^+(i) = \prod_{j=1}^{h}(1 - P^+(k_j)), \quad \text{or} \quad P^+(i) = (1 - P^+(k)) \cdot \prod_{j=1}^{h}(1 - P^+(k_j)).$$  \hspace{1cm} (5)

This equation also uses the notations in the right figure of Fig.1, which has a correspondence with cases (a-b) respectively.

Step 3: Note that all the $P^+(i)$s except $P^+(r)$ in this process are not the marginal probability $P_i^+$ of the whole graph but only some intermediate variables. Finally, the local environment of vertex $r$ can be fixed, and $P^+(r)$ is obtained which is just the marginal probability $P_r^+$.

After the above steps, we can obtain the marginal probability of different vertices by choosing different roots, and all the marginal probabilities can be obtained in about $O(n^2)$
FIG. 4. The Vertex-Cover marginal probability distribution for random graphs with \( c = 1, 2, 3 \) and scale-free graphs with \( \gamma = 2, 2.5, 3 \). In the insets, mean entropy densities (1RSB results for random graph and our algorithmic results for scale-free graph) are shown separately. The horizontal axis gives the probability of a randomly chosen vertex being uncovered \( P(x_i = +1) \), and the vertical axis gives the ratio of vertices having the same probability. The horizontal axis is uniformly divided into 10 intervals, with the left and right data for negative and positive backbones. The results are achieved by 10000 instances with \( n = 1000 \).

steps. However, this method can be (almost) accurate only on the (almost) tree structures, the validity conditions of which are the same as the cavity method.

By the above steps, marginal probabilities of random graph with different \( c \) are given in the left figure of Fig.4, and the vertices can be nearly classified into 3 classes: negative backbones \( P(x_i = +1) = 0 \), nearly positive backbones \( P(x_i \approx +1) = 1 \), and completely unfrozen vertices \( P(x_i = +1) = 0.5 \). Besides, other unfrozen vertices occupy a small proportion and the ratio of backbones increases with the average connectivity. Thus, in Vertex-cover, the statuses of the vertices possess strong polarization phenomenon, so survey propagation algorithm can have good performance in finding the minimal vertex covers [7, 8, 15].

At last, to see the effect of our algorithm on graphs with different structures, we perform it on Vertex-Cover of scale-free graphs [19]. For a randomly generated scale-free graphs with degree distribution \( P(k) \sim k^{-\gamma} \), the solution number counting and marginal probability calculating algorithms are done separately, and the mean entropy density and marginal probabilities are shown in the right figure of Fig.4 with \( 2 \leq \gamma \leq 3 \), in which there are similar phenomena with marginal probabilities of random graphs but the ratio of completely
unfrozen vertices monotonically increases.

Based on the mutual-determination and the backbone structures, our algorithm can accurately calculate the solution number of Vertex-Cover in polynomial time when the unfrozen subgraph is accurate and has fewer cycles. Though its performance is not as well as the 1RSB results when $c > e$ for random graphs, it can give solution number for instances, does not rely on the graph structures heavily and works better than the replica symmetric method. When the replica symmetric breaking phenomenon works, it is still hard work to distinguish whether the obtained results are for ground or meta-stable states, even to estimate the degree of approximation is quite difficult, which needs technical tackling and optimized strategies. Besides, further research on the breaking strategies of odd-node-number cycles will make better coverage approximations and more accurate solution counting results, which can lead to better understanding on the formation and statistics of the hardness of NP-complete and \textit{#P}-complete problems.

This work is supported by the Fundamental Research Funds for the Central Universities and the Natural Science Foundation of China (Grant No. 11201019).

[1] S.A. Cook, Proceedings Third Annual ACM Symposium on Thoery of Computing 151 (1971).
[2] M. Garey, D.S. Johnson, Computers and Intractability: A Guide to the Theory of NP-Completeness, W. H. Freeman, San Francisco (1979).
[3] J. Gomez-Gardenes, P. Echenique, and Y. Moreno, Eur. Phys. J. B 49 (2006) 259.
[4] K. Park and H. Lee, Proc. ACM SIGCOMM (2001).
[5] Y. Breitbart, C. Chan, M. Garofalakis, R. Rastogi, and A. Silverschatz, Proc. IEEE INFOCOM (2001), pp.15-26.
[6] M. Bauer and O. Golinelli, Eur. Phys. J. B 24, 339 (2001).
[7] M. Weigt, A.K. Hartmann, Phys. Rev. Lett. 84 (2000) 6118.
[8] M. Weigt, A.K. Hartmann, Phys. Rev. E 63 (2001) 056127.
[9] W. Barthel, A.K. Hartmann, Phys. Rev. E 70 (2004) 066120.
[10] S. Mertens, M. Mézard, R. Zecchina, Random. Struc. Algor. 28 (2005) 3.
[11] A. A. Bulatov, in Proc. ICALP (2008), pp.646-661.
[12] N. Creignou and M. Hermann, Inf. Comput. 125(1) (1996) 1-12.
[13] C. Greenhill, Comput. Complex. 9(1) (2000) 52-72.
[14] L.G. Valiant, Theor. Comp. Sci. 8(2) (1979) 189-201.
[15] J. Zhou and H. Zhou, Phys. Rev. E 79, 020103(R) (2009).
[16] W.Wei, R. Zhang, B. Guo, and Z. Zheng, Phys. Rev. E 86, 016112 (2012).
[17] H. Zhou, Phys. Rev. Lett. 94, 217203 (2005).
[18] F. Krzakala, A. Montanari, F. Ricci-Tersenghi, G. Semerjian, and L. Zdeborova, Proc. Natl. Acad. Sci. USA 104, 10318 (2007).
[19] A. Vazquez and M. Weigt, Phys. Rev. E 67 ,027101 (2003).