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LETTER TO THE EDITOR

Towards the solution of the graph bipartitioning problem

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Abstract. In this letter, we present the replica symmetric solution of the graph bipartitioning problem. We point out the possibility of many solutions, even with the replica symmetry assumption. We also comment on the possibility of constructing a model with an arbitrary finite number of transition temperatures.

Recently, there has been much interest in applying techniques of the statistical mechanics of random systems to hard optimisation problems. Generally, these problems can be mapped onto certain spin Hamiltonians. Then the quantity to be optimised, hereafter referred to as the cost function, is related to the ground-state energy of the corresponding spin Hamiltonian.

In a recent paper, Fu and Anderson [1] solved the graph bipartitioning problem with N-independent bond probability ($P = O(1)$) distribution. They showed that it is equivalent to the SK spin glass. By considering local field distribution, Kanter and Sompolinsky [2] found the replica symmetry solution of the graph bipartitioning problem with bond probability distribution scaled as α/N, where α is a finite number. Using the cavity field method, Mézard and Parisi [3] had obtained the same results. In this letter, we point out the possibility of the existence of many solutions, even with the replica symmetry assumption. We also work out the most naive replica symmetry breaking scheme. Unfortunately, we have not been able to find a replica symmetry breaking scheme that works.

The problem that we consider is the following. We are given a set of vertices $V = (V_1, V_2, \ldots, V_N)$, with N even, and a set of edges $E = \{(V_i, V_j)\}$. Let each edge be present with probability P. The bipartitioning problem is to divide V into two parts of equal size, in such a way as to minimise the number of edges N_c connecting these two parts. N_c is thus our cost function. We are then interested in the behaviour of N_c/N, in the limit $N \to \infty$, as a function of $\alpha = NP$.

As pointed out in [1], it is easily seen that

$$\langle N_c \rangle_{av} = \left\langle \sum_{i<j}^{N} \frac{J_{ij}}{J} \frac{(1 - S_i S_j)}{2} \right\rangle_{av} = \frac{\alpha(N-1)}{4} + \frac{1}{2J} \langle H \rangle_{av} \tag{1}$$

$$H = -\sum_{i<j}^{N} J_{ij} S_i S_j \tag{2}$$

with constraint

$$\sum_{i=1}^{N} S_i = 0 \tag{3}$$

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where $\langle\ldots\rangle_{av}$ means the average over the bond probability distribution. Hence, to minimise $\langle N_c\rangle_{av}$ is to find the ground-state energy of the Hamiltonian in equation (2), subject to the constraint of equation (3). Using the replica method:

$$\langle \ln Z\rangle_{av} = \lim_{m\to 0} \frac{\langle Z^m\rangle_{av} - 1}{m} \tag{4}$$

$$Z = \mathop{\mathrm{Tr}}_{\Sigma_{i=1}^N S_i = 0} \exp\left(\beta \sum_{i<j}^{N} J_{ij} S_i S_j\right). \tag{5}$$

Similar to the derivation presented in [1, 6], we have

$$\langle Z^m\rangle_{av} = \mathop{\mathrm{Tr}}_{\Sigma_{i=1}^N S_i^{\alpha m}=0} \cdots \mathop{\mathrm{Tr}}_{\Sigma_{i=1}^N S_i^{\alpha 1}=0}$$
$$\times \exp\left\{ \sum_{l=1}^{\infty} \left[\frac{1}{l!} \sum_{a=1}^{\infty} (-1)^{a+1} a^{l-1} \left(\frac{P}{1-P}\right)^a\right] \sum_{i<j}^{N} \left(\beta J \sum_{\alpha=1}^{m} S_i^\alpha S_j^\alpha\right)^l \right\}. \tag{6}$$

It is easy to see that J must be scaled as $J_0/\sqrt{NP}$, with J_0 some finite number, in order for the free energy to be extensive. This is true for any P as a function of N. Hence we see that as long as $\lim_{N\to\infty} NP = \alpha \to \infty$, we only have to keep the first term, namely $l = 2$. We then recover Fu and Anderson's result. If we are interested in the case $\lim_{N\to\infty} P \to 0$ and $\lim_{N\to\infty} \alpha < \infty$, we see that

$$\frac{1}{l!} \sum_{a=1}^{\infty} (-1)^{a+1} a^{l-l} \left(\frac{P}{1-P}\right)^a \simeq \frac{P}{l!}. \tag{7}$$

In that case, we have

$$\langle Z^m\rangle_{av} = \mathop{\mathrm{Tr}}_{\Sigma_{i=1}^N S_i^{\alpha m}=0} \cdots \mathop{\mathrm{Tr}}_{\Sigma_{i=1}^N S_i^{\alpha 1}=0} \exp\left\{P \sum_{i<j}^{N} \left[\exp\left(\beta J \sum_{\alpha=1}^{m} S_i^\alpha S_j^\alpha\right) - 1\right]\right\} \tag{8}$$

$$\exp\left(\beta J \sum_{\alpha=1}^{m} S_i^\alpha S_j^\alpha\right) - 1 = A_0 + \sum_{l=1}^{\infty} A_l \sum_{\alpha_1<\ldots<\alpha_l}^{m} (S_i^{\alpha_1}\ldots S_i^{\alpha_l})(S_j^{\alpha_1}\ldots S_j^{\alpha_l}) \tag{9}$$

$$A_0 = \cosh^m(\beta J) - 1 \tag{10}$$

$$A_l = \tanh^l(\beta J)\cosh^m(\beta J). \tag{11}$$

We now replace the constraint in equation (3) by the penalty term

$$\exp\left[-\lambda\left(\sum_{i=1}^{N} S_i^\alpha\right)^2\right] \tag{12}$$

with $\lambda \to \infty$. Then after Gaussian transformation (or Hubbard–Stratonovich transformation), the constraints means $\langle S^\alpha\rangle = 0$. Under the replica symmetry assumption, the saddle-point approximation gives

$$\langle \ln Z\rangle_{av} = \tfrac{1}{2}\alpha N \ln\cosh(\beta J) + \max \lim_{m\to 0} \frac{N}{m}\left[-\frac{1}{2}\sum_{l=2}^{\infty} \binom{m}{l} \alpha A_l Q_l^2\right.$$
$$\left. + \ln \mathop{\mathrm{Tr}}_{\{S^m\}} \exp\left(\sum_{l=2}^{\infty} \alpha A_l Q_l \sum_{\alpha_1<\ldots<\alpha_l}^{m} S^{\alpha_1}\cdots S^{\alpha_l}\right)\right]. \tag{13}$$

The saddle-point condition is

$$Q_l = \lim_{m\to 0}\left\{\frac{\mathrm{Tr}_{\{S^m\}} S^{\beta_1}\ldots S^{\beta_l} \exp(\Sigma_{l=2}^{\infty} \alpha A_l Q_l \Sigma_{\alpha_1<\ldots<\alpha_l}^{m} S^{\alpha_1}\ldots S^{\alpha_l})}{\mathrm{Tr}_{\{S^m\}} \exp(\Sigma_{l=2}^{\infty} \alpha A_l Q_l \Sigma_{\alpha_1<\ldots<\alpha_l}^{m} S^{\alpha_1}\ldots S^{\alpha_l})}\right\}. \tag{14}$$

Let us assume that

$$\exp\left(\sum_{l=2}^{\infty} \alpha A_l Q_l \sum_{\alpha_1<\ldots<\alpha_l}^{m} S^{\alpha_1}\ldots S^{\alpha_l}\right)$$
$$= \sum_{k=-\infty}^{\infty} h_k(\alpha, \beta J, \boldsymbol{Q}) \exp\left(g_k(\alpha, \beta J, \boldsymbol{Q})\beta J \sum_{\alpha=1}^{m} S^{\alpha}\right) \tag{15}$$

where g_k, h_k are some functions depending on the form of A_l and the value of α, βJ, $\boldsymbol{Q}=(Q_2, Q_3\ldots)$. Then

$$Q_l = \frac{\sum_{k=-\infty}^{\infty} h_k(\alpha, \beta J, \boldsymbol{Q}) \tanh^l[g_k(\alpha, \beta J, \boldsymbol{Q})\beta J]}{\sum_{k=-\infty}^{\infty} h_k(\alpha, \beta J, \boldsymbol{Q})}. \tag{16}$$

So we see that in the replica symmetry assumption, as long as $\lim_{\beta\to\infty,}\, g_k\beta J \to \infty$, we have

$$\lim_{\beta\to\infty} Q_{2l} = Q \qquad \lim_{\beta\to\infty} Q_{2l-1} = R \tag{17}$$

for all $l = 1, 2, 3, \ldots$. But our constraint says $Q_1 = \langle S^{\alpha}\rangle = 0$. Therefore all odd-spin order parameters are zero at $T=0$. Using

$$\cosh\left(\beta J \sum_{\alpha=1}^{m} S^{\alpha}\right) = \cosh^m(\beta J) + \sum_{l=1}^{\infty} A_{2l} \sum_{\alpha_1<\ldots<\alpha_{2l}}^{m} S^{\alpha_1}\ldots S^{\alpha_{2l}} \tag{18}$$

we get

$$Q = 1 - \exp(-\alpha Q) I_0(\alpha Q) \tag{19}$$

$$\lim_{N\to\infty} N_c/N = \tfrac{1}{4}\alpha(2Q - Q^2) - \tfrac{1}{2}\alpha Q \exp(-\alpha Q)[I_0(\alpha Q) + I_1(\alpha Q)]. \tag{20}$$

Results of equation (19) and (20) were derived in [2, 3] using a different method. However, we notice that equation (17) only says that, as $T\to 0$, all even-spin order parameters reach the same value. If we assume

$$\lim_{\beta\to\infty} Q_{2l} = Q + Q'\left(1 - \frac{\tanh^{2l}(\beta J a)}{\tanh^{2l}(\beta J)}\right) \tag{21}$$

where $0 \leqslant a \leqslant 1$, then we arrive at a different saddle-point equation and cost function. The $\beta\to\infty$ limit in equation (21) has to be carefully interpreted. As it stands, it means that we have to know how the even-spin order parameters reach the common value as $\beta\to\infty$. Mézard and Parisi [3] have reached the same conclusion, that it might be necessary to know how the saddle point evolves as $T\to 0$.

The motivation for introducing equation (21) is more clearly illustrated by considering local field distribution, in the replica symmetry assumption, as defined by

$$Q_k \equiv \langle S^{\alpha_1}\ldots S^{\alpha_k}\rangle = \int_{-\infty}^{\infty} P(h) \tanh^k(\beta h)\, \mathrm{d}h. \tag{22}$$

The assertion in equation (17) means that at $T=0$, as derived in [2],

$$P(h) = P_0\delta(h) + \sum_{l=1}^{\infty} P_l^+ \delta(h - lJ) + \sum_{l=1}^{\infty} P_l^- \delta(h + lJ) \tag{23}$$

$$Q = \sum_{l=1}^{\infty} P_l^+ + \sum_{l=1}^{\infty} P_l^- \tag{24}$$

$$R = \sum_{l=1}^{\infty} P_l^+ - \sum_{l=1}^{\infty} P_l^-. \tag{25}$$

However, it is not certain that $P(h)$ has a continuous part at $T=0$. This point has also been raised in [3]. The ansatz in equation (21) amounts to introducing $\delta(h\pm aJ)$, with $0\leqslant a\leqslant 1$, in the local field distribution function $P(h)$. Indeed, in the letter by Mottishaw and De Dominicis [4], they have concluded that an extra term is needed in the local field distribution to restore the stability, even in the replica symmetric subspace. We believe that the extra term they introduced is closely related to our ansatz in equation (21).

According to an exact result by Erdos and Renyi [5], and pointed out by Fu and Anderson [1], $\lim_{n\to\infty} N_c/N=0$ for $\alpha\leqslant 2\ln 2$ and $\lim_{N\to\infty} N_c/N>0$ for $\alpha>2\ln 2$. Equation (20) gives $\lim_{N\to\infty} N_c/N>0$ for $\alpha>1$ and $\lim_{N\to\infty} N_c/N=0$ for $\alpha\leqslant 1$. We have tried a variation of the type shown in equation (21). We found that

$$\lim_{N\to\infty} N_c/N=\tfrac{1}{4}\alpha[2(Q+Q')+2(Q+Q')Q'a+a-a(Q'+1)^2-(Q+Q')^2]$$
$$-\frac{e^{-\alpha Q}}{2}\sum_{k=0}^{\infty}\sum_{u=0}^{k}\frac{[\frac{1}{2}\alpha(Q+Q')]^k}{(k-u)!u!}\sum_{l=0}^{\infty}\sum_{v=0}^{l}\frac{(-1)^l(\frac{1}{2}\alpha Q')^l}{(l-v)!v!}|(k-2u)+(l-2v)a|. \tag{26}$$

We then have to find the saddle point for this expression. We notice that the cost per site is not analytic as a function of a. We do not fully understand its significance at this moment. We found that for all $\alpha\geqslant 1$, $a=\frac{1}{2}$ gives the lowest cost function (considerably less than that in equation (20)). The percolation threshold is still at $\alpha=1$. However, we still have a cost function greater than 0 for $\alpha\geqslant 1$, with nothing special happening at $\alpha=2\ln 2$.

Another possibility is replica symmetry breaking. Viana and Bray [6] had shown that replica symmetry must be broken near T_c, by including the first few order parameters. However, it is not clear whether replica symmetry is still broken at $T=0$. It might be possible that, due to the emergence of infinitely many order parameters, replica symmetry is restored. In any case, we have considered the following replica symmetry breaking scheme. Following the logic leading to equation (16), we see that for any scheme of breaking m replicas into groups, what matters is whether the number of replica indices in each group is even or odd. (This is true only at $T=0$.) As a naive attempt, let us break m replicas into two equal groups, G_1 and G_2. For $l=1,2,3,\ldots$ (we have set $Q_1\equiv\langle S^\alpha\rangle=0$), let

$$\lim_{\beta\to\infty} Q_{\alpha_1,\ldots,\alpha_{2l+1}}=\begin{cases} R-R\dfrac{\tanh^{2l+1}(\beta Jb)}{\tanh^{2l+1}(\beta J)} & \text{iff all } \alpha_1,\ldots,\alpha_{2l+1}\in G_1 \text{ (or } G_2) \\ R & \text{otherwise} \end{cases} \tag{27}$$

and

$$\lim_{\beta\to\infty} Q_{\alpha_1,\ldots,\alpha_{2l}}=\begin{cases} Q+Q'\dfrac{\tanh^{2l}(\beta Ja)}{\tanh^{2l}(\beta J)} & \text{iff odd number of } \alpha_1,\ldots,\alpha_{2l}\in G_1 \text{ and odd number of } \alpha_1,\ldots,\alpha_{2l}\in G_2 \\ Q & \text{otherwise.} \end{cases} \tag{28}$$

Equation (27) guarantees that the constraint $Q_{2l+1}=0$ at $T=0$ is satisfied. ($Q_1=0$ for all T, but Q_{2l+1}, for $l=1,2,\ldots$, need not be 0 for $T\neq 0$.) We have computed the ground-state energy under the assumption of equations (27) and (28). Interestingly, the ground-state energy does not depend on Q' or a. However, we recover the same saddle point as given in equations (19) and (20). Other replica symmetry breaking schemes are under consideration.

Finally, we would like to comment on the possibility of constructing a model with an arbitrary finite number of transition temperatures. In the course of studying this problem, we have noticed that, if we just keep the first few finite number of terms in equation (6), we might have a model with a finite number of transition temperatures. We also demonstrated that, if there is a bond probability distribution producing a finite number of terms in the replicated Hamiltonian, then there is no percolation in the problem, in the sense that all order parameters, with the replica symmetry assumption, approach 1 as $T\to 0$, regardless of the variation of any other parameters in the Hamiltonian. Let us consider the following specific example. Can we find a bond probability distribution $P(J)$ such that, for instance,

$$\int_{-\infty}^{\infty} P(J)\exp\left(\beta J\sum_{\alpha=1}^{m} S^{\alpha}\right)\mathrm{d}J=\exp\left[a\left(\beta\sum_{\alpha=1}^{m} S^{\alpha}\right)^{2}+b\left(\beta\sum_{\alpha=1}^{m} S^{\alpha}\right)^{4}+c\left(\beta\sum_{\alpha=1}^{m} S^{\alpha}\right)^{6}\right] \tag{29}$$

for some coefficients a, b, c, with $c>0$? It is easy to see that

$$\exp(aS^2+bS^4+cS^6)=\int_{-\infty}^{\infty}\exp(Sx)\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(-\mathrm{i}tx-at^2+bt^4-ct^6)\,\mathrm{d}t\right)\mathrm{d}x. \tag{30}$$

Then by Bochner's theorem,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(-\mathrm{i}tx-at^2+bt^4-ct^6)\,\mathrm{d}t \tag{31}$$

will be a probability distribution iff $\exp(-at^2+bt^4-ct^6)$ is positive definite [7]. When $c<0$, no bond probability distribution will produce such a replicated Hamiltonian. This is true for all cases with leading power in S even and the corresponding coefficient negative. If the leading power in S is odd, we again have to prove positive definiteness of a certain function. However, in general it is very hard to prove that a function is positive definite. The Gaussian case is an exception. This fact is the reason why it is relatively easy for the SK model to be constructed. Indeed, De Dominicis and Mottishaw [8] had considered a toy model with the replicated Hamiltonian

$$\exp\left[\tfrac{1}{2}\lambda^2\left(\beta\sum_{\alpha=1}^{m} S_i^{\alpha}S_j^{\alpha}\right)^{2}+\tfrac{1}{2}\lambda^4\left(\beta\sum_{\alpha=1}^{m} S_i^{\alpha}S_j^{\alpha}\right)^{4}\right]. \tag{32}$$

However, there is no bond probability distribution that would correspond to their interesting conclusion, which happens only when ρ is negative enough [8].

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