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1988 J. Phys. A: Math. Gen. 21 L1043

(http://iopscience.iop.org/0305-4470/21/22/001)

J. Phys. A: Math. Gen. 21 (1988) L1043–L1049. Printed in the UK

LETTER TO THE EDITOR

q-partitioning of graphs with finite coordination number

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Received 6 July 1988

Abstract. The NP-complete optimisation problem of q-partitioning of graphs with finite connectivity is discussed. Using the effective local field method, we obtain the local field distributions with and without the continuous part and use them to calculate the ground-state energies of the three-state Potts spin glass on lattices with finite coordination number equal to three. This in turn gives analytic results for the optimal cost of the 3-partitioning of graphs. We perform simulations of actual 3-partitions of random graphs to compare with our theoretical results and obtain very good agreement. Ways for further improvement of the estimates are discussed.

Recently, there has been much interest in applying statistical mechanical concepts and techniques to NP-complete optimisation problems. In particular, attention has been focused on the graph bi-partitioning optimisation problem [1–3] which is related to the Ising spin glass. The optimisation problem consists of dividing a given graph into subgraphs such that the intersubgraph connections are minimised. Special attention has been focused on partitioning of graphs with a finite number of neighbours [2, 4] because of its practical importance and its relation to the short-ranged spin glasses. In this letter, we investigate the problem of q-partitioning of graphs with finite coordination number, and in particular the problem of 3-partitioning. For graphs with extensive connectivity, this problem has been shown [5] to be equivalent to the q-state Potts spin glass at zero temperature. Here we evaluate the ground-state energy of the three-state Potts spin glass on a lattice with coordination number equal to three within the replica symmetric theory using the effective local field treatment [4, 6]. This gives an analytic prediction for the minimal cost of the corresponding graph 3-partitioning problem. We also simulate random graphs and find the near-optimal cost to compare well with our analytic result.

First, we consider the q-state Potts spin-glass Hamiltonian

$$H = -\sum_{\langle ij\rangle} J_{ij}(q\delta_{\sigma_i\sigma_j} - 1) \tag{1}$$

where σ_i is the Potts spin at the ith site which can take q values. The model is defined on a random graph, i.e. the spins are located at the vertices of the graphs and J_{ij} are the bond strengths. The sum is over distinct pairs of sites i and j that are connected by a bond. The random couplings J_{ij} follow a certain probability distribution $P(J_{ij})$.

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0305-4470/88/221043+07$02.50

For the case of graphs with a finite and fixed number of neighbours c, the probability distribution of the effective local fields is given by the recursion relation [7]

$$p(\eta^{(1)},\ldots,\eta^{q})=\int \mathrm{d}J\,P(J)\prod_{\gamma=1}^{q}\mathrm{d}h^{(\gamma)}\,p^{(c-1)}(h^{(1)},\ldots,h^{(q)})\prod_{\alpha=1}^{q}\delta(\eta^{(\alpha)}-X^{(\alpha)}) \tag{2a}$$

where

$$X^{(\alpha)}=\frac{1}{\beta q}\ln\frac{\exp[\beta q(J+h^{(\alpha)})]+\Sigma'_{\mu}\exp(\beta q h^{(\mu)})}{\Pi_{\nu}\{\exp[\beta q(J+h^{(\nu)})]+\Sigma'_{\mu}\exp(\beta q h^{(\mu)})\}^{1/q}} \tag{2b}$$

and

$$p^{(m)}(h^{(1)},\ldots,h^{(q)})$$
$$=\int\prod_{j=1}^{m}(\mathrm{d}\eta_j^{(1)}\ldots\mathrm{d}\eta_j^{(q)}p(\eta_j^{(1)},\ldots,\eta_j^{(q)}))\prod_{\alpha=1}^{q}\delta\left(h^{(\alpha)}-\sum_{j=1}^{m}\eta_j^{(\alpha)}\right). \tag{2c}$$

β is the inverse temperature and Σ' denotes the sum over μ excluding α. Notice that replica symmetry is not broken in this kind of effective local field treatment [4]. The free energy per site is given by [7]

$$\begin{aligned}\frac{F}{N}=\frac{c-1}{\beta}&\int\prod_{\alpha=1}^{q}\mathrm{d}h^{(\alpha)}\,p^{(c)}(h^{(1)},\ldots,h^{(q)})\ln\left(\sum_{\alpha=1}^{q}\exp(\beta q h^{(\alpha)})\right)\\&-\frac{c}{2\beta}\int\prod_{\alpha=1}^{q}(\mathrm{d}h_1^{(\alpha)}\,\mathrm{d}h_2^{(\alpha)})\,\mathrm{d}J\,P(J)\\&\times p^{(c-1)}(h_1^{(1)},\ldots,h_1^{(q)})p^{(c-1)}(h_2^{(1)},\ldots,h_2^{(q)})\\&\times\ln\left(\exp[(q-1)\beta J]\sum_{\alpha=1}^{q}\exp[\beta q(h_1^{(\alpha)}+h_2^{(\alpha)})]\right.\\&\left.+\exp(-\beta J)\sum_{\gamma\neq\delta}\exp[\beta q(h_1^{(\gamma)}+h_2^{(\delta)})]\right).\end{aligned} \tag{3}$$

For evaluating the ground-state energy, we need to find the zero-temperature solution of equations (2). Taking $P(J)$ to be ±1, i.e.

$$P(J)=\tfrac{1}{2}\{\delta(J-1)+\delta(J+1)\} \tag{4}$$

a solution to equation (2) in the $\beta\to\infty$ limit has been given in [7] for general q. Notice that the same equations hold for a Potts spin glass on a Bethe lattice with c nearest neighbours. We now give the results for the three-state Potts model with a fixed number of neighbours. As shown in [7], the local effective field distribution is given by (adding the permutations assures that $p(\eta^{(1)},\ldots,\eta^{(q)})$ is invariant under permutations of its arguments)

$$\begin{aligned}p(\eta^{(1)},\eta^{(2)},\eta^{(3)})&=c_0\delta(\eta^{(1)})\delta(\eta^{(2)})\delta(\eta^{(3)})\\&+c_1[\delta(\eta^{(1)}-\tfrac{1}{3})\delta(\eta^{(2)}-\tfrac{1}{3})\delta(\eta^{(3)}+\tfrac{2}{3})+2\text{ permutations}]\\&+c_2[\delta(\eta^{(1)}-\tfrac{2}{3})\delta(\eta^{(2)}+\tfrac{1}{3})\delta(\eta^{(3)}+\tfrac{1}{3})+2\text{ permutations}]\end{aligned} \tag{5}$$

where the coefficients also satisfy the normalisation condition

$$c_0+3c_1+3c_2=1. \tag{6}$$

By substituting (5) into (2), algebraic equations for the coefficients have been obtained [7] for the case of coordination number $c=3$. These equations possess only one solution with all c_n positive, their values are

$$
\begin{aligned}
c_0 &= 157/307 - 6\sqrt{11}/307 \simeq 0.4466 \\
c_1 &= 178/307 - 42\sqrt{11}/307 \simeq 0.1261 \\
c_2 &= -128/307 + 44\sqrt{11}/307 \simeq 0.0584.
\end{aligned}
\tag{7}
$$

Substituting (5) into (3), we worked out, after some tedious algebra, the ground-state energy for the three-state Potts spin glass on a graph with fixed coordination number equal to three:

$$
\begin{aligned}
F(T=0)/N = {} & 2[9c_0^2(c_1+2c_2)+54c_0(c_1^2+c_2^2) \\
& +108c_0c_1c_2+189c_1^2c_2+216c_1c_2^2+63c_1^3+72c_2^3] \\
& -\tfrac{3}{4}(3c_0^4+378c_0^2c_1^2+414c_0^2c_2^2+60c_0^3c_1+84c_0^3c_2+828c_0^2c_1c_2+900c_0c_1^3 \\
& +1008c_0c_2^3+2736c_0c_1^2c_2+2880c_0c_1c_2^2+747c_1^4+828c_2^4+3060c_1^3c_2 \\
& +4716c_1^2c_2^2+3204c_1c_2^3).
\end{aligned}
\tag{8}
$$

Using the normalisation constraint (6) to eliminate c_2, we have verified that the solution (7) satisfies the saddle-point equations

$$
\frac{\partial F}{\partial c_0} = \frac{\partial F}{\partial c_1} = 0. \tag{9}
$$

With the values of the c given by (7), we have

$$
F(T=0)/N \simeq -2.2193. \tag{10}
$$

This is the ground-state energy of the three-state Potts spin glass on a lattice with three nearest neighbours described by (1) and (4) without replica symmetry breaking, and without including a continuous part in the solution (5).

We now consider the inclusion of a continuous part in the solution (6). In the case of the Ising spin glass ($q=2$), a continuous part does exist and the δ-function solution has been shown [8, 9] to be unstable to the inclusion of a small continuous part. The continuous part has been obtained numerically [9, 10] and analytically [11]. It was shown [9, 10] to affect very little the value of the ground-state energy as compared with the solution with no continuous part (less than 0.5%). From general considerations we expect a continuous part to exist also in the Potts spin-glass case. This is because the appearance of such a continuous piece reflects the sensitivity of the system to a small change in the boundary conditions in the glass phase which is not likely to occur if the effective fields are locked only onto a few rational values. To determine the entire local field in the present case, we simulate the recursion relation (2) numerically using a method similar to [9]. We start with some arbitrary initial field distribution on a two-dimensional square corresponding to $-\frac{2}{3} \leq h^{(1)}, h^{(2)} \leq \frac{2}{3}$ and then iterate (2) to obtain a new field distribution. This is done by combining two values of the field via (2) to produce two new values (corresponding to $J=\pm 1$) and then replacing two old values chosen at random with the new values. After some passes for the distribution to become stationary, statistics is taken by accumulating the effective field values on a 20×20 grid to produce the distribution $p(h^{(1)}, h^{(2)})$ ($h^{(3)}$ is fixed by the condition $h^{(1)}+h^{(2)}+h^{(3)}=0$). The form of $p(h^{(1)}, h^{(2)})$ is depicted in figure 1. The seven δ

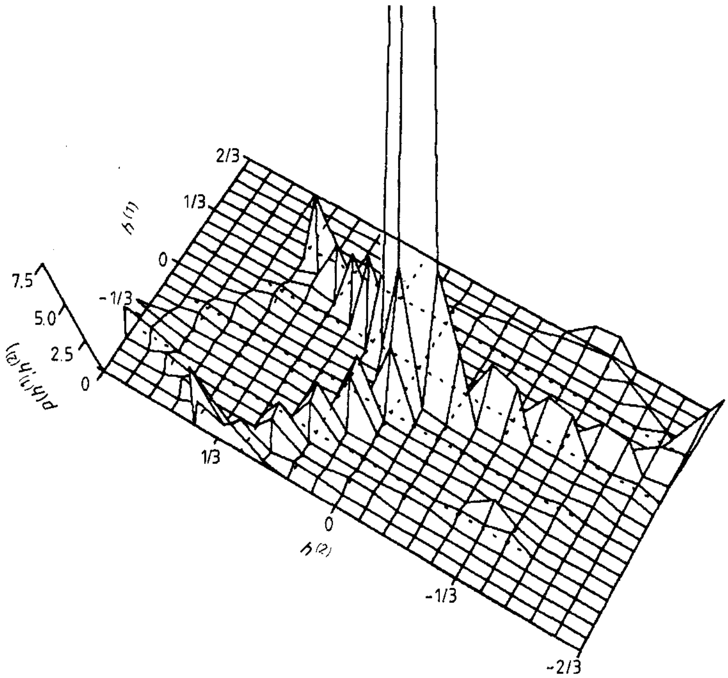

Figure 1. Effective field distribution $p(h^{(1)}, h^{(2)})$ for $q=3$ and $c=3$. The δ functions peak at positions given by equation (6).

functions corresponding to (5) are prominent. In addition, there is quite a rich structure due to the continuous part. It is clear from the figure that there are ridges joining the δ functions. Thus, we explicitly demonstrate the existence of a continuous part in the effective field solution. Using this effective field solution, we calculate the zero-temperature free energy through (3) using Monte Carlo integration by drawing effective fields from the distribution $p(h^{(1)}, h^{(2)})$ which has been determined previously. We obtained

$$F(T=0)/N=-2.0986. \tag{11}$$

Next we consider the optimisation problem of q-partitioning of a graph. It is an NP-complete optimisation problem which can be described by the Potts spin glass [5]. This problem is specified by a graph G with N vertices where N is an integral multiple of q. One is then asked to divide the N vertices into q groups of equal size such that the total number of intergroup edges is minimised. This problem can be described by the Hamiltonian in (1). In this case, $J_{ij}=1$ if the corresponding edge of G exists and is zero otherwise. In the case of graphs with fixed coordination number c, the J_{ij} also satisfy

$$\sum_{j=1}^{N} J_{ij}=c. \tag{12}$$

Thus the problem is essentially a dilute ferromagnetic Potts system but subjected to the antiferromagnetic constraint

$$\sum_{ij}^{N}\left(\delta_{\sigma_i\sigma_j}-\frac{1}{q}\right)=0. \tag{13}$$

When G is partitioned into q equal subgraphs, all the spins that take the same value belong to the same subgraph. Constraint (13) simply follows from the requirement that the q subgraphs are equal in size and mutually disjoint. The cost to be minimised is the intersubgraph connections. It can be shown following the steps in [5] that the minimal cost is related to H via

$$C_{\min}=\frac{q-1}{2q}Nc+\frac{F(T=0)}{qJ}. \tag{14}$$

The first term in (14) corresponds to the expected number of intersubgraph edges without minimisation and the second term (which is negative) is the improvement due to optimisation. It is worth noting that in this case the free energy F is extensive and the improvement is of the same order in N as the first term, whereas in the case of extensive connectivity [5], the improvement is of $O(\sqrt{N})$ less than the unoptimised term. Hence, the effect of minimisation is much more important in the present finite-connectivity case, especially in the large-N limit.

In the case of extensive connectivity, the q-partitioning problem is shown to be equivalent to the infinite-ranged Potts spin glass in the zero-temperature limit [1, 5]. However, in the case of finite connectivity, there were suggestions that the spin glass solution is not the correct solution [3, 12]. We will come back to this issue later. If we take the spin-glass solution and hence the value of the ground-state energy given by (10) and (11), we have for $q=3$ and fixed coordination number $c=3$, the optimised cost

$$\begin{aligned} &C_{\min}=0.260N && \text{no continuous part}\\ &C_{\min}=0.300N && \text{with continuous part.}\end{aligned} \tag{15}$$

To check the above analytic result, we performed simulations for 3-partitioning of graphs with coordination number fixed to be three. We use an iterative improvement algorithm to find the near-optimal cost. In order to get the best minimal cost, we started, for each graph, with several initial partitionings and picked the best result. The procedure is repeated for several realisations of graphs generated randomly and the quenched average is then taken. Table 1 shows the results of the simulations. The agreement with the analytic result with the inclusion of the continuous part is very good and is better for larger N. This is expected since (15) holds in the large-N limit. As $N\to\infty$, the simulation value seems to approach very closely our analytic value.

We now discuss the possible sources that can give rise to corrections to our analytic result for the graph partitioning problem. These are:

(i) the effect of replica symmetry breaking (RSB);

Table 1. Simulation results for 3-partitioning of graphs with number of neighbours of each vertex equal to 3. N is the number of vertices of the graph. C_{simul} is the simulation result obtained by averaging ten random graphs. C^{δ} is the cost obtained analytically using solution (6). C^{cont} is the cost with the inclusion of the continuous part in the effective field distribution.

N	C_{simul}	C_{simul}/N	$C_{\text{simul}}/C^{\delta}$	$C_{\text{simul}}/C^{\text{cont}}$
48	15.4	0.321	1.23	1.068
102	31.7	0.311	1.20	1.035
198	61.3	0.310	1.19	1.032

(ii) the possibility that permutation symmetry in the effective fields is broken for the graph partitioning problem unlike the spin-glass case.

In view of the good agreement between the result obtained using the spin-glass solution (6) and the numerical simulation of 3-partitioning, we expect the effect of the possible corrections to be very small (a few per cent). We now review them in turn. Inclusion of these corrections is the subject of future work.

(i) It was shown [13] that RSB does occur for a Potts spin glass on the Bethe lattice at temperatures just below the spin-glass transition. It is plausible that replica symmetry is still broken at $T=0$ and hence the value of the ground-state energy is altered as in the long-range Potts spin glass. A first step towards constructing a solution with RSB for the Ising spin glass at $T=0$ has been proposed recently [14]. It was found that in that scheme the improvement in the ground-state energy is less than 1%. In the long-ranged Potts spin glasses, the ground-state energy difference between the replica symmetric solution and the RSB solution is about 5% [5].

(ii) Lastly, in the case of bi-partitioning of a graph with finite coordination number, Liao [3, 12] found a solution that has a lower cost than the Ising spin-glass solution and it was suggested that the spin-glass solution may not be the correct solution for the graph partitioning problem for graphs with finite connectivity. However, a stability analysis has not been carried out for this solution; the mere fact that it leads to a lower cost function is not sufficient to demonstrate its validity. A trivial example is that the paramagnetic spin-glass solution gives an even lower cost for the graph partitioning. In terms of the effective field distribution, the spin-glass solution is equivalent to the solution of q-partitioning of a graph if the effective local field distribution $p(h^{(1)}, \ldots, h^{(q)})$ of the graph partitioning problem is permutationally symmetric in its arguments. In the case of graphs with an average (but not fixed) finite coordination number c, we find that, when

$$c \leqslant q \ln \frac{q}{q-1} \tag{16}$$

$p(h^{(1)}, \ldots, h^{(q)})$ loses its permutational symmetry. This is a generalisation of the bi-partitioning case [3, 4]. The physical picture is that in this case the infinite cluster can be fitted into one of the subgraphs and hence the system is not frustrated and the cost is zero. However, in the present case of fixed coordination number $c \geqslant 3$, the probability that the random graph is connected approaches one as $N \to \infty$ [15] and the above argument does not apply. Liao [12] claims that, in the Ising case, the symmetry is broken even in the fixed-connectivity case. But his solution does not include RSB and it is not yet known if the situation will remain the same when RSB is included.

This work has been supported in part by the National Science Foundation under grant number DMR-8709704.

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