Graph optimisation problems and the Potts glass

1987 J. Phys. A: Math. Gen. 20 L673

(http://iopscience.iop.org/0305-4470/20/11/001)

J. Phys. A: Math. Gen. **20** (1987) L673-L679. Printed in the UK

LETTER TO THE EDITOR

Graph optimisation problems and the Potts glass

I Kanter† and H Sompolinsky‡

† Department of Physics, Bar-Ilan University, Ramat-Gan, Israel 52100
‡ Racah Institute of Physics, Hebrew University, Jerusalem, Israel

Received 21 April 1987

Abstract. The *NP*-complete problems of partitioning and colouring of random graphs, with p partitions and colours respectively, are mapped onto the statistical mechanical problem of p-state Potts glasses. An estimate of the cost functions of these optimisation problems has been derived using the Potts glass mean-field theory. This estimate applies to *dense* graphs in the thermodynamic limit. An exact expression for the cost function in the large-p limit is given.

Methods and results of spin-glass theory have recently been applied to the study of complex optimisation problems. A particularly simple application [1] has been the graph bisection problem [2]. It has been shown that this problem, which is *NP* complete, is equivalent to an infinite-range spin glass. A graph consists of a set of vertices $V=\{V_1, V_2, \ldots, V_N\}$ and a set of edges $E=\{(V_i, V_j)\}$. In one version of the problem the graph is assumed to be random: each edge in E has a probability c of being connected, and $1-c$ of being disconnected. The problem consists of dividing V into two subsets of vertices V_1 and V_2 of equal size so that the number of edges connecting V_1 and V_2 is minimised. In the case of dense graphs, i.e. c and $1-c$ are of O(1), the cost function of the problem is directly related [1] to the ground-state energy of the Sherrington-Kirkpatrick (SK) Ising spin-glass model [3].

In this letter we extend the result of Fu and Anderson [1] to a more general class of graph optimisation problems which have numerous applications in engineering: graph partitioning and graph colouring [2]. These *NP*-complete problems are mapped onto infinite-range Potts glass (PG) models [4-6]. The results of mean-field theory (MFT) [5, 6] as well as numerical simulations of the Potts glass (PG) are applied to study the cost function of these graph optimisation problems.

We consider here the following problems.

(i) *Graph partitioning.* A random graph is partitioned into p subsets of vertices $V_1, V_2, \ldots, V_p$, of equal size, so that the total number of edges that connect vertices which belong to different subsets is minimised. The case of $p=2$ is the above-mentioned graph bisection problem. The average cost function $C(p, N)$ of the problem is the average minimum number of edges that connect vertices of different sets.

(ii) *Graph colouring.* Here the random graph is divided into p sets of vertices of equal size in such a way that the total number of edges connecting vertices which belong to the same subset (i.e. having the same colour) is minimised. Here the cost function $C'(p, N)$ is the average minimim number of edges that connect vertices of the same colour. These two optimisation problems, the graph partitioning and the graph colouring problems are not independent.

0305-4470/87/110673+07$02.50

It is straightforward to show that the average cost functions obey

$$C'(p, N, c) = C(p, N, 1-c) - \tfrac{1}{2}N^2[1 - 1/p - c(1-1/N)] \tag{1}$$

where c is the concentration of edges. An interesting problem in graph colouring is the value of the chromatic number, p_0. This number is the minimum number of colours which have to be introduced (for a given graph) in order that it will be possible to divide the graph without connecting vertices of the same colour. In our notation, the average p_0 is the minimum value of p for which $C'(p, N, c)$ vanishes.

The problem of graph partitioning can be mapped onto a system of N interacting Potts spins, $\{\sigma_i, i = 1, \ldots, N\}$, where each σ_i can take the values $1, 2, \ldots, 4p$. The Hamiltonian of the system is given by

$$H = -\tfrac{1}{2}\sum_{i \neq j} J_{ij}(p\delta_{\sigma_i,\sigma_j} - 1) \tag{2}$$

where each J_{ij} is a quenched random variable with the distribution

$$P(J_{ij}) = c\delta(J_{ij} - 1) + (1-c)\delta(J_{ij}). \tag{3}$$

The restriction of partitioning to p subgraphs of equal size (N/p) implies the following p global constraints:

$$m_r \equiv \frac{1}{N}\sum_{i=1}^{N}(p\delta_{\sigma_i,r} - 1) = 0 \qquad r = 1, 2, \ldots, p. \tag{4}$$

In order to prove the mapping let us denote by N_1 the total number of edges connecting vertices inside the subgraphs in a given partitioning, and by N_0 the total number of edges connecting vertices belonging to different subgraphs. The average total number of edges equals $(N-1)c/2$, hence

$$N_1 + N_0 = \tfrac{1}{2}N(N-1)c. \tag{5}$$

Each bond inside a subgraph contributes $-(p-1)$ to H whereas a bond connecting vertices of different subgraphs contributes $+1$. Therefore,

$$N_0 - N_1(p-1) = H. \tag{6}$$

Equations (5) and (6) yield, for the cost function C,

$$C = N_0 = \frac{N^2(p-1)c}{2p} - \frac{N(p-1)c}{2p} + \frac{H}{p}. \tag{7}$$

The first term on the RHS of equation (7) represents the cost in the case of random partitioning into p subgraphs, each of which will contain $c(N/p)[(N/p)-1]/2$ bonds. This yields a cost which equals

$$\tfrac{1}{2}cN(N-1) - \tfrac{1}{2}pc\frac{N}{p}\left(\frac{N}{p} - 1\right) = \frac{N^2(p-1)c}{2p}. \tag{8}$$

This is consistent with equation (7) since, in a random configuration,

$$\langle\delta_{\sigma_i,\sigma_j}\rangle = \frac{1}{p}\left(1 - \frac{(p-1)}{p}\frac{1}{(N-1)}\right)$$

where angle brackets denote an average over configurations. Thus the (negative) contribution H/p in (7) represents the reduction in cost by the optimisation of the partitioning.

The graph partitioning problem is then equivalent to finding the ground state of the Hamiltonian (2) subject to the constraints (4). Instead of considering the rigid constraints (4) it is sometimes convenient to represent them by soft constraints. This amounts to adding to the Hamiltonian, equation (2), the term

$$\frac{gH}{2p}\sum_{r=1}^{p} m_r^2 \qquad g>0 \tag{9}$$

with m_r defined by (4). This is equivalent to using the Hamiltonian (2) with the following distribution of bonds:

$$P(J_{ij}) = c\delta(J_{ij}-1+g)+(1-c)\delta(J_{ij}+g). \tag{10}$$

For sufficiently large g this modification will ensure that the optimised partitioning obeys the constraints (4).

The cost in the graph colouring problem is N_1. Minimising N_1 is equivalent to maximising N_0 of the same graph, or minimising N_0 of the graph which is formed by the missing edges in the original graph. The concentration of the missing bonds is $1-c$.

Using (5) and the fact that the number of all possible edges connecting the p groups is $N^2(1-1/p)/2$, one obtains the relation (1).

Although the Hamiltonian (2) describes an infinite-ranged system, calculating its ground-state energy is a complex task. Here we will focus on the case of dense graphs defined by c and $1-c$ being of order unity, in the limit $N\to\infty$. In this case, a direct connection can be made between the Hamiltonian (2) and the mean-field theory (MFT) of infinite-ranged Potts glasses [5].

The argument for the connection with the MFT is the same as in the case of Fu and Anderson. When the average number of bonds per site is proportional to N, the local fields are sums of N terms and are not sensitive (in the $N\to\infty$ limit) to the details of the distribution of the individual J_{ij}. The macroscopic properties of the system depend only on the first two moments of the distribution. Using the distribution (10), the first moment is

$$J_0 \equiv \langle\langle J_{ij}\rangle\rangle = -g+c. \tag{11}$$

Double angle brackets denote an average of $P(J_{ij})$. The second moment is

$$J^2 \equiv \langle\langle J_{ij}^2\rangle\rangle - \langle\langle J_{ij}\rangle\rangle^2 = c(1-c). \tag{12}$$

Therefore, in the case of dense graphs the cost function is identical, in the $N\to\infty$ limit, to an infinite-range PG Hamiltonian of the form (2) with a Gaussian distribution of bonds:

$$P(J_{ij}) = \left(\frac{1}{2\pi J^2}\right)^{1/2} \exp\left(-\frac{1}{2J^2}(J_{ij}-J_0)^2\right) \tag{13}$$

where J_0 and J are given by equations (11) and (12). Furthermore, once J_0 is made sufficiently negative that the ground state obeys the constraints (4), the energy E of the Hamiltonian (2) with J_{ij} of (13) is independent of the magnitude of J_0, since the latter couples only to the 'magnetisations' m_r which vanish. In such a case,

$$E = -JN^{3/2}U(p, N) \tag{14}$$

where $U(p)\equiv\lim_{N\to\infty} U(p, N)$ is a positive number of O(1) which does not depend on J or J_0 (i.e. on c and g). Substituting equations (13) and (14) in equation (7)

yields, for the $N \to \infty$ limit,

$$C = \frac{N^2 c(p-1)}{2p} - N^{3/2} c^{1/2} (1-c)^{1/2} \frac{U(p)}{p}. \tag{15}$$

For the graph colouring problem one obtains, using equations (1) and (15),

$$C' = \frac{N^2 c}{2p} - N^{3/2} c^{1/2} (1-c)^{1/2} \frac{U(p)}{p}. \tag{16}$$

Thus the non-trivial correction to the cost function is the same for both the partitioning and the colouring problems in the case of dense graphs and the $N \to \infty$ limit, and it is simply related to the ground-state energy of the infinite-range PG with Gaussian bonds.

In order to evaluate the ensemble-averaged value of $U(p)$ we apply the results of the replica MFT, previously developed [5, 6] for evaluating the PG free energy [5]. The ensemble-averaged free energy per site is defined as

$$f = -\frac{1}{N\beta} \langle\langle \ln \operatorname{Tr}_{\{\sigma_i\}} \exp(-\beta H) \rangle\rangle \tag{17}$$

where H is given by (2) and the ensemble average is performed over the distribution of bonds, equation (13). The parameter β is the inverse temperature. When β approaches infinity f approaches the minimum energy per spin, i.e. $-JN^{1/2}U(p)$ (see equation (14)). Using Parisi's replica symmetry breaking (RSB) theory [7] with an ansatz of a one step of RSB [5, 6] one obtains the following expression for f:

$$f = -\tfrac{1}{4}(p-1)\beta[1-2q+(1-x)q^2] - \frac{1}{\beta x} \ln \int_{-\infty}^{\infty} \prod_{K}^{p} \frac{\mathrm{d}t_K}{(2\pi p)^{1/2}} \delta\left(\sum_{K=1}^{p} t_K\right)$$
$$\times \exp\left[-\frac{1}{2p} \sum_{K=1}^{p} t_K^2 + x \ln\left(\sum_{K=1}^{p} \exp(\beta q^{1/2} t_K)\right)\right]. \tag{18}$$

The 'order parameters' q and x, $0 \leqslant q \leqslant 1$, $0 \leqslant x \leqslant 1$, are determined by the equations $\partial f/\partial x = \partial f/\partial q = 0$. In the limit of $\beta \to \infty$, $q \to 1$, $x \to 0$ and equation (18) reduces to

$$U(p) = -\tfrac{1}{4}(p+1)a + \frac{1}{a} \ln\left[\left(\frac{p}{2\pi}\right)^{1/2} 2^{-p+1} \int_{-\infty}^{\infty} \mathrm{d}t \exp\left(-\frac{t^2}{2p} + at\right)\left(1 + \operatorname{erf}\left(\frac{t}{\sqrt{2p}}\right)\right)^{p-1}\right]. \tag{19}$$

The parameter $a = \lim_{\beta \to 0} (x\beta)$ is determined via $\partial U/\partial a = 0$. We have calculated $U(p)$ by numerical maximisation of (19). A few examples are $U = 1.39$, 2.43 and 6.02 for $p = 3$, 5 and 15 respectively. The results for general p are shown in figure 1.

An interesting limit is the case of $p \to \infty$. Evaluating equation (19) by a saddle-point method one obtains

$$U = \lim_{p \to \infty} U(p) = (p \ln p)^{1/2}. \tag{20}$$

At finite temperature $T = \beta^{-1}$ the free energy (18) exhibits a phase transition from a 'high-temperature' value $f/JN^{1/2} = -T \ln p - \beta(p-1)/4$, $\beta < \beta_c$, to the 'low-temperature' value $f/JN^{1/2} = -U_\infty$, $\beta > \beta_c$. The value of β_c is

$$\beta_c = 2(\ln p / Np)^{1/2}. \tag{21}$$

The results (18)-(21) are exact in the large-p limit. In the case of finite p, $p > 2$, the 'one-step' ansatz (and hence the result (18)) is exact only at high and intermediate

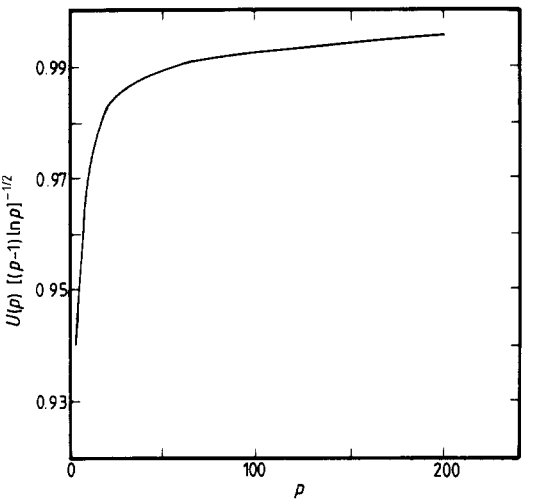

Figure 1. Results of numerical maximisation of equation (19). The results show the convergence of U to its large-p limit $(p \ln p)^{1/2}$, equation (20).

temperatures, but breaks down below $T = T_2 < T_c$, where the nature of the RSB is more complex. Nevertheless the corrections due to this additional complication are expected to remain small even as $T \to 0$. This is particularly true for large values of p, where the actual values of $U(p)$ are expected to be very close to the large-p result. Note also that $T_2 \to 0$ as $p \to \infty$.

In order to check the quality of the approximation (19) for $U(p)$ we have performed Monte Carlo simulations of the ground-state energy E of the infinite-range Potts glass, equations (2) and (13), with $p = 7$. In the simulations, systems of sizes $N = 35$, 70 and 200 were slowly annealed from high temperatures using a heat-bath algorithm. The results for $E = -U$ are shown plotted against N in figure 2.

In the simulation, the value of J has been chosen for convenience to be $J = 1/\sqrt{N}$. As for J_0, the MFT predicts [4] that in the case of $J_0 = 0$ the PG ground state possesses a ferromagnetic (FM) long-range order, thus violating the constraints. Putting $J_0 N = \bar{J}_0$, the FM order is suppressed at a temperature T if [4]

$$\bar{J}_0 < -\beta(p-2)/2. \tag{22}$$

Note that in the bipartitioning case ($p = 2$), choosing $J_0 = 0$ is sufficient to guarantee that the ground state obeys the constraint. This prediction has been borne out by our simulations. Choosing $J_0 = 0$ resulted in an FM ground state. Using small negative values for J_0, a spin-glass state has been achieved at intermediate temperature $T \leqslant 1.3$ but an FM order appeared at lower temperatures. In practice, choosing $\bar{J}_0 \leqslant -5$ was sufficient to guarantee the suppression of the magnetisation in the temperature regime $T \geqslant 0.4$, in which significant thermal fluctuations were still observed. A detailed presentation of the finite-temperature results of the simulations will be given elsewhere. Although the statistical errors are not negligible, the results seem to be consistent with a finite-size correction of E, of order $1/N$. This should be contrasted with the $1/\sqrt{N}$ corrections seen in simulations of the Ising spin glass [8]. The fact that the finite-size corrections seem to be smaller here may be related† to the fact that there are less

† We thank M Mézard for a discussion on this point.

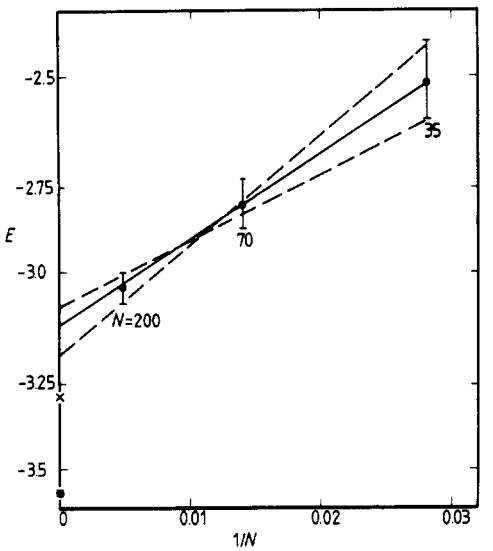

Figure 2. Monte Carlo simulation of the ground-state energy (per spin) of the seven-state infinite-range Potts glass, equations (2) and (13). The choice of J and J_0 is discussed in the text. N denotes the system size, and × and ■ denote the values of E (in the thermodynamic limit) according to the one-step MFT [5, 6] and the replica symmetric MFT [4], respectively.

marginal fluctuations in the ordered state of the Potts model relative to the Ising case [5, 6]. The results of figure 2 yield $\lim_{N\to\infty} U(p=7) = 3.15 \pm 0.05$ which differs by only 4% from the 'one-step' approximation, $U(7) = 3.3$. Part of this discrepancy may be due to incomplete equilibration of the systems in the simulations. Note that the naive MFT (the replica symmetric theory) [4] yields a much worse estimate for U ($U(7) = 3.56$). As mentioned above, the discrepancy between equation (19) (figure 1) and the actual value of $U(p)$ is expected to decrease as p increases.

Returning to graph partitioning we obtain for the ensemble-averaged cost function in the large-p limit,

$$\lim_{p\to\infty}\lim_{N\to\infty} C(p, N, c) = \tfrac{1}{2}N^2 c - N^{3/2}\left(\frac{c(1-c)\ln p}{p}\right)^{1/2} \tag{23}$$

(see equations (15) and (20)). In the case of finite large p, the result (15), together with equation (19), is expected to yield a good approximation for the cost function.

In the case of graph colouring, equation (16) yields

$$\lim_{p\to\infty}\lim_{N\to\infty} C' = \frac{N^2 c}{2p} - N^{3/2}\left(\frac{c(1-c)\ln p}{p}\right)^{1/2}. \tag{24}$$

Note that the positive random contribution to the cost decreases more rapidly with p than the contribution from the optimisation. The two terms cancel each other at

$$P_0 \simeq \frac{N}{4\ln N}\left(\frac{c}{1-c}\right). \tag{25}$$

It is tempting to identify p_0 as the chromatic number. However, equation (25) violates

the rigorous bounds [9, 10] for the chromatic number p_0 for all values of c:

$$\frac{N}{2 \ln N} \ln\left(\frac{1}{1-c}\right) < p_0 < \frac{N}{\ln N} \ln\left(\frac{1}{1-c}\right) \tag{26}$$

valid for the case of dense graphs. Although we obtain the correct scaling with N, namely $p_0 \propto N/\ln N$, the coefficient predicted by (25) is incorrect. The likely reason for this failure is that the mapping between the graph problem and the PG with Gaussian bonds (equation (13)) breaks down when p is as large as $N/\ln N$. In this case, the real bond distribution (equation (10)) must be taken into account.

In conclusion, we have presented in this letter a mapping between graph partitioning and graph colouring problems (with p partitions or colours) and the statistical mechanical problems of p-state Potts glasses. The ensemble-averaged cost functions of dense graphs can be calculated using the MFT of Potts glasses. Using the results of the MFT, an exact expression (equations (23) and (24)) for the average cost function in the limit of large p has been derived. To our knowledge this result is new.

In addition, we have derived an estimate of the cost function for all $p > 2$ (in the thermodynamic limit), based on an approximate MFT. This estimate is believed to be within only a few per cent of the exact cost for all values of $p > 2$. It would be interesting to compare these results with numerical optimisation of the graph problems performed by either heuristic algorithms or simulated annealing.

Discussion with D J Gross, D S Johnson, M Mézard and E Shamir are gratefully acknowledged. We also thank E Shamir for bring references [9] and [10] to our attention. The research has been supported in part by the Fund for Basic Research of the Israeli Academy of Science and Humanities and by the US-Israel Binational Science Foundation.

Note added. After the completion of this work, we received an interesting preprint by P Y Lai and Y Y Goldschmidt which also discusses the mapping between the graph partitioning and colouring problems and the Potts glass.

References

[1] Fu Y and Anderson P W 1986 *J. Phys. A: Math. Gen.* **19** 1605
[2] Gary M R and Johnson D S 1979 *Computers and Intractability* (San Francisco: Freeman)
[3] Kirkpatrick S and Sherrington D 1978 *Phys. Rev.* B **17** 4384
[4] Elderfield D and Sherrington D 1983 *J. Phys. C: Solid State Phys.* **16** L497
[5] Gross D J, Kanter I and Sompolinsky H 1985 *Phys. Rev. Lett.* **55** 304; 1987 to be published
[6] Kanter I 1987 *PhD Thesis* Bar-Ilan University
[7] Parisi G 1980 *J. Phys. A: Math. Gen.* **13** 1101
[8] Palmer R G and Pond C M 1979 *J. Phys. F: Metal Phys.* **9** 1451
[9] Erdos P and Spencer J 1974 *Probabilistic Methods in Combinatoxics* (New York: Academic)
[10] Bollobas B and Erdos P 1976 *Math. Proc. Camb. Phil. Soc.* **80** 419