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LETTER TO THE EDITOR

Graph bipartitioning and the Bethe spin glass

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Abstract. The problem of the equipartitioning of a random graph of fixed finite valence is studied by comparison with a ferromagnetic Bethe lattice with random boundary conditions. The simplicity of recursion relations for effective fields due to descendents on Bethe lattices provides simple approximations for the optimal cost, in quite good agreement with simulations.

Recently, there has been much interest in applying techniques from the physics of disordered and frustrated systems to the study of complex optimisation problems. One example is the graph bipartitioning problem [1] in which one has a set of randomly connected vertices and the issue is to partition them into two subsets of equal size, so that the number of connections between the two sets, or 'cost' N_{ct}, is minimised. By associating an Ising spin with each vertex, so that it takes the value $+1$ if the vertex belongs to one set and -1 if otherwise, this problem can be mapped into that of finding the ground state of a ferromagnetic Ising model on the network with an identical configuration of bonds, subject to the constraint that the total magnetisation is zero [1, 2]. The energy E of the Ising system (in units of the coupling strength J) and the cost N_{ct} of the graph partitioning are related by $E = -N_b + 2N_{ct}$, where N_b is the total number of bonds.

In the thermodynamic limit (i.e. as the total number of vertices becomes infinite), we consider the cost per vertex averaged over an ensemble of graphs having the same constraints of connectivity but different explicit configurations. For the case of extensive connectivity (in which the probability p that any two vertices are connected is independent of the total number of vertices N) the graph bipartitioning problem is equivalent to finding the ground-state energy of the infinite-range Sherrington-Kirkpatrick (SK) spin glass [3] and has been solved [1, 4, 5].

This letter is concerned with intensive connectivity with every vertex connected to the same number α of other vertices; we refer to α as the valence. This problem has been studied numerically by Banavar *et al* [6] and an empirical formula proposed for the ground-state energy. We present here some simple approximate analytic procedures for estimating this quantity, obtaining results in quite good agreement with the simulations.

The key basis for our approximations is the observation that paths between connected vertices on a graph of random intensive connectivity are effectively tree-like over finite numbers of steps, the average length of closed loops increasing with N. Indeed, Banavar *et al* [6] have demonstrated that a system of unconstrained Ising spins, located on the vertices of such a graph and interacting ferromagnetically where

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a connecting edge exists, have in the thermodynamic limit the same transition temperature as for spins on a Bethe lattice of the same valence and exchange strength. In the present problem, with its equipartition or zero-magnetisation constraint, we therefore simulate the problem of graph partitioning by that of spins on Bethe lattices interacting ferromagnetically (with identical neighbouring exchange strengths) but subjected to quenched random fields on the boundary spins. The advantage of a Bethe lattice lies in the simple recursive evaluation of local fields due to descendents. With quenched random boundary fields, having a symmetric distribution, the recursive relation ensures the zero-magnetisation constraint to be held among the spins of each ascending generation. Furthermore, a Bethe spin glass of random $\pm J$ bonds can be gauge transformed into this ferromagnetic Bethe system with random boundary fields [7], hence also suggesting a basis for the features of non-self-averaging and ultrametricity [8] found in the simulations [6].

We start by considering an Ising ferromagnet on a Bethe lattice

$$H = -J \sum_{(ij)} \sigma_i \sigma_j \tag{1}$$

where (ij) denotes the pair of neighbouring sites i, j. The Bethe lattice is constructed as follows. A central site (zeroth generation) branches out to α 'neighbouring' sites (first descendents) with thereafter each site branching out to $K = (\alpha - 1)$ further sites until the Nth generation. To simulate the constraint of zero magnetisation and the random connectivity of the graph bipartitioning problem we impose random fields on the boundary (surface) spins with a symmetric distribution

$$P(h) = P(-h). \tag{2}$$

Once the boundary fields are assigned, the effective field at any site due to its descendents follows recursively from [9, 10]

$$\beta h = \sum_{i=1}^{K} \tanh^{-1}(\tanh \beta J \tanh \beta h_i) \tag{3}$$

where the h_i on the right-hand side are the corresponding fields on the immediate descendents, or the boundary fields in the case of the Nth generation. In the case of random boundary conditions this leads to a recursive relation between the effective field distributions of sequential generations

$$P_s(h) = \int \mathrm{d}h_1 \ldots \mathrm{d}h_K \, P_{s+1}(h_1) \ldots P_{s+1}(h_K) \times \delta\left(h - \beta^{-1} \sum_{i=1}^{K} \tanh^{-1}(\tanh \beta J \tanh \beta h_i) \right) \tag{4}$$

where $P_s(h)$ is the distribution at the sth generation. Far from the surface $P_s(h)$ tends towards a 'fixed-point' distribution. At high temperatures this fixed-point distribution is a delta function at $h = 0$, corresponding to a paramagnet, whilst beneath a critical temperature $T_c = J/\tanh^{-1}(K^{-1/2})$ the $P(h)$, which retains its $P(h) = P(-h)$ symmetry, acquires a finite width, characteristic of a spin glass [10, 11].

The recursion relations simplify at $T = 0$. Thus equation (3) becomes

$$h = \sum_{i=1}^{K} \operatorname{sgn} h_i \min(J, |h_i|) \tag{5}$$

where the right-hand side refers to the immediate descendents of the site on the left-hand side. It is clearly natural to restrict the boundary fields to $h_i = nJ$; n integral, $|n| \leqslant K$. Then, at earlier generations, h is similarly restricted and given by

$$h = J \sum_{i=1}^{K} \operatorname{sgn} h_i. \tag{6}$$

Now $P(h=0) = p_0$ suffices as a measure from which all other quantities of interest follow. p_0 at generation s, $p_0^{(s)}$, is given in terms of that at generation $(s+1)$ by the simple recursion relation

$$p_0^{(s)} = f(p_0^{(s+1)}) = \sum_{r=0}^{\operatorname{int}(K/2)} \frac{K!}{(K-2r)!(r!)^2} (p_0^{(s+1)})^{K-2r} \left(\frac{1-p_0^{(s+1)}}{2}\right)^{2r} \tag{7}$$

where $\operatorname{int}(x)$ means the integral part of x. The corresponding expression for the full field distribution is

$$P^{(s)}(nJ) = \sum_{r=0}^{\operatorname{int}[(K-n)/2]} \frac{K!}{(K-n-2r)!(n+r)!r!} (p_0^{(s+1)})^{K-n-2r} \left(\frac{1-p_0^{(s+1)}}{2}\right)^{n+2r}$$
$$= P^{(s)}(-nJ) \qquad n = 0, 1, \ldots, K. \tag{8}$$

The recursion relations (7) for $K=2$ and 3 are shown in figures 1(a) and (b) respectively. Note that for $K=2$ (and other even K) there exist two fixed points of the relation $f(p_0^*) = p_0^*$, of which $p_0^* = 1$ is unstable whilst the other fixed point is stable. For K odd there are three fixed points, those at $p_0^* = 0$ and 1 being unstable and the remaining one being stable.

Consider an arbitrary $p_0 (\neq p_0^*)$ at the boundary. As one goes generation by generation inward, the iterated p_0 will approach the stable fixed point p_0^{**}. Table 1 gives the values of p_0^{**} for $3 \leqslant \alpha \leqslant 8$.

We now turn to the calculation of the ground-state energy. In the thermodynamic limit, the free energy per site for the sth generation is given by [10]

$$-F_s/N_s J = (T/2J)\langle \ln[4 \cosh \beta(J+h) \cosh \beta(J-h)] \rangle_s \tag{9}$$

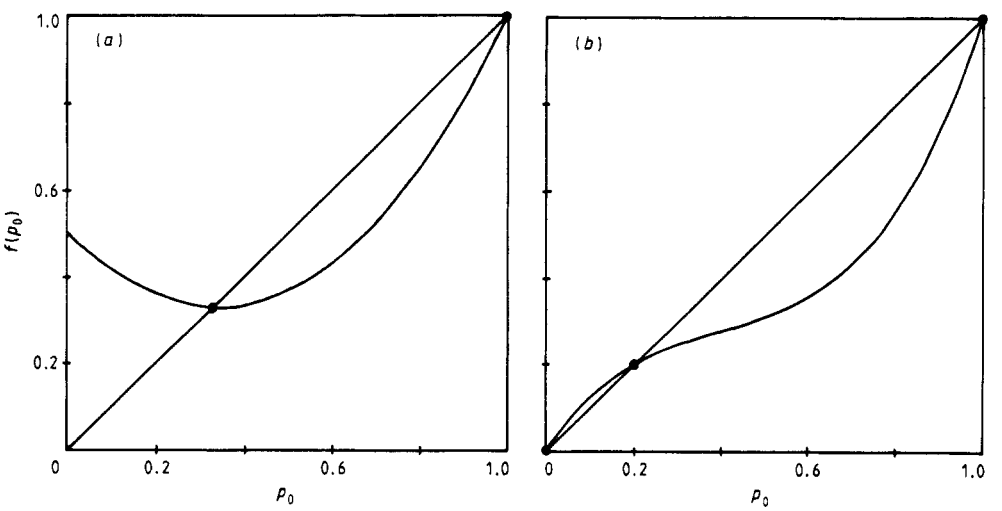

Figure 1. Plots of $f(p_0)$ showing fixed points (●) of the recursion relation (7) for (a) $k=2$, $f(p_0) = \frac{1}{2}(3p_0^2 - 2p_0 + 1)$ and (b) $k=3$, $f(p_0) = \frac{1}{2}p_0(5p_0^2 - 6p_0 + 3)$.

Table 1. Values p_0^{**} of stable fixed points and estimates of the ground-state energy per bond for graph partitionings of valences $3 \leqslant \alpha \leqslant 8$.

α	Source	3	4	5	6	7	8
p_0^{**}		0.333	0.200	0.229	0.167	0.183	0.146
E_{BSS}	Reference [6]	0.840	0.732	0.663	0.605	0.564	0.528
$E(p_0^{**})$	Equation (12)	0.778	0.616	0.575	0.494	0.475	0.425
ε_α	Equation (13)	0.778	0.670	0.619	0.567	0.533	0.501
$\tilde{\varepsilon}_\alpha$	Equation (15)	0.815	0.724	0.645	0.600	0.554	0.525
E_{MP}	Reference [15]	0.852	0.734	0.677	0.618	0.578	0.541

where $\langle\ \rangle_s$ refers to an average over the sth generation. At $T=0$, the energy is the same as the free energy and equation (9) takes the simple form

$$-E_s/N_sJ = \sum_{n=1}^{K} (P^{(s)}(nJ) + P^{(s)}(-nJ))n + P^{(s)}(0)$$
$$\equiv E(p_0^{(s+1)}) \tag{10}$$

where the form of $E(p_0)$ follows from the use of equation (8). This expression is interpreted as follows. In order to avoid double counting, in calculating the total energy of the system, we add up the coupling energy of each site with only its K descendents or, for the surface sites, the imposed boundary fields, except that when the field due to its descendents is zero an energy $-J$ must be added to allow for interaction with the immediate ancestor†. The total energy is given by summing over all the sites. It is often convenient to separate out the exchange contribution to the energy from the boundary field contribution and to treat interior and boundary spins on equal footings. To this end we consider an alternative procedure, associating the exchange energy per spin in any generation with interaction only with its immediate ancestors

$$-\tilde{E}_s/N_sJ = K^{-1} \sum_{n=1}^{K} (P^{(s-1)}(nJ) + P^{(s-1)}(-nJ))n + P^{(s)}(0). \tag{11}$$

The energy due to the applied boundary fields is additional. Because of the one-to-one relationship between the number of sites in a generation and the number of bonds to the immediate ancestors, this expression also yields the exchange energy per bond ascendent from generation s. Clearly, the expression on the right-hand side is a function of $p_0^{(s)}$. Formally we write it as

$$-\tilde{E}_s/N_sJ = E(p_0^{(s)}) = K^{-1}(E(p_0^{(s)}) - f(p_0^{(s)})) + p_0^{(s)}. \tag{12}$$

Let us now use the above to estimate the ground-state energy of the randomly connected ferromagnetic network with zero magnetisation, the graph partitioning problem. A first simple approximation is to assume that the energy per bond of the network is given by equation (12) with $p_0^{(s)} = p_0^{**}$, the stable fixed point value. A reason for this choice is the observation that any typical set of a finite number of connected vertices of the random graph looks like a section of a Bethe lattice away from its surface, where the field distribution tends towards its stable fixed-point form. This assumption leads to energies 10–20% higher than those found by Banavar *et al* [6] for $3 \leqslant \alpha \leqslant 8$, as shown in table 1.

† Note that $h=0$ does not imply $\langle\sigma\rangle = 0$. In the case of $h=0$ the mean spin is determined by the ancestral behaviour.

A possible reason that the above calculation gives energies higher than expected is that the energy due to boundary fields has been neglected. While this contribution is usually negligible for conventional lattices, this is not true for Bethe lattices in view of its notoriously significant fraction of boundary spins. To better simulate the complete connectedness of the graph problem (as opposed to the behaviour over a finite number of steps on the graph) we now, instead of imposing random boundary fields on the system, consider the Bethe lattice to have its boundary spins randomly interconnected, so that they also have the coordination number α of the rest, with the constraint of zero magnetisation. In the spirit that the probability of forming small loops is infinitesimally small, we can treat this random connection among the boundary spins as another Bethe lattice but of valence $(\alpha-1)$. This $(\alpha-1)$ Bethe lattice is similarly terminated by one of valence $(\alpha-2)$ and so on until the valence 2 lattice is reached. A valence 2 random graph is simply a randomly connected necklace. We refer to this construction as a Bethe hyperlattice and the procedure as valence reduction†.

We now argue that the zero-magnetisation ground state of the hyperlattice is given, at least to a good approximation, in the thermodynamic limit by assuming that the $(\alpha-1)$ 'core' of an α hyperlattice is in one of its zero-magnetisation ground states and the boundary spin values are given by independent random choices from the sites of the core. This amounts to neglecting the effects on the core of the loops formed by the core with the ascendents on the α lattice. We expect this to be a good approximation for two reasons. First, because $(\alpha-2)/(\alpha-1)$ of the sites of a Bethe lattice are on the surface, this procedure minimises the energy of a considerable fraction of the spins, whilst adjusting the rest accordingly. Second, if further correlations are ignored, no overall reduction in energy arises from changing the state of a boundary spin to match its siblings with the same immediate ancestor. Thus, for $\alpha=3$, say, the core necklace is in a state consisting of two large equal-sized domains of opposite spin; although there is an ancestral interaction energy improvement of $-2J$ when a pair of boundary spins with a common ancestor is switched from $+-$ into $++$ (or $--$) to align with its $+$ (or $-$) ancestral spin, this is normally offset by a greater energy increase due to the necessary insertion of extra domain walls in the boundary system‡. This approximation is in the spirit of the effective random field approximations to conventional spin glass theory [13, 14].

The above approximation, giving $p_0=0$ on the termination lattice, provides the energy associated with the ancestral sites of the main lattice via equations (12) and (7), yielding finally for the energy per bond of the α hyperlattice

$$\varepsilon_\alpha=-\frac{E}{N_b J}=\left(\tfrac{1}{2}(\alpha-1)\varepsilon_{\alpha-1}+\sum_{r=0}^{\infty}\frac{1}{K^{r+1}}\tilde{E}(f^r(0))\right)\left(\tfrac{1}{2}(\alpha-1)+\sum_{r=0}^{\infty}\frac{1}{K^r}\right)^{-1} \tag{13}$$

where N_b is the total number of bonds and

$$f^r(p_0)=\begin{cases}p_0 & r=0\\ f(f^{r-1}(p_0)) & r\geqslant 1.\end{cases} \tag{14}$$

† We might note in passing that this analogy suggests the variant of the travelling salesman problem [12] in which, given a randomly connected network, one looks for the path (or paths) which visits the greatest number of sites before returning to its starting point while passing through any site once at most. This path is the analogue of the terminating necklace and has a length (in terms of the number of sites visited) proportional to the total number of sites; for the hyperlattice the length of the terminating necklace is $N/(\alpha-1)$ where N is the total number of sites.

‡ For an $\alpha=2$ necklace termination, the domain wall penalty is $4J$.

Again, the results for $3 \leqslant \alpha \leqslant 8$ are displayed in table 1. Compared with the simulations of Banavar *et al* [6], the energies obtained are 5-9% higher.

In comparison with the simulation results it is also intriguing to note that if $E(p_0^{**})$ is taken as the energy per site and, with the number of bonds per site being $\alpha/2$, the ground-state energy per bond is estimated from

$$\tilde{\varepsilon}_\alpha = 2\alpha^{-1} E(p_0^{**}) \tag{15}$$

the resulting energies are of the order of only 1-3% higher than those found in the simulations for $3 \leqslant \alpha \leqslant 8$; again see table 1 for details. Although the apparent agreement is remarkable for such a simple evaluation, this comparison must be viewed with caution since a corresponding procedure for the energy of an unrestricted ferromagnet ($2\alpha^{-1}$ times the result of equation (10)) would yield an incorrect result (unlike the use of equation (11)).

Finally, we comment that in a study of graph partitioning Mézard and Parisi [15] have reported equations (derived within an undetailed cavity method) which are identical in form to some of ours but have been given slightly different interpretations. Thus they reported an equation identical to our equation (4) at self-consistency but with h defined as $h_i = \beta^{-1} \tanh\langle\sigma_i\rangle$, an effective field due to all influences on σ_i, whereas our h_i is due to descendents only and does not necessarily determine $\langle\sigma_i\rangle$. Similarly they give an equation identical to our equation (7) at its fixed point with p_0^* identified as the number of 'crazy spins', whereas in our analysis $h = 0$ does not imply an ill-defined spin. Thus the full significance of the similarity of these equations is unclear. Mézard and Parisi also give an expression for the ground-state energy per spin which, when expressed in terms of $P(h)$, takes the form

$$E_{\mathrm{MP}} = -E_0/NJ = \alpha p_0^{*2}/2 + p_0^*(1-p_0^*) + \sum_{n=1}^{K} (P(nJ) + P(-nJ))n \tag{16}$$

reminiscent of our equation (10) but differing in the $h = 0$ term. This expression also gives very good agreement with the simulations (see table 1), now lying slightly lower in energy. We have re-derived equation (16) within replica theory [3, 13] but with an interpretation closer to that of the Bethe glass, but we defer further discussion to a separate publication [16].

In summary, we have shown that Bethe lattices with appropriate random boundary conditions provide reasonable approximations to partitioning of graphs of random connectivity. An advantage of Bethe lattices lies in the simplicity of recursion relations between generations. At zero temperature, for given boundary conditions, a single recursively determined parameter suffices to determine the ground-state properties.

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