Computer-intractability of the frustration model of a spin glass

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LETTER TO THE EDITOR

Computer-intractability of the frustration model of a spin glass

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Abstract. We prove that finding a ground state of the three-dimensional frustration model of a spin glass is an NP-complete optimisation problem, and hence probably intractable in the sense that no algorithm requiring a time bounded by a polynomial of the volume can exactly solve it.

Some time ago Kirkpatrick *et al* (1983) pointed out an interesting similarity between spin glass models, and a class of combinatorial optimisation problems known as NP-complete: both are characterised by a large number of nearly degenerate locally optimal configurations, fluctuating with disorder and separated by large energy barriers. This feature presumably accounts for the failure of local-search algorithms to find the true ground state in a reasonable amount of time, as well as for the experimentally observed long (infinite?) relaxation times of real spin glasses (dilute magnetic alloys) at low temperatures‡.

Even though necessary, the existence of a large number of metastable fluctuating states does not, however, suffice by itself to render an optimisation problem NP-complete, nor does it guarantee the existence of a distinct spin glass phase at thermodynamic equilibrium. This is clearly illustrated by the two-dimensional Ising model with competing interactions whose ground state can always be found by a non-local algorithm in time bounded by a polynomial of the volume (Bieche *et al* 1980, Barahona *et al* 1982), and which, furthermore, does not—according to current wisdom—exhibit a spin glass phase, despite the presence of both disorder and frustration. A much subtler feature should therefore be responsible both for rendering optimisation problems intractable, and for the appearance of a spin glass phase, and the question naturally arises whether the analogy between spin glasses and NP-complete problems is deeper than it was originally meant to be§.

A natural first step towards answering this question would be a classification of proposed spin glass models according to their algorithmic complexity. Barahona (1982) has already shown that finding the ground state of an Ising model with random

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‡ For a brief review of spin glasses see for instance Binder (1980), and references therein.

§ This is further supported by the observed ultrametricity of locally optimal paths in the Travelling Salesman Problem (Kirkpatrick and Toulouse 1984), a property also characterising Parisi's solution of the Sherrington–Kirkpatrick model (Mézard *et al* 1984a, b).

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nearest-neighbour couplings in three or more dimensions at zero magnetic field, as well as in two or more dimensions in the presence of a magnetic field, is an NP-complete optimisation problem. In this letter we will extend his results to the three- (or higher-) dimensional frustration model, defined by the Hamiltonian:

$$\mathcal{H} = -\sum_{\text{NN}} J_{ij}\sigma_i\sigma_j \tag{1}$$

where the σ_i are again Ising spins, the summation runs over a nearest neighbours (NN) on a hypercubic lattice, but the couplings J_{ij} can now only take the values ± 1. Except for its finite residual entropy, this model is believed to share most properties of realistic spin glasses†, and by virtue of its simplicity is most widely used for numerical simulations. Proving its NP-completeness might therefore also save the time of physicists trying to devise exact algorithms to generate its ground states‡.

We begin by stating, in a slightly modified language, a known NP-complete optimisation problem, Restricted Maximum Cut (RMC) (Yannakakis 1978)§: Given a graph $G = (V, E)$ where V is the set of vertices and E the set of undirected edges (unordered pairs of vertices), such that no vertex has a degree higher than three (i.e. no more than three lines emanate from each vertex), minimise the cost function:

$$G = \sum_{(v_1, v_2) \in E} \sigma_{v_1}\sigma_{v_2} \tag{2}$$

where the σ_v are Ising spins. We will now assign to every instance (i.e. graph G) of RMC, an instance (i.e. configuration of coupling J_{ij}) of the three-dimensional frustration model, so that minimising the cost function of the former is equivalent to minimising the energy function of the latter. This will prove that finding the ground state of the frustration model is at least as hard as solving RMC, and hence belongs to the class of NP-complete problem.

Indeed, given an instance G of RMC, we first construct a new graph $\tilde{G}$ by doubling each edge of G and then adding loops (i.e. edges starting and finishing at the same point) until each vertex has degree six, as shown in figure 1 (for the field-theorist $\tilde{G}$ is thus a vacuum diagram for a φ^6 interaction). Next we embed $\tilde{G}$ into a three-dimensional lattice, so that to each vertex $\tilde{v}$ corresponds a lattice site (node) $l(\tilde{v})$, to each edge $\tilde{e} = (\tilde{v}_1, \tilde{v}_2)$ a path on the lattice ('wire') $l(\tilde{e})$, going from $l(\tilde{v}_1)$ to $l(\tilde{v}_2)$, and such that the distance of any two distinct wires is always larger than a lattice spacing, except possibly in the vicinity of a node. In particular the wire network never overlaps, and can only intersect at the nodes; this is always possible in three or more dimensions. Finally we set $J_{ij} = +1$ for all but the following special links for which $J_{ij} = -1$:

(a) one link in the middle of each wire which is not a loop (we shall call these links 'valves'), and

(b) two links for each lattice site on the network which is not a node, chosen so that all four transverse plaquettes at this site (i.e. plaquettes touching but not containing any link of the network) are frustrated. This is easier to explain with a picture (see figure 2).

† See for instance Toulouse (1979) and references therein.

‡ It is currently believed that no algorithm with polynomially bounded time-requirement can solve an NP-complete problem. Proving (or disproving) this statement remains one of the main challenges for computer scientists and mathematicians.

§ For a detailed discussion and listing of NP-complete problems see Garey and Johnson (1979).

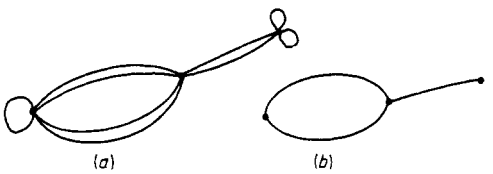

Figure 1. (*a*) a graph G and (*b*) the corresponding $\tilde{G}$ obtained by doubling each edge, and then adding three loops.

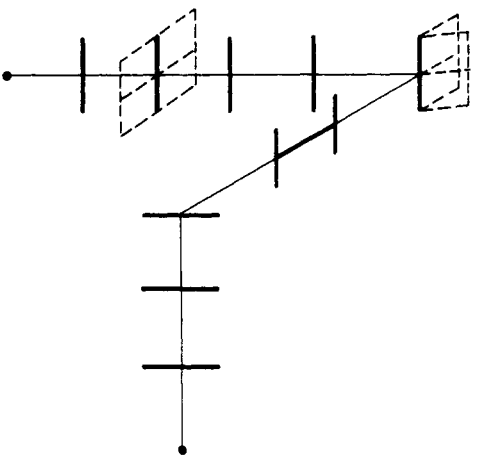

Figure 2. The distribution of coupling constants in the vicinity of a wire: links for which $J_{uj} = -1$ are drawn in thick ink. They are chosen so as to make all four transverse plaquettes, at each site on the wire other than the two nodes, frustrated (transverse plaquettes are drawn with broken lines at two typical points on the wire). The valve—the single negative link along the wire—is absent if the wire is a loop.

The virtue of this construction is that, as we will now argue, in order to minimise the energy (1), one needs only to choose an optimal configuration of spins on the nodes. Indeed, let $\bar{\sigma}_{l(\tilde{v})}$ be a given, fixed configuration of spins on the nodes. Extend this to a complete spin configuration by setting all spins outside the network equal to +1, and letting spins propagate from the nodes along the network without changing sign except possibly at a valve (see figure 3). The energy of this configuration is

$$E = -3V + N + 2n(\bar{\sigma}_{l(\tilde{v})}) \tag{3}$$

where V is the total number of lattice sites, N the number of plaquettes transverse to the network, and $n(\bar{\sigma}_{l(\tilde{v})})$ the number of wires: $l(\tilde{e}) = (l(\tilde{v}_1), l(\tilde{v}_2))$ other than loops, for which:

$$\bar{\sigma}_{l(\tilde{v}_1)}\bar{\sigma}_{l(\tilde{v}_2)} = +1.$$

Now since the N transverse plaquettes and the $n(\bar{\sigma}_{l(\tilde{v})})$ wires must each have at least one violated link (a link is violated if $J_{ij}\sigma_i\sigma_j = -1$), and since no link can be shared by more than two transverse plaquettes, or a single wire at a time, we conclude that the energy of any configuration with $\sigma_{l(\tilde{v})} = \bar{\sigma}_{l(\tilde{v})}$ is larger than or equal to (3). Thus, finally, to minimise the energy, one needs only to minimise $n(\sigma_{l(\tilde{v})})$, which is equivalent to minimising the cost function (2) for the graph G. This completes the proof of NP-completeness for the three-dimensional frustration model. We conclude with a series of remarks:

(a) The problem of finding the ground state of the frustration model remains NP-complete, even if the size of the lattice in one direction is kept fixed (and equal, say, to 4 or 5), since the embedding of any graph $\tilde{G}$ as described in the proof can still be effected. It might thus be amusing to search for a spin glass phase in this essentially two-dimensional (albeit non-planar) model.

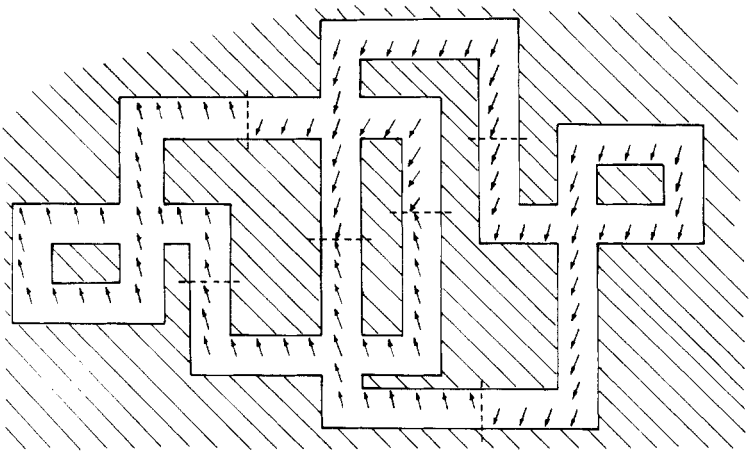

Figure 3. A two-dimensional cross-section of an optimal configuration, for a fixed configuration of spins on the nodes. The shaded region is a sea of up-spins. Spins are explicitly drawn on the network; they can only flip sign at the valves (broken transverse lines). The role of the construction of figure 2 was to insulate the wires from the surrounding sea of up spins, in the sense that the transverse energy is independent of the spin configuration on the network.

(b) Our proof can also be trivially extended both to the frustration model in higher dimensions, and to the Sherrington–Kirkpatrick model even if couplings are restricted to be 0 or -1.

(c) More work needs to be done to clarify the analogy between spin glasses and NP-complete problems. Measure considerations are particularly important: if, for instance, the algorithmic complexity of a model is relevant to its statistical mechanics, it should be unchanged by the exclusion of a set of instances whose measure, in the thermodynamic limit, vanishes.

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References

Barahona F 1982 *J. Phys. A: Math. Gen.* **15** 3241

Barahona F, Maynard R, Rammal R and Uhry J P 1982 *J. Phys. A: Math. Gen.* **15** 673

Bieche I, Maynard R, Rammal R and Uhry J P 1980 *J. Phys. A: Math. Gen.* **13** 2553

Binder K 1980 in *Fundamental Problems in Statistical Mechanics V* ed E G D Cohen (Amsterdam: North-Holland)

Garey M and Johnson D 1979 *Computers and Intractability* (New York: Freeman)

Mézard M, Parisi G, Sourlas N, Toulouse G and Virasoro M 1084a *Phys. Rev. Lett.* **52** 1156

—— 1984b *J. Physique* **45** 843

Kirkpatrick S, Gelatt C D and Vecchi M P 1983 *Science* vol 220 number 4598, 671

Kirkpatrick S and Toulouse G 1984 in preparation

Toulouse G 1979 in *Modern Trends in the Theory of Condensed Matter (Kapacz Proc.)* ed A Pekalski and J Przystawa (Berlin: Springer)

Yannakakis M 1978 *Node-and-Edge Deletion, NP-complete Problems in Proc. 10th Annual ACM Symp. on Theory of Computing* (New York: Association for Computing Machinery) p 253