Intractable Computations without Local Minima

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An *NP*-complete problem which is not a spin-glass is exhibited. The *NP*-complete problem 3-satisfiability is also embedded into a continuous analog system with no hills in the energy landscape obstructing solution of the problem. There is, however, a large flat plateau. This shows how sculpting of the energy surfaces of continuous analog systems to remove hills may fail to aid solution of embedded combinatorial optimization problems.

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Hard combinatorial optimization problems have been related to spin-glasses. Finding the ground state of a spin-glass is an *NP*-complete problem.[1] *NP*-complete problems,[2] such as the traveling salesman problem,[3] graph partitioning,[4] and graph coloring[5] have been studied as spin-glasses. Simulated annealing, an algorithm arising from spin-glass considerations, has been applied to optimization problems.[6] The free energy landscape of spin-glasses contains many metastable states,[7] and also an infinite hierarchy[8] of thermodynamic equilibrium states, i.e., valleys infinitely deep in the limit of infinite system size. This ultrametricity seems characteristic of many combinatorial optimization problems as well[9] and may be exploitable by heuristics.[10]

Because of the multiplicity of equilibrium states, spin-glasses relax very slowly towards their ground state. This has suggested[11] that *NP*-complete problems may be computationally hard because they are spin-glasses.[12] In this paper I exhibit an *NP*-complete problem which has only one equilibrium state, at least at zero temperature. Its energy landscape is like a putting green in the game of golf[13]; that is, broad and flat with one hole. This occurs because all the frustrated loops involve a certain unique spin, so that if it is removed there is no frustration in the system. This construction shows that computational intractability does not imply spin-glass nature.

To consider a combinatorial optimization problem as a spin-glass, one must choose a topology, i.e., specify which configurations are neighbors. I require the set of neighbors to be listable in polynomial time. There is, however, no canonical choice. Under different topologies the same optimization problem can correspond to several thermal systems.[14] These can also be regarded as generalized Monte Carlo algorithms. I define the temperature as determining the probability to flip, rather than a single spin, a cluster of spins simultaneously. This definition is crucial to my result. My clusters are defined with use of a generalization of Kempe chaining.[15]

To generate heuristics, physicists have suggested embedding hard discrete problems into continuous analog systems whose ground state determines the optimum solution.[16] Cleverly chosen analog systems fall into poor local optima more rarely than the original discrete system. As a version of the discrete system with some constraints removed, the continuous system has more degrees of freedom, and thus more directions to decrease from any given point. Perhaps more importantly, the constraints on the discrete system prevent free propagation of forces. The continuous system can develop a collective action preventing small parts of the system from getting stuck independently of the rest, and forcing local optima to have a more global nature.[16] Many authors have reported that continuous embeddings lead to useful algorithms.[17] Such embeddings have suggested hardwiring of a special computer as these neural net circuits also relax rapidly, in parallel. It still seems dubious, however, whether these circuits can beat digital algorithms.[18] By embedding discrete problems one also gains the ability to compute a gradient direction in the differentiable systems. This has been applied in learning networks.[19]

Ideally one would embed a hard combinatorial optimization problem into a system where simply proceeding downhill in energy yields the optimal solution. I embed 3-satisfiability (3-SAT), an *NP*-complete problem,[2,20] into a potential with no hills. I present both a discrete and a continuous embedding. In both cases a path leads to the optimum without ever increasing the energy. The potential, however, is a golf-course potential—flat but for a hole at the global optimum. The only known way to find the hole is exhaustive search. I view this interesting manifestation of intractability as the likely end result of sculpting energy landscapes to remove local minima.

NP is a broad class of decision problems, i.e., problems with answer yes or no.[21] Problem B is *mapped* into problem A if for every instance b of B we can construct in polynomial time an instance a of A such that a is yes if and only if b is yes. A is then at least as hard as B since, given a p-time algorithm for A, we map b into a and solve it. If every problem in *NP* can be mapped into A then A is *NP-complete.* Cook proved that 3-SAT is *NP*-complete.[20] Thus, by composition of maps, any problem C into which I map 3-SAT is *NP*-complete.

An instance of 3-SAT is comprised of a collection of Boolean variables and a collection of clauses. Each clause takes the form (a or b or d), where a, b, and d represent three of the boolean variables, or their negations. A *satisfying truth assignment* is a particular choice of values for the variables such that every clause is true. The problem of 3-SAT is, given an instance, is there a satisfying truth assignment?

I now proceed in three steps. First I map 3-SAT into graph three-coloring to produce an *NP*-complete problem. Second I define an energy function taking the same value ε at configurations corresponding to nonsatisfying truth assignments, and energy 0 at satisfying truth assignments. Finally I define a topology, i.e., a set of transformations from a configuration to neighboring configurations. My topology contains only transforms which do not increase the energy, and yet allows exhaustive search of the energy ε plateau looking for energy 0 holes.

Let $C=\{c_1,\ldots,c_p\}$ be any set of three-clauses in the variables $\{v_1,\ldots,v_n\}$ given as an instance of 3-SAT. Let $c_i=(a_i \vee b_i \vee d_i)$. I describe a graph G, three-colorable[22] if and only if C is satisfiable.[23]. The set N of nodes of G is

$$N=\{u_1,u_2,\}\cup\{v_i,\bar{v}_i:1\le i\le n\}\cup\{w_{ij}:1\le i\le p,1\le j\le 5\}.$$

The set E of edges is

$$E=\{(u_1,u_2),(u_1,u_2)\}\cup\{(v_i,\bar{v}_i):1\le i\le n\}\cup\{(u_2,v_i),(u_2,\bar{v}_i):1\le i\le n\}$$
$$\cup\{(a_i,w_{i1}),(b_i,w_{i2}),(d_i,w_{i4}):1\le i\le p\}\cup\{(w_{i1},w_{i2}),(w_{i1},w_{i4}),(w_{i2},w_{i4}):1\le i\le p\}$$
$$\cup\{(w_{i3},w_{i5}),(w_{i3},u_1),(w_{i5},u_1),(w_{i4},w_{i5}):1\le i\le p\}.$$

G is fabricated from subgraphs H_i shown in Fig. 1, consisting of w_{i1} w_{i2}, w_{i3}, w_{i4}, w_{i5}, and u_1 (common to all the H_i), and the variable nodes a_i, b_i, d_i. The subgraphs H_i correspond to the clauses c_i in the instance of 3-SAT, and the variable nodes a_i, b_i, d_i take values among the $\{v_i,\bar{v}_i\}$ accordingly. I describe nodes a_i, b_i, d_i as *inputs* of the subgraph H_i, and u_1 as its *output*.

To each node j of G associate a spin (or color) variable $s(j)$ taking one of three values: $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, or $\hat{\mathbf{z}}$. Define a *conflict* to be an edge connecting two nodes with like spin. Now map any truth assignment to a partial spin assignment by $\mathbf{s}(v_i)=\hat{\mathbf{x}}$ if v_i is true and $\hat{\mathbf{y}}$ if v_i is false. Note (by inspection) that the H subgraph acts as a clause in that any assignment of $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ spins to its three inputs extends without conflict so that $s(u_1)=\hat{\mathbf{x}}$ if and only if at least one input spin is $\hat{\mathbf{x}}$. Thus any satisfying truth assignment can be extended to a three-coloring of the graph, and conversely any three-coloring is seen to yield a satisfying truth assignment.[23]

I now construct the golf course. The point is that excising vertex u_1 removes frustration from the graph. To exploit this I allow $\mathbf{s}(u_1)$ to take in addition a fourth value, $\hat{\mathbf{e}}$. Picture these spins as unit vectors pointing along one of four orthogonal axes, and define the usual dot product: $\hat{\mathbf{x}}\cdot\hat{\mathbf{x}}=\hat{\mathbf{y}}\cdot\hat{\mathbf{y}}=\hat{\mathbf{z}}\cdot\hat{\mathbf{z}}=\hat{\mathbf{e}}\cdot\hat{\mathbf{e}}=1$, $\hat{\mathbf{x}}\cdot\hat{\mathbf{y}}=$all other dot products $=0$. Define for this system the energy:

$$E=\sum_{\text{edges}(j,k)}\mathbf{s}(j)\cdot\mathbf{s}(k)+\varepsilon\hat{\mathbf{e}}\cdot\mathbf{s}(u_1). \qquad (1)$$

Choose $\varepsilon<1$, say $\frac{1}{2}$. The ground-state energy is zero if and only if the original instance of 3-SAT is satisfiable. Every nonsatisfying truth assignment maps to an assignment of $\mathbf{s}(v_i)$ extendable to a spin configuration with $\mathbf{s}(u_1)=\hat{\mathbf{e}}$, no conflicts, and energy ε.

Call two nodes $\hat{\mathbf{x}}$-$\hat{\mathbf{y}}$ *connected* if a chain of nodes connects them along which the spins alternate between $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ (including the two nodes themselves). I describe this as an $\hat{\mathbf{x}}$-$\hat{\mathbf{y}}$ chain. Define a *contiguous x-y transform at site i* to be the replacement of the spin $\hat{\mathbf{x}}$ at site i by $\hat{\mathbf{y}}$ together with the simultaneous interchange $\hat{\mathbf{x}}\leftrightarrow\hat{\mathbf{y}}$ of the spin of all nodes which are $\hat{\mathbf{x}}$-$\hat{\mathbf{y}}$ connected to i. Figure 2 shows an example of the effect of such a transform. The effect of this transform can be computed in time bounded by N^2, if there are N nodes in the graph.[24]

I take as transform set the contiguous a-b transforms, with a and b taking any values in $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$, $\hat{\mathbf{e}}$, except that I allow only $\mathbf{s}(u_1)$ to take the value $\hat{\mathbf{e}}$. There are $2N+1$ such transforms. No contiguous transform ever changes

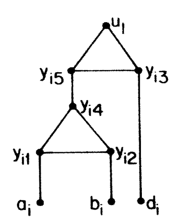

FIG. 1. The subgraph H_i.

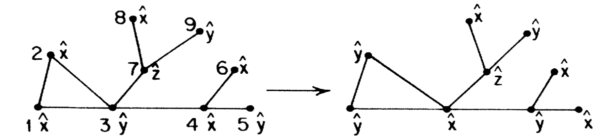

FIG. 2. The effect of a contiguous $\hat{\mathbf{y}}$-$\hat{\mathbf{x}}$ transform at node 3. Nodes 6,7,8,9 are unaffected. The total number of conflicts is lowered by 1.

any nonconflict edge to a conflict[24]; thus only the transform rotating $\mathbf{s}(u_1)$ to $\hat{\mathbf{e}}$ can increase the energy.

Theorem 1.— There exists a sequence of contiguous transforms which render any configuration with $\mathbf{s}(u_1) = \hat{\mathbf{e}}$ to the ground state.

The proof, presented in detail elsewhere,[24] is by exhaustive construction. If $\mathbf{s}(u_1) = \hat{\mathbf{e}}$, transforms do not propagate through u_1 and chains connect different H subgraphs only through their inputs. I use preparatory contiguous transforms to break dangerous chains and thus deal with one subgraph at a time. I first exhibit a sequence of contiguous transforms which render any initial state to a configuration with no conflicts. All inputs have spin either $\hat{\mathbf{x}}$ or $\hat{\mathbf{y}}$, and all such configurations correspond to truth assignments.

I must now show that we can slide freely on this plateau of energy ε. I can arrange each H_i to have $\hat{\mathbf{z}}$ strategically located so that no input is $\hat{\mathbf{x}}$-$\hat{\mathbf{y}}$ connected to another. This allows one to transform freely any v_i without affecting any other v_j or $\bar{v}_j$ except $\bar{v}_i$. This means that I can change the $\mathbf{s}(v_k)$ to any existing satisfying truth assignment. I may then transform $\mathbf{s}(u_1)$ to $\hat{\mathbf{x}}$, and reach the zero-energy ground state.

Corollary.— Any configuration can reach the ground state by a path with energy cost $\leq \varepsilon$. There are no deep valleys.

To remove all metastable states from the system, I slightly modify the energy and the transformation set, without disturbing the property of *NP*-completeness. I leave the details for a longer treatment,[24] where I prove the following theorem.

Theorem 2.— With modified transformation set, any configuration can be brought to the ground state without an increase in the modified energy.

I next extend this construction to a continuous embedding. Instead of spins, assign to each vertex j of the graph G a unit vector $\mathbf{r}(j) \in \mathscr{R}^4$. Every vector except that associated with u_1 lies in an $\mathscr{R}^3$ spanned by three orthonormal basis vectors $\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}}$. $r(u_1)$ lies in the $\hat{\mathbf{x}}$-$\hat{\mathbf{e}}$ plane, where $\hat{e}$ is a fourth orthonormal basis vector. The graph is modified to G' by the addition of edges connecting w_{i2} to w_{i3}. Define energy as

$$E = \sum_{\text{edges}(j,k)} [r(j)\cdot r(k)]^2 + \varepsilon[\hat{e}\cdot r(u_1)]^2. \tag{2}$$

I need to choose $\varepsilon \ll 1$. The dot products now represent ordinary inner products.

I describe a starting point which is the ground state if the 3-SAT instance is unsatisfiable. Let $r(u_1) = \hat{e}$, $r(u_2) = \hat{z}$; $\forall i$, $r(v_i) = \hat{x}$, $r(\bar{v}_i) = \hat{y}$, and now trivially choose the $r(y_i)$ to fill in so that there are no conflicts, i.e., edges connecting vertices with nonorthogonal vectors. The energy of this configuration is ε. Configurations with smaller energy have no edge containing energy greater than ε. Elsewhere[25] I showed that G' could be orthogonalized[26] if and only if it could be colored. Similar analysis shows that, for unsatisfiable instances no configuration has energy less than ε.[24]

I define a *contiguous rotation about $\hat{a}$ by angle θ* to be a rotation of one vector about axis $\hat{a}$ together with the simultaneous rotation of all neighbors, together with rotation of their neighbors except that chains do not propagate through unaffected vectors (in this case $\hat{a}$). Contiguous rotations preserve orthogonality. Proof similar to that of theorem 1 now establishes[24] the following theorem.

Theorem 3.— The configuration described is the ground state whenever the instance is unsatisfiable, and can relax to the ground state without increasing the energy otherwise.

I do not know whether other local minima exist. This is unimportant for purposes of using a continuous embedding to solve a hard problem, as one may specify initial conditions for the system.

I have given an *NP*-complete problem and a reasonable topology such that a path along which energy never increases leads from any configuration to the ground state.[27] To accomplish this I constructed an *NP*-complete problem with frustration involving only a single vertex. This demonstrates that not every *NP*-complete problem can be regarded as a spin-glass. This mapping does not appear to help solve 3-SAT, which was put into a golf course where no clue points the way towards the ground state. My analysis has all been at zero temperature. At finite temperature, the hole in the golf course will wash out. I believe it will remain true that there is one equilibrium state.

This example raises the following question.[28] In the thermodynamic limit, spin-glasses have many stable states. Does a path connect these equilibrium states which only rises finitely high in energy, but is so narrow as to require exponential time for finite temperature annealing to discover?

I have also mapped an *NP*-complete problem into a continuous system with a distinguished state which is either the ground state, or able to reach it without increasing the energy. In short, if the system can evolve so as to lower the energy, then the answer to my problem is yes. I believe I found the generic consequence of embedding hard combinatorial problems into continuous media without local minima; namely, such systems will stick on table tops, unable to roll because the energy landscape is flat.

I do not wish to discourage continuous embeddings. I expect that they may be useful for heuristics if one does not attempt to remove all local valleys. I regard the extent of the energy surface crafting I was able to accomplish as surprising. Finally my work indicates that embedding discrete problems in continuous systems can suggest useful topologies for the original problem.

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[1]F. Barahona, J. Phys. A **15**, 3241 (1982); C. P. Bachas, J. Phys. A **17**, L709 (1984).

[2]See, e.g., M. R. Garey and D. S. Johnson, *Computers and Intractibility: A Guide to the Theory of NP-completeness* (W. H. Freeman, New York, 1979).

[3]S. Kirkpatrick, C. D. Gelatt, Jr., and M. P. Vecchi, Science **220**, 671 (1983); S. Kirkpatrick, and G. Toulouse, J. Phys. (Paris) **46**, 1277 (1985); G. Baskaran, Y. Fu, and P. W. Anderson, to be published.

[4]Y. Fu and P. W. Anderson, to be published; Kirkpatrick, Gelatt, and Vecchi, Ref. 3.

[5]J. P. Bouchaud and P. Le Doussal, to be published.

[6]See Kirkpatrick, Gelatt, and Vecchi, Ref. 3.

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[9]See Refs. 4 and 5.

[10]E. B. Baum, to be published.

[11]See Bachas, Ref. 1.

[12]It is widely believed that no polynomial-time (p-time) algorithm can exist for any NP-complete problem. For many NP-complete problems, however, known heuristics will almost always solve a randomly chosen instance, failing only on a set of measure zero. It may be that every problem in NP will be solvable in p time in the average case. If so, physicist's methods, which ignore sets of measure zero, are unlikely to cast light on why NP-complete problems are intractable.

[13]The term "gold" seems to have first been applied to potentials of this type by T. J. Sejnowski and G. E. Hinton, in *Vision, Brain, and Computer,* edited by M. A. Arbib and A. R. Hanson (MIT Press, Cambridge, MA, 1986).

[14]Proper choice of topology is far more important than choice of annealing schedule in practical heuristics. See, for example, Ref. 10.

[15]A. B. Kempe, Nature **20**, 275 (1979), and **21**, 399 (1880), cited in T. L. Staaty and P. C. Kainen, *The Four Color Problem* (McGraw-Hill, New York, 1977).

[16]J. J. Hopfield and D. W. Tank, Biol. Cybernetics **52**, 141 (1985); E. B. Baum, unpublished, and address at Workshop on Neural Networks Models for Computing, 1 May 1985, Santa Barbara, California (unpublished); E. B. Baum, to be published.

[17]J. J. Hopfield and D. W. Tank, Ref. 16, and IEEE Trans. Circuits Syst. (to be published); L. Jackel, private communication; W. Jeffrey and R. Rosner, Astrophys. J. (to be published); E. Mjolsness, Ph.D. dissertation, California Institute of Technology, 1985 (unpublished).

[18]Baum, Ref. 16, and to be published.

[19]D. E. Rumelhart, G. E. Hinton, and R. J. Williams in *Paralle Distributed Processing: Explorations in the Microstructure of Cognition.* edited by D. E. Rumelhart and J. L. McClelland (MIT Press, Cambridge, MA, 1986), Vol. 1.

[20]For definition of NP see, e.g., Ref. 2. To any optimization problem corresponds a decision problem of form, "Is the optimum value greater than X?" (given any X). A p-time algorithm for the optimization problem extends to a p-time algorithm for the decision problem, and the converse is usually true as well. See Ref. 2.

[21]S. A. Cook in *Proceedings of the Third Annual ACM Symposium on the Theory of Computing* (Association for Computing Machinery, New York, 1971).

[22]A graph is three-colored if one of three colors is assigned to each node so that no edge connects two like colored nodes.

[23]M. R. Garey, D. S. Johnson, and L. Stockmeyer, Theoret. Comput. Sci. 1, 237 (1976).

[24]E. B. Baum, to be published.

[25]E. B. Baum, to be published.

[26]A graph is orthogonalized when it has no conflicts.

[27]My construction suggests the following simple energy which, although horribly nonlocal and unnatural, has the golf-course property. Given any NP-complete optimization problem with natural energy E, take $E' = \theta(E - X)$ for X a constant and θ the Heaviside function. The problem of finding the minimum of E' will remain NP-complete for appropriate X, and has a golf-course landscape. I am indebted to D. A. Huse for this remark.

[28]J. J. Hopfield, private communication.