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The Ising Model Is NP-Complete

By Barry A. Cipra

Enormous herds of naked souls I saw,
lamenting till their eyes were burned of tears;
they seemed condemned by an unequal law,

for some were stretched supine upon the ground,
some squatted with their arms about themselves,
and others without pause roamed round and round.
—*The Inferno, Canto XIV* (Ciardi translation)

In 1925, the German physicist Ernst Ising introduced a simple mathematical model of phase transitions, the abrupt changes of state that occur, for example, when water freezes or a cooling lump of iron becomes magnetic. In the 75 years since, the Ising model has been analyzed, generalized, and computerized—but never, except in special cases, solved. Researchers managed to get exact answers for physically unrealistic, two-dimensional systems, but have never been able to make the leap out of the plane.

There could be a good reason: The Ising model, in its full, nonplanar glory, is NP-complete.

The complexity result was announced in May by Sorin Istrail, a theoretical computer scientist at Sandia National Laboratories (who subsequently joined Celera Genomics in Rockville, Maryland). Extending earlier work of Francisco Barahona of the University of Chile, Istrail showed that essentially all versions of the Ising model are computationally intractable when the setting is three-dimensional.

Moreover, the new results show that the computational barrier lies not so much in the extra dimension as in the nonplanarity of an essential underlying graph—which explains why physicists have been stymied even in certain two-dimensional generalizations of the Ising model. Although it doesn't completely put the kibosh on the search for exact solutions (for one thing, the P-versus-NP question is still famously open), Istrail's work sheds new light on the likely limitations of techniques that, because of their success in the plane, had theorists chasing wild geese into the third dimension.

Ground States

I turned like one who cannot wait to see
the thing he dreads, and who, in sudden fright,
runs while he looks, his curiosity

competing with his terror—and at my back
I saw a figure that came running toward us
across the ridge, a Demon huge and black.
—*The Inferno, Canto XXI*

The Ising model itself can be formulated in any dimension. The model is conveniently described in graph-theoretic terms, in which vertices represent atoms in a crystal and edges represent bonds between adjacent atoms. In the classic model, the graph is the standard "square" lattice in one, two, or three dimensions, so that each atom has two, four, or six "nearest neighbors," respectively. There are two key sets of variables. First, each vertex i can be in one of two states, usually written as $\sigma_i = \pm 1$. Second, each edge has an assigned coupling constant, usually written as J_{ij}, where i and j are the two vertices.

When neighboring vertices i and j are in states σ_i and σ_j, the interaction between them contributes an amount $-J_{ij}\sigma_i\sigma_j$ to the total energy H (the Hamiltonian) of the system, so that

$$H(\sigma) = -\sum_{(i,j)} J_{ij}\sigma_i\sigma_j,$$

where the sum is taken over all pairs of neighbors (i.e., edges of the graph). If J_{ij} is positive, then having neighbors in the same state ($\sigma_i = \sigma_j$) decreases the total energy. In particular, if all the coupling constants are positive, the system has a clear-cut lowest-energy configuration, in which all vertices are in the same state (either all +1 or all –1). But if the coupling constants are a mix of positive and negative numbers—as they are for the class of Ising models known as spin glasses—finding the "ground state" can be a frustrating experience.

That's where computational complexity comes in. If a graph has N vertices, and one of two values, say $+J$ or $-J$, is assigned to each edge, then finding the ground state can clearly be done by computing $H(\sigma)$ for all 2^N possible σ's, much as the traveling salesman problem can be solved by testing all possible routes among N cities. The spin glass Ising model is thus clearly in the class NP. But is it NP-complete?

For planar graphs, the answer is No. There is, in fact, a polynomial-time algorithm for computing what's called the partition function, which summarizes the number of states at each possible energy level, from lowest to highest.

The central premise of statistical physics is that the probability of finding the system in state σ is proportional to $e^{-H(\sigma)/kT}$, where k is Boltzmann's constant and T is the (absolute) temperature. This focuses attention on the expression

$$Z(T) = \sum_\sigma e^{-H(\sigma)/kT},$$

which physicists call the partition function. A phase transition, more or less by definition, is a singularity in the limit of $\log(Z(T)/N$ as N, the size of the lattice, goes to infinity. The goal of the Ising model is to understand how local interactions can give rise to long-range correlations.

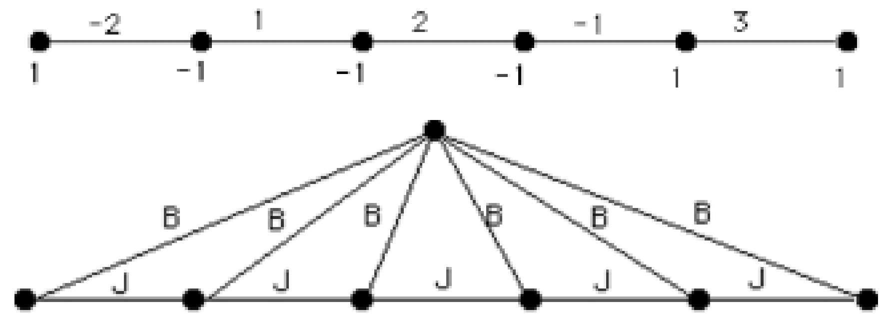

Figure 1. *(a) States and coupling constants for a one-dimensional lattice. The ground state is easy to find. (b) One-dimensional Ising model with an external magnetic field.*

The computation of the partition function is essentially trivial in the one-dimensional case (see Figure 1a). It becomes a little more interesting with the addition of an "external field," which can be viewed as an extra vertex with edges to all the other vertices (Figure 1b). This was the subject of Ising's original work, which constituted his PhD dissertation. Ising solved the "ferromagnetic" case of the model, in which all the coupling constants are J (for nearest neighbors) or B (for the external field).

Ising's one-dimensional ferromagnet fails to exhibit a phase transition—the limit of the partition function is a nice, smooth function of T. But a phase transition *is* seen in the two-dimensional model. In 1944, Norwegian chemist (and later Nobel laureate) Lars Onsager obtained a closed-form solution to the ferromagnetic model in the no-external-field case. Over the next two decades, Onsager's breakthrough was refined and extended to a complete solution of the Ising model for any planar graph. But three-dimensional models, and the planar case with an external field, continued to elude theorists' grasp.

Nonplanar Key

I stood now where the souls of the last class
(with fear my verses tell it) were covered wholly;
they shone below the ice like straws of glass.

Some lie stretched out; others are fixed in place
upright, some on their heads, some on their soles;
another, like a bow, bends foot to face.
—The Inferno, Canto XXXIV

In 1982, Barahona uncovered the cause of the problem: The three-dimensional spin glass model for the standard square lattice, and the planar model with an external field, are NP-complete. More precisely, for the three-dimensional result, Barahona showed that a graph-theoretic problem known to be NP-complete—the task of finding a maximum set of independent edges (i.e., with no vertices in common) in a graph for which each vertex has degree 3—can be reduced to the problem of finding a ground state for the three-value coupling constant ($J_{ij} = -1, 0,$ or 1) on a cubic grid. For the planar problem, he showed that computing the minimum value of $H(\sigma) = \sum_{ij}\sigma_i\sigma_j + \sum_i \sigma_i$—in effect, the anti-ferromagnetic case with an external magnetic field—is tantamount to solving the NP-complete problem of finding the largest set of vertices in a planar, degree-3 graph with no two vertices in the set connected by an edge.

Istrail has shown that the essential ingredient in the NP-completeness of the Ising model is nonplanarity. This criterion includes two-dimensional models with next-nearest-neighbor interactions in addition to the nearest-neighbor kind, which researchers had found as vexing to solve as their three-dimensional cousins. Every nonplanar lattice in two or three dimensions, Istrail shows, contains a subdivision of an infinite graph he calls the "basic Kuratowskian" (see Figure 2). He then shows that, for the basic Kuratowskian with weights –1, 0, and 1 assigned to the edges, the problem of computing a minimum-weight "cut" (i.e., set of edges joining vertices in opposite states) is NP-complete.

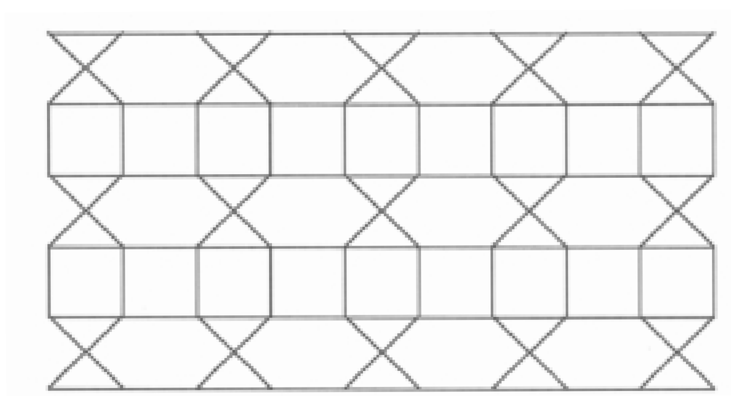

Figure 2. *The "basic Kuratowskian" is a nonplanar, two-dimensional mix of bonds between nearest and next-nearest neighbors.*

It's easy to see that $H(\sigma) = -\sum_{ij\in E^+} J_{ij} - \sum_{ij\in E^-} J_{ij} = -\sum_{ij\in E} J_{ij} + 2\sum_{ij\in E^-} J_{ij}$, where E^+ is the set of edges connecting vertices i and j in the same state (i.e., with $\sigma_i\sigma_j = 1$), E^- is the cut, and E is the set of *all* edges. This shows that computing the ground state boils down to finding a minimum-weight cut and, consequently, that computation for the Ising model with coupling constants –1, 0, and 1 is NP-complete.

Related complexity arguments take care of various cases with just two coupling constants. (When both are positive, the intractable problem is computing the *highest* energy state. Either way, computing the partition function is NP-complete.) Overall, the results show that the general, spin glass Ising model is (barring a P = NP surprise) exactly solvable only in planar cases.

NP-completeness, however, doesn't mean things are completely hopeless. The complexity result bars algorithms only from solving *all* instances of the problem in polynomial time. Typical spin glasses are random mixtures of coupling constants. It's entirely possible that the *average* spin glass problem can be solved in polynomial time, even though the worst case may be exponential. Finally, Ising's original, ferromagnetic model, in which all coupling constants are equal (and positive), is a special case, so it too might yet fall within polynomial time. Only time—but possibly an agonizing, exponential amount of it—will tell.

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