AN APPLICATION OF COMBINATORIAL OPTIMIZATION TO STATISTICAL PHYSICS AND CIRCUIT LAYOUT DESIGN

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We study the problem of finding ground states of spin glasses with exterior magnetic field, and the problem of minimizing the number of vias (holes on a printed circuit board, or contacts on a chip) subject to pin preassignments and layer preferences. The former problem comes up in solid-state physics, and the latter in very-large-scale-integrated (VLSI) circuit design and in printed circuit board design. Both problems can be reduced to the max-cut problem in graphs. Based on a partial characterization of the cut polytope, we design a cutting plane algorithm and report on computational experience with it. Our method has been used to solve max-cut problems on graphs with up to 1,600 nodes.

Operations research, due to its historical development, is closely linked to the fields of economics, management science and engineering. However, since the models developed by operations researchers and mathematical programmers are abstract mathematical models, they quite frequently apply to real-world situations other than those from which they arose. Unfortunately, OR professionals are often unaware of these potential applications, and, conversely, professionals in other fields do not know about the models and solution methods developed by operations researchers and mathematical programmers, or about the present state of the art of our discipline. This lack of mutual awareness is due mainly to insufficient communication on both sides, and has led to many reinventions and rediscoveries of models, theorems and algorithms. In this article, we will report on several such cases in the field of physics and VLSI circuit design.

Cuts (in graphs and digraphs) have played an important role in combinatorial optimization since the early days of network flow theory. The efficient solvability of minimum-cut problems follows from the work of Ford and Fulkerson, while the max-cut problem was among the first problems to be shown to be NP-complete (Karp 1972). In this paper, we will consider the latter problem. In can be stated as follows. Given an undirected graph $G = (V, E)$ with edge weights $c_{ij} \in \mathbb{R}$ for all $ij \in E$, find a cut $\delta(W)$ in G such that $c(\delta(W)) := \sum_{ij \in \delta(W)} c_{ij}$ is as large as possible. For any subset $W \subseteq V$, $\delta(W)$ denotes the set of edges $ij \in E$ (the cut associated with W) with $i \in W$ and $j \in V \setminus W$. If all weights c_{ij} are nonpositive, then the max-cut problem is trivial, and also a nonempty cut of maximum weight can be found in polynomial time using any good min-cut algorithm. Orlova and Dorfman (1972) and Hadlock (1975) independently found a method that transforms the max-cut problem in planar graphs into a so-called T-join problem (using the duality theory of planar graphs) for which a beautiful polynomial time solution method had been invented by Edmonds and Johnson (1973). Their algorithm is based on a combination of shortest-path and matching algorithms. Barahona (1983) showed the max-cut problem to be polynomially solvable for graphs not contractible to K_5 (these graphs include planar graphs); Grötschel and Pulleyblank (1981) did likewise for the case $c_{ij} \geq 0$ for all ij, for weakly bipartite graphs. The latter two results are based on polyhedral combinatorics; this theory also forms the background of the algorithm we will present and discuss in Sections 4 and 5. On the negative side, Barahona (1983) proved that for "almost planar" graphs, i.e., graphs G that contain a node v such that $G - v$ is planar, the max-cut problem is NP-complete.

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Let us now describe two applications in which the max-cut problem arises in a rather natural way. A very interesting problem in statistical physics (within the theory of magnetism) is the determination of ground states of spin glasses, and the study of their properties; for details see Section 1. Some models of spin glasses, in particular, (according to Kinzel and Binder 1984) the most successful model introduced by Edwards and Anderson, which is based on the Ising model, led to formulations of the ground state problem that are optimization problems in ± 1-variables. In fact, an easy transformation shows that these problems can be reduced to max-cut problems.

The reduction of Orlova and Dorfman, and of Hadlock, has been rediscovered in the field of physics. Toulouse (1977) introduced concepts such as curved plaquettes, frustrated contours, and so forth, that correspond to notions such as odd nodes, and odd cuts used by Edmonds and Johnson. Based on Toulouse's observation, Bieche et al. (1980) realized that a ground state (in two dimensions) can be found by means of matching techniques.

Barahona et al. (1982) described a primal version of the Edmonds-Johnson algorithm. A primal algorithm is especially useful in performing postoptimality analysis—in this case, to study the existence of long distance order. This algorithm has been heavily used; as far as we know, it can successfully handle spin glass problems on grids of size 50×50 (see Angles d'Auriac and Maynard 1984).

Working on some problems in very-large-scale-integrated (VLSI) circuit design, we recently found that a rather parallel development has occurred in this field. One important problem here is to reduce the number of vias (holes in a printed circuit board, contacts on a chip). Over the years, many heuristics for this problem have been proposed in the electrical engineering and computer science literature, and researchers believed the problem to be NP-complete. Then Pinter (1984) and Chen, Kajitani and Chan (1983) found independently that the 2-layer problem (without preassignments and preferred layers) can be reduced to a max-cut problem in planar graphs. So again the Orlova-Dorfman-Hadlock reduction can be used to apply the Edmonds-Johnson algorithm to obtain a polynomial time algorithm. We will show in Section 2 that pin-and-wire preassignments and preferred layers can also be handled within the max-cut model, though polynomial time solvability is lost, by using an analogy to the planar spin glass problem with exterior magnetic field.

We were quite surprised to discover this (rather simple and obvious) analogy between two such unrelated problems. But this situation shows again the importance of two basic components of operations research/mathematical programming: a good knowledge of the abstract theory, and a sound familiarity with modeling techniques in various fields of application.

We learned a number of things from our study. For example, our interactions with physicists provided us with some new and interesting applications. The corresponding mathematical models (here, the max-cut problem) are well known but had not been extensively studied. The applications gave rise to interesting mathematical questions which we turned into problems concerning the polyhedral structure of cut polytopes that could be solved—at least partially. Moreover, we used the theory to derive algorithms that, we hope, can solve some of the open questions in the applications. It is our feeling that many discrete phenomena in nature have not been studied seriously from an optimization perspective. We believe that the techniques developed recently in our field—and unknown to most practitioners or scientists in other areas—could help to solve some of the new, larger, real-world problems. In particular, some areas in physics, chemistry, biology, computer science and engineering have little contact with our science, and many problems in these fields are waiting to be addressed using the techniques of operations research and mathematical programming.

1. Spin Glasses

One of the most flourishing branches of physics at present is the study of order-disorder phenomena. A central topic in this area is the investigation of properties of spin glasses. Researchers have developed a number of theories to model spin glasses and explain their behavior. Some of these theories predict contradicting phenomena. These phenomena occur in situations that are hard to realize experimentally. In order to test the theories and guide the design of experiments, researchers have developed computer models to simulate the behavior of spin glasses and then observe which phenomena occur. Some aspects studied in these models lead, in fact, to optimization problems.

A spin glass is an alloy of magnetic impurities diluted in a nonmagnetic metal. Alloys that show spin glass behavior are, for instance, CuMn; the metallic crystal AuFe; the insulator EuSrS; and the amorphous metal GdAl. One characteristic of spin glasses is a

peak in magnetic susceptibility at a certain temperature. This peak indicates a phase transition. Another phase transition may take place at very low temperature. However, it is an open question at present whether or under what conditions on the spin glass such a phase transition occurs, and what kind of order phenomena appear at low temperature.

We will now present a mathematical model of spin glasses. We assume a given spin glass that contains n magnetic impurities (atoms). Each magnetic atom i has a magnetic orientation (spin) that is represented by a 3-dimensional unit-length vector S_i. Between each pair i, j of magnetic atoms there is an interaction J_{ij} that depends on the nonmagnetic material and on the distance r_{ij} between the atoms. Several proposals in the literature model this interaction. One common feature of these models is that the absolute value of the interaction decreases rapidly with distance and that small changes of distance may result in a change of sign of the interaction. One example of such an interaction function (used frequently) is

$$J_{ij} = J(r_{ij}) = A\,\frac{\cos(Dr_{ij})}{B^3 r_{ij}^3},$$

where A, B, and D are material-dependent constants. (We remark at this point that the choice of the function J is irrelevant for our purposes. Our methods handle any function.) If atoms i and j have spins S_i and S_j, the energy interaction between i and j is given by

$$H_{ij} = J_{ij} S_i \cdot S_j,$$

where $S_i \cdot S_j$ denotes the Euclidean inner product. Given a spin configuration ω, the energy of the whole system is given by the hamiltonian,

$$H(\omega) = -\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} J_{ij} S_i \cdot S_j - h \sum_{i=1}^{n} S_i \cdot F,$$

where a unit length vector $F \in \mathbb{R}^3$ represents the orientation of an exterior magnetic field and h represents the strength of this field. The study of this hamiltonian is a major issue in statisical physics. Its difficulty has led to considering various simplifications. One such simplification is to replace the 3-dimensional vectors S_i and the magnetic field F by 1-dimensional vectors s_i, respectively f, with values $+1$ or -1 (called "Ising spins"), meaning magnetic north pole "up" and magnetic north pole "down." Such a representation is called the Ising model. There are, in fact, substances that show an up/down behavior and for which the Ising model is the "correct" model and not just a simplification.

If we consider interactions between all pairs of impurities, we can speak of a long range model. But, as just noted, the absolute value of the interaction decreases rapidly with distance. So a number of models consider only interactions between "close" impurities (so-called nearest neighbor interactions), and set to zero the interactions between impurities that are far apart. These models are called short range models. Many physicists consider short range models more realistic (see Young 1984, and Kinzel 1984). Moreover, a number of substances show short range interactions only: next-neighbor and second-next-neighbor, say. In our computational study, presented in Section 5, we will therefore investigate short range models, although our methods are equally well suited for other models.

It is customary to make further simplifications and to consider the spins regularly distributed, say on a two- or three-dimensional grid. In a typical short range model of such a grid structure, interactions are nonzero only along edges of the grid, so, for instance, in two-space, an impurity interacts only with (at most) four other impurities, its neighbors in the grid graph. Two grid models of this type have been studied intensively: the Gaussian model, where the interactions are chosen from a Gaussian distribution, and the $\pm J$-model, where interactions between impurities attain only the values $+J$ and $-J$, J a fixed positive number, according to some distribution. In a real spin glass (an alloy), the magnetic impurities are randomly distributed. Note that in the models just introduced, the spins are regularly distributed in a grid, but the interaction values are considered random.

Let Ω be the set of all the possible configurations of Ising spins on a grid. So $|\Omega| = 2^n$, if there are n spins. The behavior of such a system at temperature T is (basically) described by the so-called magnetic partition function

$$f(T) := \sum_{\omega \in \Omega} \exp\left(\frac{-H(\omega)}{KT}\right),$$

where K is the Boltzmann constant. Analytic expressions of this function are, in general, not known. But for the two-dimensional grid model with only $+J$ interactions (the so-called ferromagnetic case), Onsager derived a simple formula for f. He predicted a phase transition (at the so-called Curie temperature) that could be observed experimentally. This discovery was honored with a Nobel prize. Onsager's results, and those of many other researchers, indicate the suitability of the short range Ising model of spin glasses.

At 0°K, the spin glass system attains a minimum energy configuration. Such a configuration is called a ground state. This state can be found by minimizing the Hamiltonian associated with the system. We will now present the reduction, mentioned in the introduction, of the problem of finding a minimum energy spin configuration in the Ising model to a max-cut problem in graphs.

Suppose we have magnetic impurities 1, 2, ..., n and an exterior magnetic field, 0. We set $V = \{0, 1, \ldots, n\}$ and consider V as the node set of a graph $G = (V, E)$. For a pair i, j of impurities, G constains an edge ij if the interaction J_{ij} between i and j is nonzero. An edge $0i$ links every impurity i, $1 \leq i \leq n$, to the magnetic field 0. An Ising spin $s_i \in \{-1, +1\}$ is associated with each impurity. The Ising spin s_0 of the exterior magnetic field can be set to $+1$ without loss of generality. Let h be the strength of the magnetic field and set $J_{0i} := h$ for $i = 1, \ldots, n$; then we can write the hamiltonian of this model as a quadratic function in ± 1-variables in the following way:

$$H(\omega) = -\sum_{\substack{ij \in E \\ i,j>0}} J_{ij} s_i s_j - h \sum_{i=1}^{n} s_i$$

$$= -\sum_{ij \in E} J_{ij} s_i s_j.$$

Each spin configuration ω corresponds to a partition of V into V^+ and V^-, where $V^+ = \{i \in V \mid s_i = +1\}$ and $V^- = \{i \in V \mid s_i = -1\}$. So we can write the energy of the spin configuration ω in the form

$$H(\omega) = -\sum_{ij \in E(V^+)} J_{ij} s_i s_j$$

$$-\sum_{ij \in E(V^-)} J_{ij} s_i s_j - \sum_{ij \in \delta(V^+)} J_{ij} s_i s_j$$

$$= -\sum_{ij \in E(V^+)} J_{ij} - \sum_{ij \in E(V^-)} J_{ij} + \sum_{ij \in \delta(V^+)} J_{ij},$$

where, for each subset W of V, we define $E(W) := \{ij \in E \mid i, j \in W\}$ and, as before, $\delta(W) = \{ij \in E \mid i \in W, j \in V \setminus W\}$. Setting $C := \sum_{ij \in E} J_{ij}$, we see that

$$H(\omega) + C = 2 \sum_{ij \in \delta(V^+)} J_{ij},$$

and defining $c_{ij} := -J_{ij}$ for all $ij \in E$, we find that the problem of minimizing H is equivalent to maximizing

$$c(\delta(V^+)) := \sum_{ij \in \delta(V^+)} c_{ij}$$

over all $V^+ \subseteq V$. This problem is a weighted max-cut problem in the graph G associated with the spin glass system. Thus, finding a ground state in the Ising model of a spin glass is equivalent to finding an optimum solution of the corresponding max-cut problem.

It is impossible to survey in this article all the important properties of spin glasses and the unsolved problems related to them. Some recent papers that serve this purpose are those of Kinzel, and Young. Van Hemmen and Morgenstern (1983) give a broad overview of all theoretical and experimental issues discussed in this area. Kinzel has counted about 2,000 publications on this subject and estimates a present production rate of one paper per day on spin glasses. (Ours is the one for May 2, 1986!)

We would, however, like to mention a few open or controversial questions to acquaint the reader with this area. Some of these problems can be approached using the algorithm developed in this paper.

An important problem is the behavior of spin glasses at temperatures close to zero. Kinzel writes: "Lowering the temperature of spin glasses, one usually finds that below a rather well-defined freezing temperature T_f, the magnetic moments freeze into randomly distributed directions. One of the main problems in spin glasses is the question: Is this transition into the spin glass phase a true static phase transition or is it a gradual freezing process far from thermal equilibrium," and further, "... the two-dimensional Edwards-Anderson model describes real spin glasses qualitatively surprisingly well. However, recently more and more experiments seem to favor a true phase transition at a nonzero critical temperature T_f, whereas the model has a nonequilibrium freezing temperature...."

It is interesting to see that two-dimensional and three-dimensional spin glasses seem to behave differently: theories and experiments are more in agreement with respect to the planar case. In particular, some power law hypotheses about phase transitions seem to be generally accepted in dimension two, while the three-dimensional case is open. Moreover, there are controversies between theory and practice. Young points out: "In the last three years, then, theorists have become more than ever convinced that (the lower critical dimension) $d_L = 4$ and experimentalists more than ever sure that a transition occurs in $d = 3$. Hence this paradox is no nearer being solved." Moreover, Morgenstern and Binder (1980a) explain: "The nonexistence of a phase transition at nonzero temperature in two dimensions is in agreement with high-temperature series extrapolation ..., with most (but not all) real space renormalization group treatments and other arguments. For three-dimensional Ising systems, the situation is much more controversial:

series ... and other arguments ... again imply nonexistence of a transition, while all real-space renormalization methods ... now imply the existence of a transition with $T_f \neq 0$."

There are a number of open questions (in two and three dimensions) concerning the behavior of the $\pm J$ model. Angles d'Auriac and Maynard write: "In the $\pm J$ model, the ferromagnetic ($+J$) and antiferromagnetic ($-J$) bonds are distributed at random on a square lattice of Ising spins. By increasing the concentration x of antiferromagnetic bonds from 0 to 0.5 at very low temperatures, the ferromagnetism disappears and a dislocated phase appears which resembles a superparamagnet. This property is well established, but there has been some controversy as to whether the random antiphase occurs between the ferromagnetic phase and superparamagnetic at $T = 0°K$. This postulated phase has been suggested ... from the observation of a series of exact ground states exhibiting both rigidity and a magnetic wall at intermediate concentrations $0.1 < x < 0.15$." In fact, these observations have only been made in the planar case without exterior magnetic field, and it is interesting to see whether or not similar phenomena occur in three dimensions or with a magnetic field.

Reger, Binder and Kinzel (1984) express further interest in exact ground-state calculations with exterior magnetic field: "Thus, there is considerable interest in estimating the ground-state magnetization $M(T = 0, H)$ accurately. So far the information on $M(T = 0, H)$ rests on Monte Carlo simulations where the temperature T of the model system is slowly cooled down to $T = 0$. These simulations are very time consuming... More efficient alternative methods to study ground-state properties of spin glass models would be highly desirable."

Here we come to an interesting issue. Ground-state calculations were the starting point of the Monte Carlo methods (currently running under the name of simulated annealing) that now invade many branches of optimization. Although many physicists believe that some stochastic processes such as simulated annealing reflect the evolution of real spin glass systems rather accurately, there have been some doubts. For instance, Van Hemmen and Sütö (1985) point out: "Most glassy materials show an extremely slow relaxation to equilibrium once they are below glass transition regime. This behavior is due to local anisotropies which make a local change inadvantageous unless other particles also participate and a whole cluster is flipped." The flipping of one spin at a time is the usual random change used in simulated annealing. Morgenstern and Binder (1980b) write, with respect to this method: "It is an open question to identify the times necessary to simulate equilibrium properties of spin glasses," and furthermore: "There has been considerable discussion in the literature ... concerning ground-state properties obtained from Monte Carlo simulations."

A more elaborate discussion of this topic can be found in Barahona et al. (1982). We have done some preliminary testing and found that simulated annealing comes up with spin configurations whose energy is only slightly larger than the minimum energy, but the spin configurations often differ considerably from the optimal ones. Our observations agree with the findings of Morgenstern and Binder (1980b). We will report elsewhere on this subject.

As we have mentioned, there is considerable interest in obtaining exact ground states. So far, physicists use almost exclusively (approximative) Monte Carlo methods. A completely different approach is described in the recent paper by Canisius and Van Hemmen (1986). Here a nonlinear programming algorithm (based on Rosen's projected-gradient method) is designed to minimize the hamiltonian $H(\omega)$ directly. This method produces a series of local minima from which the best is selected. It can handle quite large two- and three-dimensional grids (problems of size up to 30×30 and $10 \times 10 \times 10$ are reported) and provides good approximations of the ground state.

We have found very few reports mentioning exact algorithms for spin glass systems different from planar grids. Hartwig, Daske and Kobe (1984) report on a branch-and-bound method that is able to solve systems with up to 60 spins. With the same algorithm, Kaschner and Kobe (1984) handled 80 spins. For a special planar grid model with exterior magnetic field, Morgenstern and Binder (1980b) invented an enumeration method—which is quite time-and-space consuming—with which optimal ground states could be found for 18×18 grids. (Their study needed about 500 hours of computing time on an IBM 370/168.) Barahona and Maccioni (1982) have designed an algorithm for three-dimensional spin glasses which can handle $5 \times 5 \times 5$ grids.

The algorithm we have designed has been used successfully for toroidal grids of up to 40×40 with exterior magnetic field—see Section 5 for details. This grid size is acceptable for many applications in physics, though larger grid sizes are desirable in certain instances. We hope that our approach will provide the means to also address these larger applications.

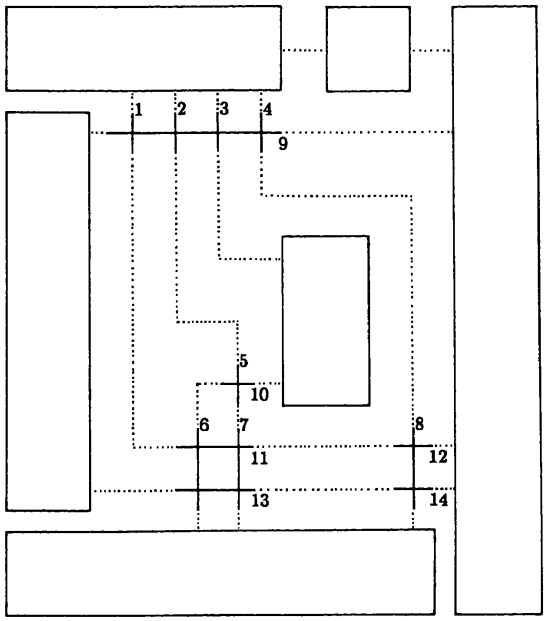

Figure 1. A chip with six cells and nine nets.

2. Via Minimization

We now want to outline another application of the max-cut problem that has interesting parallels to the ground-state minimization of spin glasses. This problem comes up in VLSI design and in the design of printed circuit boards. A chip construction is usually broken into several phases, among which are placement, routing and layer assignment. We suppose that all cells are placed on a chip and all nets have been routed but that the assignment of wire segments to layers has not been performed (this is called transient routing). A net may connect two or more pins. Figure 1 shows six cells with nine nets. All nets connect two pins.

In a transient routing, wires belonging to different nets may cross. A feasible layer assignment must have the property that such crossing wire segments are assigned to different layers. Thus some wires necessarily have to be routed on different layers. Physically, a change of layers is achieved by placing a "via"—in printed circuit board design, a hole to be drilled; in VLSI design, a contact that needs special treatment in the production process. In printed circuit board fabrication, vias cause additional costly work and often contribute to failure of the board due to cracking. In VLSI design, vias need additional space, are obstacles in compaction, and decrease the yield in the fabrication process. Thus, it is desirable to find a layer assignment such that the number of vias is as small as possible. Further design rules (for example, two wires that run parallel at minimum feasible distance within a certain interval may not contain a via within this interval) restrict the placement of vias. In general, each wire may be partitioned into free and critical segments, such that vias are allowed on free segments but are forbidden on critical segments. In Figure 1 there are 14 critical segments (drawn solid and numbered $1, \ldots, 14$) and 23 free segments (drawn dotted).

We want to treat the case where only two layers are available. Let us first assume that all nets connect exactly two pins, so each net consists of one wire. We partition each wire into its free and critical segments. The critical segments correspond to the node set V of a layout graph $G = (V, E)$ which has two kinds of edges. Nodes i and j are joined by a conflict edge ij whenever the associated critical segments must be on different layers. Nodes i and j are joined by a continuation edge ij whenever the associated critical segments are connected by a free segment. So $E = A \cup B$, where A are the conflict edges and B the continuation edges. In our example, the layout graph looks as shown in Figure 2. In it, the conflict edges are represented by solid lines and the continuation edges by broken lines.

If the "conflict graph" $H = (V, A)$ of G is not bipartite, it is easy to see that there is no feasible

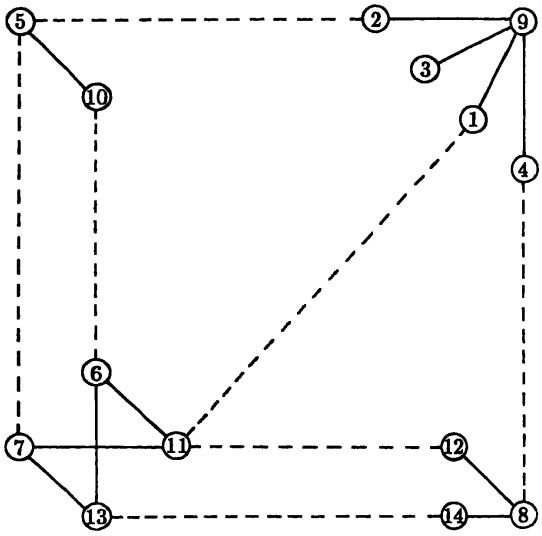

Figure 2. The layout graph for the chip shown in Figure 1.

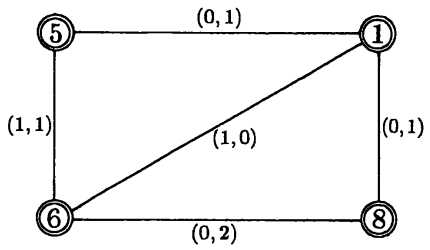

Figure 3. The reduced layout graph of the graph shown in Figure 2.

assignment of segments to the two layers (in this case the transient routing has to be changed). Otherwise H partitions into connected bipartite components $(V_1, A_1), \ldots, (V_k A_k)$. Clearly, the assignment of one node of a component (V_i, A_i) to a layer implies the assignment of all other nodes of V_i. We can now phrase the via minimization problem in terms of the layout graph G as follows. Find a cut C of G that contains all conflict edges A and contains as few continuation edges as possible. To formulate this as a max-cut problem, we proceed as follows.

We construct a reduced layout graph $R = (W, F)$ in the following way. For each component (V_i, A_i) of H, we arbitrarily select a "representative" node v_i and set $W = \{v_1, \ldots, v_k\}$. F contains an edge linking v_i and v_j, $i \neq j$, if and only if G contains a (continuation) edge linking some node in V_i to some node in V_j. In graph theoretical terminology, the reduced layout graph is constructed from the layout graph by "shrinking" each component (V_i, A_i), $i \in \{1, \ldots, k\}$, to one node v_i. This way, all conflict edges disappear and the edge set F represents the continuation edges. Since, by definition, continuation edges do not cross, the reduced layout graph is planar by construction. Figure 3 shows the reduced layout graph of the graph shown in Figure 2. For each edge v_iv_j in F, we define two weights α_{ij} and β_{ij} in the following way:

α_{ij} := number of vias between V_i and V_j necessary if v_i and v_j are assigned to the same layer, and
β_{ij} := number of vias between V_i and V_j necessary if v_i and v_j are assigned to different layers.

The numbers α_{ij} and β_{ij} can be easily calculated in linear time by counting continuation edges in G between V_i and V_j. In Figure 3, the edges of the reduced layout graph are labeled $(\alpha_{ij}, \beta_{ij})$.

A layer assignment corresponds, by construction, to a partition W^+, W^- of W. Given such a partition, the number of vias is

$$\mathrm{VIA}(W^+, W^-) := \sum_{\substack{v_iv_j \in F \\ v_i, v_j \in W^+}} \alpha_{ij} + \sum_{\substack{v_iv_j \in F \\ v_i, v_j \in W^-}} \alpha_{ij} + \sum_{\substack{v_iv_j \in F \\ v_i \in W^+ \\ v_j \in W^-}} \beta_{ij}.$$

Define $C := \sum_{v_iv_j \in F} \alpha_{ij}$. Then

$$\mathrm{VIA}(W^+, W^-) - C = \sum_{\substack{v_iv_j \in F \\ v_i \in W^+ \\ v_j \in W^-}} (\beta_{ij} - \alpha_{ij}),$$

and so for $c_{ij} := \alpha_{ij} - \beta_{ij}$ the problem of minimizing the number of vias is equivalent to the max-cut problem in $R = (W, F)$, with the weights c_{ij} on the edges $v_iv_j \in F$. In our example, we have $C = 2$, and the edge weights c_{ij} are shown in Figure 4. We induce a maximum weight cut in this graph by partitioning W into $\{1, 5\}$ and $\{6, 8\}$. This cut has weight 0, and therefore at least $C - 0 = 2$ vias are needed. Our (optimal) solution consists of placing a via between the critical segments 5 and 7 and another via between the critical segments 4 and 8 of Figure 1.

The reduction outlined above is due to Pinter and to Chen, Kajitani and Chan independently. These authors also observed that the max-cut problem is solvable in polynomial time since the reduced layout graph is planar.

Pinter, and Chen, Kajitani and Chan mention that the reduction just described also works in the case of general nets (3 pins or more per net are allowed) if the transient routing contains three-way junctions only. How to handle four-way junctions is an open problem, but, fortunately, they rarely occur in practice. Figure 5 shows how a three-way junction has to be modeled in the layout graph. The triangle consists of three "continuation edges" with weights ½. In this more general framework, all other continuation edges

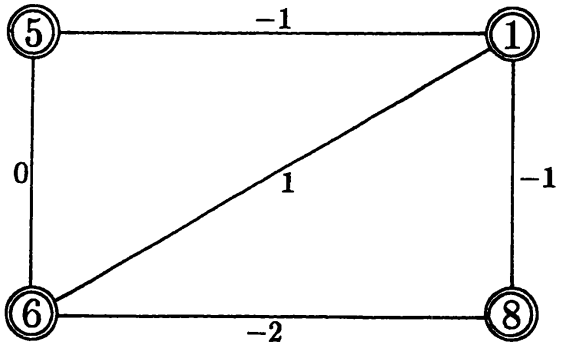

Figure 4. The reduced layout graph, showing the edge weights c_{ij}.

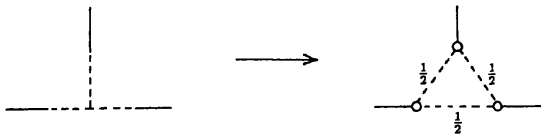

Figure 5. Model of a three-way junction in a layout graph.

are assumed to have weight 1. The modeling of the via minimization problem just described disregards an important requirement in VLSI design, where in many cases one of two layers is preferred and pins are preassigned to some layer. For instance, in standard cell design in 3-μ-CMOS-2 technology, there are a polysilicon (poly) and an aluminum (alu) layer. Preferably, wires should be in the alu-layer whereas pins are usually in the poly-layer. In ECL technology there are two metal layers (alu 1 and alu 2), and pins are usually preassigned to one of the layers.

We will now show how one can model these requirements by introducing an additional node. This node plays the role of the exterior magnetic field in the spin glass application. The graphs that result will not be planar in general, but they will be "almost planar."

First we would like to remark that via minimization and layer preference are conflicting objectives, since obviously, by increasing the number of vias, more wire segments can be placed on the preferred layer. This suggests the introduction of a parameter, to be set by the user, with which the relative emphasis given to the two goals can be controlled.

Recall that the layout graph was constructed from free and critical wire segments of the transient routing. We now add additional critical segments as follows. If the initial segment of a wire starting at a pin is free, we replace it by a critical segment (starting at the pin) followed by a free segment. Each remaining free segment is subdivided into a free segment, followed by a critical segment, followed by a free segment. From this set of critical and free segments, we construct the layout graph $G = (V, E)$, $V = \{1, \ldots, n\}$, as described previously. We introduce an additional node, called 0, and associate it to the preferred layer. We use this node as a "magnetic field" to attract wire segments to the preferred layer with "force" $h > 0$ and to preassign some wire segments and pins to any of the two layers. To do this, we join each node i, $1 \leq i \leq n$, to 0 by an edge. Let us call this graph the extended layout graph $\hat{G} = (\hat{V}, \hat{E})$. We now put weights on the edges of $\hat{E}$. All conflict edges ij in E have weight $w_{ij} := 0$, all continuation edges have weight $w_{ij} := 1$ (unless they result from the construction shown in Figure 5, in which case they have weight ½). Let M be a very large positive number. We define the weight of an edge $0i$ as follows:

$$w_{0i} := \begin{cases} -M & \text{if } i \text{ corresponds to a wire segment preassigned to the preferred layer,} \\ M & \text{if } i \text{ corresponds to a wire segment preassigned to the other layer,} \\ -h & \text{otherwise.} \end{cases}$$

A pin preassignment is handled by putting the appropriate weight (M or $-M$) on the edge $0i$, where i is the node corresponding to the initial critical segment starting at that pin.

We want to solve the following problem: Find a cut C in $\hat{G}$ such that C contains all conflict edges and $w(C)$ is as small as possible.

The parameter h is the control parameter for the user to decide on the relative emphasis given to the conflicting goals. The stipulation $h = 0$ results in a via minimization subject to preassignments of some pins and wire segments, while h large enough strongly favors the preferred layer. Clearly, some care must be given to setting h.

We now construct the reduced layout graph $\hat{R} = (\hat{W}, \hat{F})$ from $\hat{G}$ as described previously (the edges $0i$ are considered continuation edges). The definition of the weights α_{ij}, β_{ij} of the edges of $\hat{F}$ should be clear from the construction. Setting $c_{ij} = \alpha_{ij} - \beta_{ij}$, we can easily see that finding a cut $\hat{C}$ in $\hat{R}$ with maximum weight $c(\hat{C})$ is equivalent to the problem just defined.

The reduced layout graph $\hat{R}$ is not planar, but $\hat{R} - v_0$, where v_0 is the node in $\hat{R}$ corresponding to node 0 in $\hat{G}$ that is associated to the preferred layer, is planar. So we are able to reduce the via minimization problem, subject to pin preassignment and layer preference, to a max-cut problem in an "almost planar" graph. Recall that a similar problem also arose in our spin glass application, where we had a torus instead of a planar graph. As mentioned in the introduction, the max-cut problem is NP-complete for these almost planar graphs. Our computational experience (see Section 5) with the spin glass problem shows that the polyhedral approach is good enough to handle such problems in practice. This indicates that our algorithm might also be suitable for via minimization with preferred layers and preassignments. (If there is no layer preference, but possibly pin preassignments, then the problem is polynomially solvable provided that all nodes corresponding to preassigned pins are on the same face of the reduced layout graph.)

The reduction just described (in particular, the subdivision of all free segments and the addition of a critical segment at each pin) results in a rather large number of nodes. In a practical situation, not all free segments and pins are equally important, and thus the user should decide which critical segments he wants to add.

We would like to remark that, so far, we minimize the *number* of vias, respectively, maximize the *number* of wire segments, on the preferred layer. Our model also allows us to take the lengths of wire segments into account by individualizing the magnetic force, i.e., by attracting a long segment with a larger force than a short one.

3. Polyhedral Background

We will now describe the theoretical background on which we base our cutting plane algorithm for the max-cut problem.

Suppose a graph $G = (V, E)$ with edge weights c_{ij} for $ij \in E$ is given. For each cut $\delta(W)$, $W \subseteq V$, we define its incidence vector $\chi^{\delta(W)} \in \mathbb{R}^E$ by setting $\chi_e^{\delta(W)} = 1$ if $e \in \delta(W)$ and $\chi_e^{\delta(W)} = 0$ if $e \notin \delta(W)$. The cut polytope $\mathrm{CUT}(G)$ of G is the convex hull of all incidence vectors of cuts of G, i.e.,

$$\mathrm{CUT}(G) = \mathrm{conv}\{\chi^{\delta(W)} \in \mathbb{R}^E \mid W \subseteq V\}. \tag{1}$$

We can write the problem of finding a cut $\delta(W)$ in G with $c(\delta(W))$ as large as possible (considering c as a vector in $\mathbb{R}^E$) as the linear program

$$\max\{c^T x \mid x \in \mathrm{CUT}(G)\}, \tag{2}$$

since the vertices of the polytope $\mathrm{CUT}(G)$ are exactly the incidence vectors of the cuts of G. In order to apply linear programming techniques to solve this LP, we must represent $\mathrm{CUT}(G)$ as the solution set of an inequality system. Since the max-cut problem is NP-complete, we cannot expect to find a complete system describing $\mathrm{CUT}(G)$, but, as we shall see later, partial systems may also be useful in solving the max-cut problem. The polyhedral structure of $\mathrm{CUT}(G)$ and the closely related bipartite subgraph polytope has, for instance, been studied in Barahona, Grötschel and Mahjoub (1985) and Barahona and Mahjoub (1986). We now summarize some of the results known about the facial structure of $\mathrm{CUT}(G)$ mentioned in Barahona and Mahjoub.

The cut polytope is full dimensional, i.e.,

$$\dim(\mathrm{CUT}(G)) = |E|.$$

This implies that each facet-defining inequality is unique up to multiplication by a constant. Since $\mathrm{CUT}(G)$ is in the unit hypercube of $\mathbb{R}^E$, the trivial inequalities $0 \leq x_e \leq 1$ are valid for $\mathrm{CUT}(G)$.

Theorem 1. *For $e \in E$, the following statements are equivalent:*

(a) $x_e \geq 0$ defines a facet of $\mathrm{CUT}(G)$.
(b) $x_e \leq 1$ defines a facet of $\mathrm{CUT}(G)$.
(c) e does not belong to a triangle.

We know from graph theory that a cut and a cycle intersect in an even number of edges. This observation yields that the odd cycle inequalities

$$x(F) - x(C \setminus F) \leq |F| - 1$$

for all cycles $C \subseteq E$ and all $F \subseteq C$, $|F|$ odd

are satisfied by all incidence vectors of cuts. Recall that a chord of a cycle C is an edge of G that joins two nodes of C but does not belong to C.

Theorem 2. *Let $C \subseteq E$ by a cycle and $F \subseteq C$, $|F|$ odd, then $x(F) - x(C \setminus F) \leq |F| - 1$ defines a facet of $\mathrm{CUT}(G)$ if and only if C has no chord.*

A graph is called a bicycle p-wheel if it consists of a cycle of length p and two nodes adjacent to each other and to every node of the cycle.

Theorem 3. *Let (W, F) be a bicycle $(2k+1)$-wheel, $k \geq 1$, contained in G. Then the inequality*

$$x(F) \leq 2(2k+1)$$

defines a facet of $\mathrm{CUT}(G)$.

Theorem 4. *Let $K_p = (W, F)$ be a complete subgraph of order p of G. Then the K_p-inequality*

$$x(F) \leq \left\lceil \frac{p}{2} \right\rceil \left\lfloor \frac{p}{2} \right\rfloor$$

is valid for $\mathrm{CUT}(G)$; this inequality defines a facet of $\mathrm{CUT}(G)$ if and only if p is odd.

There are further known classes of facets of $\mathrm{CUT}(G)$. In particular there exist interesting methods to construct new facet-defining inequalities from given facet-defining inequalities. Especially notable are the techniques of changing the sign of a cut and of subdividing an edge. The exact definitions of these operations are technically a little complicated and are therefore omitted.

A relevant problem for our purposes is to decide whether the separation problem for the classes of

inequalities just decribed for CUT(G) is solvable efficiently. The separation problem for a class $\mathcal{X}$ of inequalities valid for CUT(G) is as follows.

Given $y \in \mathbb{Q}^E$, decide whether y satisfies all inequalities in $\mathcal{X}$, and if y does not, find an inequality in $\mathcal{X}$ violated by y.

The importance of the separation problem stems from the fact that the polynomial time solvability of the separation problem for $\mathcal{X}$ implies, by the ellipsoid method, the existence of a polynomial algorithm for the optimization problem $\max\{c^T x \mid x$ satisfies all inequalities in $\mathcal{X}\}$ (see Grötschel, Lovász and Schrijver 1981). Although the ellipsoid method is not practically efficient, experience gained in recent years shows that these optimization problems can indeed be solved reasonably well in practice (see, e.g., Crowder and Padberg 1980; Crowder, Johnson and Padberg 1983; Grötschel and Holland 1985; and Grötschel, Jünger and Reinelt 1984).

Concerning the classes of inequalities just defined, the following is known. We assume that a graph $G = (V, E)$ and a point $y \in \mathbb{Q}^E$ are given. We want to solve the separation problem for y.

Trivial Inequalities. The separation problem is trivial. We simply substitute y into the inequalities $0 \leqslant x_e \leqslant 1$, $e \in E$.

Odd Cycle Inequalities. (We can assume that $0 \leqslant y_e \leqslant 1$ holds.) We define a new graph $H = (V' \cup V'', E' \cup E'' \cup E''') = (W, F)$ that consists of two copies of G, say $G' = (V', E')$ and $G'' = (V'', E'')$, and the following additional edges E'''. For each edge $uv \in E$ we create the two edges $u'v''$ and $u''v'$. The edges $u'v' \in E'$ and $u''v'' \in E''$ are assigned the weight y_{uv}, while the edges $u'v'', u''v' \in E'''$ are assigned the weight $1 - y_{uv}$. For each pair of nodes $u', u'' \in W$, we calculate a shortest (with respect to the weights just defined) path in H. Such a path contains an odd number of edges of E''' and corresponds to a closed walk in G containing u. Clearly, if the shortest of these (u', u'')-paths in H has length less than 1, there exists a cycle $C \subseteq E$ and an edge set $F \subseteq C$, $|F|$ odd, such that y violates the corresponding odd cycle inequality. (C and F are easily constructed from a shortest path.) If the shortest of these (u', u'')-paths has length at least 1, then y satisfies all these inequalities. So the separation problem can be solved in polynomial time (Barahona and Mahjoub).

Bicycle Wheel Inequalities. Gerards (1985) has shown that the separation problem for this class of inequalities can be reduced to a sequence of shortest path calculations in a similar way as described above for the odd cycle inequalities. Hence, this separation problem is also polynomially solvable.

K_p-Inequalities. Trivially, for p fixed, one can check all K_p-inequalities in polynomial time by enumeration, but it is not known whether there is a polynomial time algorithm to solve the separation problem for all complete subgraph inequalities. It is also not known whether there is a good algorithm to solve the separation problem for the class of inequalities obtained from the K_5-inequalities by edge subdivision and changing the sign of a cut.

These remarks show that the following LP-relaxation of the max-cut problem can be solved in polynomial time.

$$\text{Max } c^T x$$
$$0 \leqslant x_e \leqslant 1 \quad \text{for all } e \in E$$
$$x(F) - x(C \setminus F) \leqslant |F| - 1$$
$$\text{for all cycles } C \subseteq E \text{ and all } F \subseteq C, \ |F| \text{ odd}$$
$$x(F) \leqslant 2(2k + 1)$$
$$\text{for all bicycle } (2k + 1)\text{-wheels } (W, F).$$

In the special application we will treat, bicycle p-wheels do not occur. (The graphs G also do not contain complete subgraphs K_p for $p \geqslant 4$, but they may contain subdivisions of K_5 that induces facets of CUT(G).) Thus we can disregard these inequalities and concentrate on the remaining two classes. Let us therefore define the following polytope.

$$P_C(G) := \{x \in \mathbb{R}^E \mid 0 \leqslant x_e \leqslant 1 \text{ for all } e \mid E,$$
$$x(F) - x(C \setminus F) \leqslant |F| - 1$$
$$\text{for all cycles } C \subseteq E$$
$$\text{and all } F \subseteq C, \ |F| \text{ odd}\}.$$

Observe that

$$\text{CUT}(G) = \text{conv}\{x \in P_C(G) \mid x \text{ integer}\},$$

so

$$\max c^T x$$
$$x \in P_C(G)$$
$$x \text{ integer}$$

is an integer programming formulation of the max-cut problem. Moreover, the following has been shown by Barahona and Mahjoub.

Theorem 5. *$P_C(G) = \text{CUT}(G)$ if and only if G is not contractible to K_5.*

This theorem and our preceding remarks prove that the max-cut problem is solvable in polynomial time for the class of graphs not contractible to K_5. Since, by Wagner's theorem, planar graphs are those graphs which are not contractible to K_5 or $K_{3,3}$, we have $P_C(G) = \mathrm{CUT}(G)$ for all planar graphs. So this observation also implies the polynomial time solvability of the max-cut problem for planar graphs.

Barahona (1981) designed a polynomial time algorithm that solves the max-cut problem for toroidal graphs with ± 1 weights. This makes it possible to find a ground state in the two-dimensional $\pm J$-model with periodic boundary conditions. However, we do not know an inequality system describing the cut polytope for toroidal graphs.

As mentioned before, for the ground state problem in spin glasses, Toulouse introduced the concept of frustrated contours and stated "There is no way of choosing the orientations of the site spins around a frustrated contour without frustrating at least one bond." If one translates this sentence into our terminology, it suggests that we consider the following system of inequalities:

$$\sum_{ij \in C} x_{ij} \geqslant 1 \quad \text{for all frustrated contours } C \subseteq E,$$

$$x_{ij} \geqslant 0 \quad \text{for all } ij \in E,$$

where frustrated contours are cycles in G with an odd number of negative interactions. For the two-dimensional case, this system defines an integral polyhedron. This follows from the Chinese-Postman-Theorem of Edmonds and Johnson, as has been pointed out in Barahona et al. For random-field Ising ferromagnets, the system also defines an integral polyhedron. This is a consequence of the max-flow min-cut theorem of Ford and Fulkerson and was shown by Barahona (1985). This system, however, is not integral for three-dimensional Ising models, but it provides a tight LP-relaxation, as can be seen from the computational experience with it reported in Barahona and Maccioni. It is also not integral for planar nor for toroidal spin glass systems with exterior magnetic field, a case we will consider later in this paper.

4. The Cutting Plane Algorithm

We have implemented a standard cutting plane algorithm based on the simplex method: i.e., we start with a very coarse LP-relaxation of the max-cut problem and use the simplex method to solve it. If the optimum solution is the incidence vector of a cut, we are done. Otherwise we enter a "separation phase" to find inequalities violated by the optimum solution. If such inequalities are found, we add them and repeat the process. If not, we have to resort to branch and bound (in principle). Our cutting plane algorithm was not implemented to treat general graphs. Our objective was to develop a special purpose computer code for max-cut problems in the spin glass application. Although we exploited the special structure of this problem class (e.g., by designing special purpose cutting plane generation heuristics) our approach is general in principle. Only a few heuristics have to be exchanged and some data structures have to be modified in order to treat arbitrary graphs.

We study two-dimensional Ising spin glasses on a grid with nearest neighbor interactions, an exterior magnetic field and so-called periodic boundary conditions. (The periodic boundary conditions are a standard way of modeling an infinite planar spin glass finitely.) This leads to the class of graphs consisting of a $k \times k$-grid embedded on a torus and a further node joined to all grid nodes (Figure 6.) Setting $n = k^2$, our graphs, thus, have $n + 1$ nodes nd $m = 3n$ edges.

Now we outline our strategy for generating and eliminating cutting planes. As mentioned previously, we restrict ourselves to trivial inequalities and odd cycle inequalities. The nonnegativity constraints and the upper bounds (of value 1) on the variables are automatically handled by the simplex method. We implemented the separation algorithm for the odd cycle inequalities outlined in Section 3. Using Dijkstra's method and labeling techniques, we can achieve an $O(n^3)$-implementation, but, for practical purposes, this approach is rather slow. Therefore, we have added faster heuristics for finding violated odd

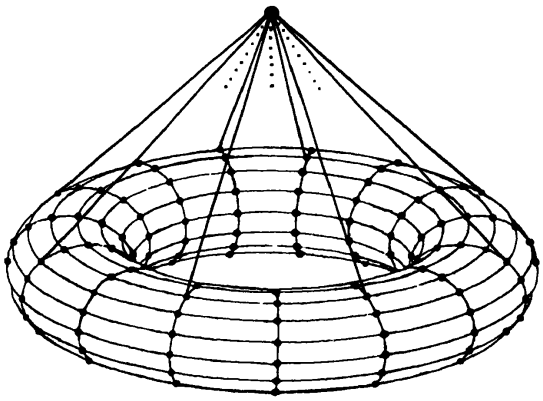

Figure 6. A $k \times k$ grid embedded on a torus, with a further node joined to all grid nodes.

cycle inequalities in order to avoid calling the "exact separation routine." We describe them in the order we call them in the algorithm.

Suppose $y \in \mathbb{Q}^E$ is the optimum solution of the last linear program. We have to check whether y is the incidence vector of a cut, and if not, find odd cycle inequalities violated by y, if there are any.

CIBCAG (*C*heck *I*ntegrality, *B*ipartiteness, *C*ut, *a*nd *G*enerate Cutting Planes). For $0 < \epsilon < \frac{1}{2}$ we define the graph $G_\epsilon = (V, E_\epsilon)$ as follows:

$$E_\epsilon := \{e \in E \mid y_e \leq \epsilon \text{ or } y_e \geq 1 - \epsilon\}.$$

We try to 2-color the nodes of G_ϵ with red and green, say. First we pick an arbitrary node $v \in V$ and color it red. For all neighbors w of v in G_ϵ we do the following: If w is not colored, w receives the color of v if $y_{vw} \leq \epsilon$, otherwise w receives the complementary color. If w is already colored, there are two cases. If w has the same color as v and $y_{vw} \leq \epsilon$ or if v and w have complementary colors and $y_{vw} \geq 1 - \epsilon$, we continue. Otherwise we have found a cycle C with an odd number of edges of value at least $1 - \epsilon$. Let F be the set of these edges. We check whether $y(F) - y(C \setminus F) > |F| - 1$. If this is the case, we have found a violated odd cycle inequality. When all neighbors of v have been considered, we pick a new, colored node, consider its neighbors, and proceed in breadth first search manner.

If y is integral, which we check on the run, and not a cut, this procedure guarantees that a violated odd cycle inequality will be found. So, if for an integral y, CIBCAG does not produce a violated inequality, y is the incidence vector of a maximum weight cut in G. The breadth first search tree built up by CIBCAG allows us to generate the violated odd cycle inequalities efficiently. The worst-case running time of our implementation of CIBCAG depends on the structure of G_ϵ and is between $O(n)$ and $O(|E| \log n)$. Empirically it is $O(n)$ and extremely fast.

GEN4CYC (*Gen*erate *4-Cyc*les). Due to the special structure of our graph, the unchorded 4-cycles of the graph correspond exactly to the grid squares. There are n such 4-cycles. We scan through all these and check each of the eight associated odd cycle inequalities for violation. This can be done in $O(n)$ time.

GEN3CYC (*Gen*erate *3-Cyc*les). All 3-cycles (triangles) in G must contain the node 0 corresponding to the exterior magnetic field. By scanning through all grid edges vw we check the four possible odd cycle inequalities that can be derived from the triangle $0vw$. This algorithm has time complexity $O(n)$.

SHOC (*S*panning Tree *H*euristic for *O*dd *C*ycles). We calculate a maximum weight spanning tree T_{max} of G with edge weights $|y_e - \frac{1}{2}|$. For any non-tree edge e, we consider its fundamental cycle C and set $F := \{e \in C \mid y_e > \frac{1}{2}\}$. We check whether $|F|$ is odd and the corresponding odd cycle inequality is violated by y. Using Kruskal's algorithm, this heuristic runs in time $O(n \log n)$ on the average, and $O(n^2)$ in the worst case.

The above decribed heuristics are used in the following order.

- CIBCAG with user specified parameter EPSILON; if no cut can be generated this way, CIBCAG tries again with EPSILON = 0.49.
- GEN4CYC if less than GENCYC-LIM cutting planes have been produced by CIBCAG.
- GEN3CYC if less than GENCYC-LIM cutting planes have been produced by CIBCAG and GEN4CYC.
- SHOC if less than SHOC-LIM cutting planes have been produced in the previous steps.

Finally, the "exact" separation routine named OC (*O*dd *C*ycles) is called if all heuristics together found less than OC-LIM cutting planes. This kind of parameterization keeps the program flexible by allowing us to test various cutting plane generation strategies.

Elimination of Cutting Planes. To keep the number of constraints small, we eliminate inequalities in the following way: Whenever the objective function value has decreased by more than the parameter DELTA compared to the previous solution value, all inequalities nonbinding at the current optimum solution are eliminated; otherwise no elimination is performed.

The features just described are the basic components of our cutting plane algorithm. The algorithm provably produces an optimum vertex of the polytope $P_C(G)$. If this algorithm finds an optimum solution which is integral, it provides a ground state of the spin glass. The algorithm, however, carries no guarantee of finding an optimum integral solution. Formally, we could add a branch-and-bound phase to give such a guarantee. But, as shown in Section 5, it turned out that this is unnecessary.

5. Computational Experience

In this section, we report our findings concerning the practical performance of the cutting plane algorithm

described in the previous section. We aim to solve ground-state problems. Thus we have generated several series of spin glass problems with spin interactions and exterior magnetic force, as used in physics. We have concentrated on the Gaussian model. The spins are located on the nodes of a toroidal $k \times k$ grid (Figure 6).

In a first series of experiments, not reported here, we have compared various choices of the parameters DELTA, EPSILON and other tactical issues. We decided to use the following features:

DELTA is set to 0.001. (3)

EPSILON is set to 0.3. (4)

To keep the number of rows small, we never add more than MAXGEN = 200 *new inequalities in one cutting plane phase. As soon as the* 200*th cutting plane is found, we terminate the current separation routine and proceed by solving the new linear program.* (5)

In case we run a series of experiments in which all spin interactions remain fixed and only the strength of the exterior field varies, we start with the problem with the strongest field and iteratively reduce the strength of the field until the lower bound (usually zero) is reached. Whenever a new problem is solved, we use the optimal (final) basis of the preceding problem as the starting basis for the new problem. (6)

If the strength of the exterior field is zero, a so-called "2Δ-phase" is inserted; i.e., we solve the problem with exterior magnetic field 2 * *DELTA before solving it with zero field.* (7)

Feature (6) resulted in considerable savings in the overall running time. If we compare (6), for instance, with the intuitively more appealing strategy of (due to complexity considerations) starting with zero field and increasing the strength of the field gradually, we see (6)'s clear superiority. Quite frequently a whole series of runs with strategy (6) took about the same time as solving the first problem of zero field of the second strategy. In addition, feature (7) turned out to speed up the solution process. This is due to the fact that, in our approach, the zero field problem is by far the "hardest" in such a series. We expected the additional 2Δ-phase to provide a good starting solution for the 0-phase; in many cases this solution turned out to be optimal for the 0-field problem.

In a second series of experiments, we tried to find a good strategy for setting the parameters GENCYC-LIM, SHOC-LIM, and OC-LIM. We tested and report the four strategies given in Table I.

Table I
Strategies for Setting the Parameters GENCYC-LIM, SHOC-LIM, and OC-LIM

Strategy	GENCYC-LIM	SHOC-LIM	OC-LIM
1	0	0	0
2	∞	0	0
3	0	∞	0
4	0	0	∞

Table I can be interpreted as follows. According to our description of the cutting plane algorithm in Section 4, given the optimum solution y of the last LP, we always call the subroutine CIBCAG first. Afterward the routines GEN4CYC, GEN3CYC, SHOC, OC are called in this order. If one of the parameters . . .-LIM is equal to l, we call the corresponding algorithm only if all separation routines preceding it have not found more than l violated inequalities.

We experimented with 10 × 10 and 20 × 20 grids with Gaussian interactions to compare the strategies. The results in all cases gave a consistent picture. So we restrict ourselves to showing a detailed report of the behavior of the four strategies on a fixed 20 × 20 Gaussian problem in which the exterior field ranges from $h = 1$ to $h = 0$ by 0.2.

The experiments we document were run on an IBM 3081-D32 at the Kernforschungsanlage Jülich. We also used the IBM 4361 of the Institut für Ökonometrie und Operations Research at the University of Bonn. The running times on this machine are about 3 times as long as those on the 3081.

The code was written in ECL (an extension of PL/I) and uses IBM's LP-solver MPSX as a subroutine.

Tables II through V contain the relevant information to compare the four strategies. These tables should be interpreted as follows.

Column 1 ≙ h
= strength of the exterior magnetic field.
Column 2 ≙ *Ph*
= number of cutting plane phases
= number of LPs solved
Column 3 ≙ 4C
= number of calls of GEN4CYC
Column 4 ≙ 3C
= number of calls of GEN3CYC
Column 5 ≙ SH
= number of calls of SHOC
Column 6 ≙ OC
= number of calls of OC

Table II
Behavior of Strategy 1 on a Fixed 20 × 20 Gaussian Problem

	Strategy 1 (0, 0, 0)									
Ph	4C	3C	SH	OC	No. Iter	Size	Time	% Cut	% LP	% Rev
20	0	0	0	0	1435	764	1:46.07	9	45	35
16	0	0	0	0	1286	764	1:32.55	5	57	31
20	1	0	0	0	2429	905	2:59.03	4	70	21
42	2	0	0	0	3183	876	4:34.48	4	62	27
93	1	0	0	0	5211	923	9:18.95	6	57	30
185	36	21	13	13	3501	1293	63:15.31	80	6	11
8	3	1	1	1	63	1310	38:33.62	99	0	0

7 ≙ No. iter
= total number of simplex pivots used for solving all the LPs
8 ≙ Size
= number of rows of the final LP
9 ≙ Time
= total computation time in min:sec including input and output
10 ≙ % Cut
= percentage of total time spent in cutting plane generation (including the feasibility check done by CIBCAG)
11 ≙ % LP
= percentage of total time spent in solving the LPs
12 ≙ % REV
= percentage of total time spent in generating MPSX revise data and revising the LP data

ercentages of a row do not add up to 100%; sing time was spent in input, output and overhead.
btained the data for columns 9–12 by calling system functions that do not seem to behave y in some cases. Although we do not completely trust the accuracy of these data, we include them because we believe that they give the right idea.

In all our runs (with a few exceptions), Strategy 2 turned out to be the best with respect to total running time. This is because the cutting plane heuristics we used (mainly GEN4CYC and GEN3CYC) generate, on the average, no fewer violated inequalities than the other algorithms but are much faster with respect to execution time. Note, however, that these routines are special purpose heuristics and may not be reasonable for other classes of graphs.

In general, the running times of cutting plane algorithms that are based on combinations of heuristics are not precisely predictable. For a given set of comparable problems, the large majority of the running times for a fixed strategy are within a relatively small time interval, but there may be a few rather poor exceptions: the running time for Strategy 4 at 0.4-field is such a runaway.

From a theoretical point of view, the strategy to use is Strategy 4 (which consists only of calls of the exact separation routine OC). However, this method is not suitable as Tables II–V show. OC runs much longer than the heuristics and generates only a few constraints. Thus many more LP phases must be executed. This outcome shows that, in order to obtain

Table III
Behavior of Stategy 2 on a Fixed 20 × 20 Gaussian Problem

	Strategy 2 (∞, 0, 0)									
Ph	4C	3C	SH	OC	No. Iter	Size	Time	% Cut	% LP	% Rev
8	6	3	0	0	939	924	0:53.32	11	46	33
2	2	2	0	0	326	1034	0:15.25	6	55	31
3	3	3	0	0	422	1107	0:23.00	5	60	28
6	6	6	0	0	929	1205	1:00.99	3	69	22
11	11	11	3	3	1178	1200	3:31.52	59	28	10
38	38	38	0	0	1566	1290	3:35.02	7	40	42
0	0	0	0	0	7	1290	0:01.90	6	31	31

Table IV
Behavior of Strategy 3 on a Fixed 20 × 20 Gaussian Problem

		Strategy 3 (0, ∞, 0)									
h	*Ph*	4C	3C	SH	OC	No. Iter	Size	Time	% Cut	% LP	% Rev
1.0	11	0	0	9	0	1157	1017	2:12.14	49	28	19
0.8	5	0	0	5	0	725	1107	1:30.62	55	27	14
0.6	0	0	6	0	0	1173	1116	2:17.69	46	40	11
0.4	23	1	0	23	0	2404	1079	7:13.40	55	31	11
0.2	42	1	0	42	0	3693	1055	12:46.63	57	30	11
2Δ	64	3	0	64	0	2497	1293	16:36.32	64	15	17
0.0	0	0	0	0	0	49	1293	0:04.30	3	70	14

practically efficient cutting plane algorithms, it is extremely important to use very fast separation heuristics. Exact separation routines should be called only as a last resort to guarantee that all inequalities of a class have been checked.

We ran all further experiments with strategy (∞, 0, 0). (We also tried to replace ∞ by numbers such as 100, 200, . . . , but the results were slightly inferior.) In different experiments, we observed that the parameter MAXGEN, which controls the number of inequalities to be added in one phase, should be adjusted to the problem size.

Tables VI–IX demonstrate the empirical behavior of our cutting plane algorithm for toroidal $k \times k$ spin glass systems (k = 10, 20, 30, 40) with exterior magnetic field. These tables have the same structure as Tables II–V, but they have two additional columns (with information relevant for physicists). The column labeled "Energy" contains the ground-state energy per spin, i.e., the ground-state energy divided by k^2. The column labeled "Mag" contains the magnetization per spin, i.e., the number of spins with north pole up minus the number of spins with north pole down (in the optimum solution found), divided by k^2.

Tables VI–IX contain experiments on 10 × 10, 20 × 20, 30 × 30 and 40 × 40 grids. MAXGEN is set to 300, 400, 500, 600, respectively. For each k, the spin interactions are chosen from a Gaussian distribution and are fixed for all runs, and the exterior magnetic field varies in strength from $h = 4$ to $h = 0$ in steps of 0.2.

Our code was defeated in the 40 × 40 problem with $h = 2\Delta$ of Table IX. We found an optimum solution of the LP relaxation after about 300 minutes, but it turned out to be nonintegral. Our code does not yet contain an additional branch-and-bound or cutting plane phase (with Gomory cuts, say). So the code gave up without producing an optimum solution to (2). For this reason, we did not attempt to solve the 0-field problem.

For all of the more than one hundred problems documented so far, the optimum LP solutions turned out to be integral, with the one exception just mentioned. We thus found (globally optimal) ground states. To test the various versions of our code and decide on tactical issues, we ran far more than a thousand spin glass problems. In the Gaussian model, we encountered only a few nonintegral optimal solutions. Figures 7 and 8 show two fractional solutions, both on a 5 × 5 grid at zero exterior magnetic field. Solving problems of the $\pm J$-model yielded a few more, but still only a marginal number, of fractional LP

Table V
Behavior of Stratgegy 4 on a Fixed 20 × 20 Gaussian Problem

		Strategy 4 (0, 0, ∞)									
h	*Ph*	4C	3C	SH	OC	No. Iter	Size	Time	% Cut	% LP	% Rev
1.0	13	0	0	0	11	1273	862	3:58.86	69	17	11
0.8	8	0	0	0	8	854	929	2:55.71	69	18	10
0.6	10	0	0	0	10	1489	904	3:49.22	56	31	10
0.4	46	1	0	0	46	4707	980	47:16.16	86	10	3
0.2	89	1	0	0	89	7253	1023	31:58.10	62	26	10
2Δ	93	0	0	0	93	3709	1205	37:01.00	76	11	11
0.0	0	0	0	0	0	20	1205	0:02.51	5	48	24

Table VI
Empirical Behavior of the Cutting Plane Algorithm for a Toroidal 10 × 10 Spin Glass System

10 × 10 Strategy (∞, 0, 0)													
h	*Ph*	4C	3C	SH	OC	No. Iter	Size	Time	% Cut	% LP	% Rev	Energy	Mag
4.0	2	2	2	0	0	102	145	0:02.02	14	30	2	−3.9876	0.9000
3.8	0	0	0	0	0	2	145	0:00.61	3	0	1	−3.8102	0.8800
3.6	0	0	0	0	0	0	145	0:00.01	80	0	20	−3.6342	0.8800
3.4	0	0	0	0	0	1	145	0:00.61	3	0	0	−3.4582	0.8800
3.2	0	0	0	0	0	4	145	0:00.01	83	0	17	−3.2822	0.8800
3.0	2	2	2	0	0	8	156	0:01.35	10	89	1	−3.1071	0.8600
2.8	0	0	0	0	0	2	156	0:00.01	100	0	0	−2.9360	0.8400
2.6	0	0	0	0	0	6	156	0:00.61	3	0	97	−2.7704	0.8000
2.4	0	0	0	0	0	4	156	0:00.01	100	0	0	−2.6105	0.8000
2.2	1	1	1	0	0	10	158	0:00.68	11	0	89	−2.4539	0.7800
2.0	1	1	1	0	0	14	170	0:01.30	8	46	46	−2.2979	0.7800
1.8	2	2	2	0	0	22	185	0:00.72	16	0	84	−2.1469	0.7000
1.6	1	1	1	0	0	21	190	0:00.64	5	0	2	−2.0069	0.7000
1.4	1	1	1	0	0	26	200	0:00.70	14	0	86	−1.8787	0.6000
1.2	0	0	0	0	0	19	200	0:00.62	4	0	0	−1.7645	0.5400
1.0	1	1	1	0	0	36	202	0:00.66	8	0	92	−1.6592	0.5200
0.8	1	1	1	0	0	50	225	0:01.27	4	94	2	−1.5590	0.5000
0.6	2	2	2	0	0	84	241	0:01.95	7	92	1	−1.4601	0.4400
0.4	3	3	3	0	0	59	255	0:02.07	12	29	59	−1.3894	0.2800
0.2	2	2	2	0	0	94	257	0:02.62	8	68	24	−1.3359	0.2600
2Δ	36	36	36	3	0	437	274	0:26.66	18	45	19	−1.2886	0.0000
0.0	0	0	0	0	0	0	274	0:00.62	4	0	96	−1.2886	0.0000

Table VII
Empirical Behavior of the Cutting Plane Algorithm for a Toroidal 20 × 20 Spin Glass System

20 × 20 Strategy (∞, 0, 0)													
h	*Ph*	4C	3C	SH	OC	No. Iter	Size	Time	% Cut	% LP	% Rev	Energy	Mag
4.0	3	3	3	0	0	509	614	0:25.70	19	49	15	−4.0099	0.9450
3.8	2	2	2	0	0	15	622	0:03.17	23	57	20	−3.8225	0.9300
3.6	1	1	1	0	0	8	627	0:02.86	15	0	43	−3.6367	0.9250
3.4	0	0	0	0	0	12	627	0:01.31	8	46	46	−3.4534	0.9100
3.2	2	2	2	0	0	17	631	0:04.41	18	0	42	−3.2726	0.9000
3.0	2	2	2	0	0	14	638	0:03.13	22	19	59	−3.0942	0.8800
2.8	1	1	1	0	0	26	647	0:02.87	16	21	43	−2.9230	0.8400
2.6	1	1	1	0	0	31	664	0:02.93	17	20	42	−2.7591	0.8050
2.4	2	2	2	0	0	34	679	0:03.77	20	32	33	−2.5994	0.7900
2.2	1	1	1	0	0	30	681	0:02.84	15	0	43	−2.4469	0.7500
2.0	1	1	1	0	0	34	688	0:03.44	13	0	53	−2.2999	0.7250
1.8	2	2	2	0	0	58	712	0:05.19	18	23	24	−2.1560	0.7150
1.6	2	2	2	0	0	82	745	0:05.00	16	48	24	−2.0166	0.6800
1.4	1	1	1	0	0	84	775	0:04.05	10	30	30	−1.8841	0.6500
1.2	2	2	2	0	0	135	810	0:06.69	19	27	36	−1.7598	0.5750
1.0	2	2	2	0	0	125	863	0:06.75	11	27	36	−1.6517	0.5250
0.8	3	3	3	0	0	215	912	0:10.98	12	55	22	−1.5498	0.4550
0.6	2	2	2	0	0	311	922	0:12.52	9	67	10	−1.4745	0.3450
0.4	5	5	5	0	0	586	1013	0:30.98	8	72	14	−1.4094	0.2750
0.2	2	2	2	0	0	679	1062	0:27.91	3	82	9	−1.3667	0.1650
2Δ	48	48	48	2	0	1804	1173	3:35.71	19	43	26	−1.3395	0.1250
0.0	1	1	1	0	0	90	1165	0:07.08	7	62	16	−1.3392	0.1250

Table VIII
Empirical Behavior of the Cutting Plane Algorithm for a Toroidal 30 × 30 Spin Glass Sys

	30 × 30 Strategy (∞, 0, 0)											
h	*Ph*	4C	3C	SH	OC	No. Iter	Size	Time	% Cut	% LP	% Rev	Energy
4.0	5	5	5	0	0	1520	1586	2:30.87	26	49	13	−4.0290
3.8	1	1	1	1	0	13	1587	0:32.58	82	4	9	−3.8371
3.6	1	1	1	0	0	22	1593	0:08.11	18	15	36	−3.6470
3.4	1	1	1	0	0	27	1606	0:08.24	20	15	44	−3.4591
3.2	1	1	1	0	0	37	1618	0:08.81	18	14	41	−3.2734
3.0	1	1	1	0	0	29	1622	0:08.03	17	15	38	−3.0916
2.8	1	1	1	0	0	56	1643	0:09.00	20	20	40	−2.9139
2.6	1	1	1	0	0	65	1659	0:08.95	19	13	41	−2.7416
2.4	1	1	1	0	0	89	1691	0:10.39	19	29	35	−2.5784
2.2	1	1	1	0	0	89	1721	0:10.30	12	29	41	−2.4200
2.0	2	2	2	0	0	115	1765	0:14.38	16	25	34	−2.2652
1.8	2	2	2	0	0	158	1798	0:16.66	20	25	33	−2.1164
1.6	2	2	2	0	0	149	1827	0:15.68	15	34	27	−1.9797
1.4	2	2	2	0	0	211	1908	0:19.11	15	41	29	−1.8511
1.2	2	2	2	0	0	259	1994	0:21.14	14	37	32	−1.7310
1.0	2	2	2	0	0	400	2112	0:30.90	12	49	26	−1.6205
0.8	3	3	3	0	0	491	2217	0:38.86	12	49	24	−1.5212
0.6	5	5	5	1	0	879	2294	1:38.81	32	46	11	−1.4373
0.4	8	8	8	1	0	1336	2405	2:52.08	21	59	11	−1.3754
0.2	7	7	7	0	0	2691	2512	5:08.57	5	80	11	−1.3334
2Δ	96	96	96	13	1	6069	2831	34:13:89	37	35	17	−1.3187
0.0	0	0	0	0	0	133	2831	0:20.21	2	71	15	−1.3187

Table IX
Empirical Behavior of the Cutting Plane Algorithm for a Toroidal 40 × 40 Spin Glass Sys

	40 × 40 Strategy (∞, 0, 0)											
h	*Ph*	4C	3C	SH	OC	No. Iter	Size	Time	% Cut	% LP	% Rev	Energy
4.0	7	7	6	0	0	3108	2901	10:20.57	39	42	10	−4.0207
3.8	1	1	1	0	0	31	2910	0:21.52	27	11	39	−3.8285
3.6	1	1	1	0	0	41	2919	0:22.04	26	14	38	−3.6387
3.4	2	2	2	0	0	37	2925	0:27.52	28	11	35	−3.4508
3.2	1	1	1	0	0	50	2942	0:22.50	28	13	38	−3.2654
3.0	2	2	2	0	0	77	2963	0:32.58	31	15	32	−3.0849
2.8	2	2	2	0	0	96	3000	0:36.83	31	15	31	−2.9082
2.6	1	1	1	0	0	130	3033	0:27.98	27	21	35	−2.7355
2.4	2	2	2	0	0	152	3079	0:40.35	31	22	29	−2.5682
2.2	2	2	2	0	0	186	3155	0:40.01	25	24	30	−2.4080
2.0	2	2	2	0	0	187	3202	0:42.00	30	21	27	−2.2547
1.8	2	2	2	0	0	253	3259	0:48.40	29	27	26	−2.1079
1.6	3	3	3	0	0	330	3339	0:59.02	25	28	26	−1.9688
1.4	2	2	2	0	0	419	3468	1:01.92	22	37	25	−1.8395
1.2	2	2	2	0	0	559	3600	1:16.51	19	45	22	−1.7195
1.0	3	3	3	0	0	719	3725	1:33.21	17	46	22	−1.6129
0.8	4	4	4	0	0	1044	3892	2:17.12	15	52	18	−1.5192
0.6	5	5	5	0	0	1372	4050	3:43.54	11	63	14	−1.4375
0.4	14	14	14	2	0	2260	4197	11:42.55	37	45	9	−1.3710
0.2	7	7	7	0	0	4668	4394	13:38.52	5	81	9	−1.3236
2Δ	—	—	—	—	—	—	—	—	—	—	—	—
0.0	—	—	—	—	—	—	—	—	—	—	—	—

solutions. These empirical observations justify our choice of the odd cycle constraints, i.e., the polytope $P_C(G)$, for the LP-relaxation of the max-cut problem.

Nonintegral optimum solutions can be handled in two ways to obtain integrality. One either adds further cutting planes (e.g., bicycle wheel inequalities—see Theorem 3; or K_p-inequalities—see Theorem 4) or one proceeds with branch and bound. For this case, we want to discuss only two small examples.

Figure 7 shows a fractional solution of a 5 × 5 grid problem with exterior field. Edges drawn with solid lines correspond to variables with value 1; edges drawn with dotted lines correspond to value ⅔; edges drawn with broken lines correspond to value ⅓; edges with value 0 are not shown. The edges connecting a spin node to the exterior magnetic field node 0 appear as short lines pointed northeast. For clarity, they are not connected to 0. Note that the graph of Figure 7 has to be embedded in a torus. So the edges leaving the top line in the northerly direction must be identified with the corresponding edges leaving the bottom line in the southerly direction (e.g., nodes 6 and 10 are connected by an edge with value ⅔); similarly, the corresponding leftmost and rightmost edges must be identified (e.g., nodes 3 and 23 are connected by an edge of value ⅓).

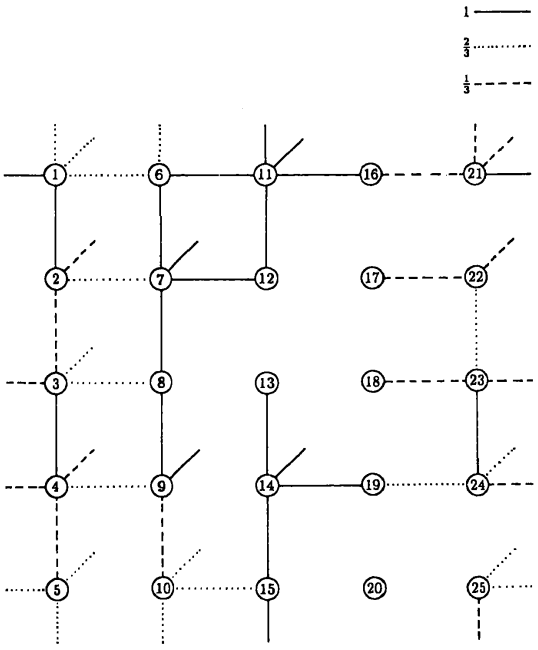

Figure 7. A fractional solution of a 5 × 5 grid problem with exterior field.

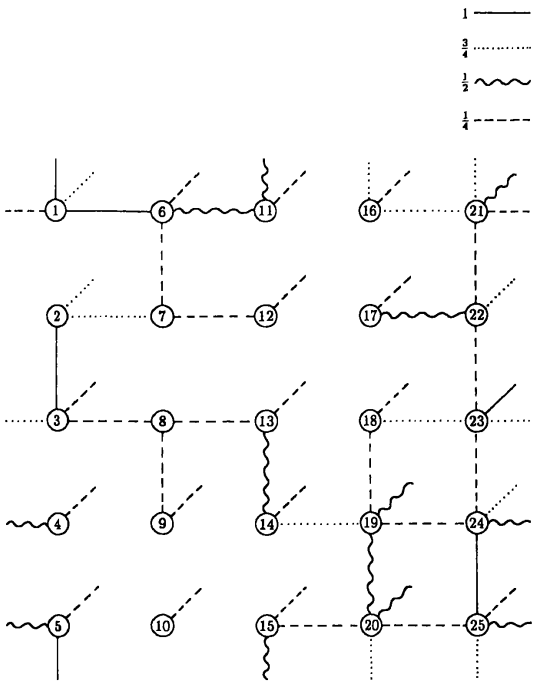

Figure 8. A fractional solution of a 5 × 5 problem in which our heuristic for detecting violated subdivided K_5 inequalities failed.

By visual inspection, we found that this fractional solution violates an inequality that can be obtained by subdividing edges of K_5. The violated inequality which, as shown by Barahona and Mahjoub, defines a facet of CUT(G), is the following (0 is the node corresponding to the exterior field, the nodes of K_5 are the nodes 0, 1, 3, 5, 25):

$$x_{0,1} + x_{0,3} + x_{0,5} + x_{0,25} + x_{1,2} + x_{1,5} + x_{1,21} - x_{2,3} + x_{3,4} - x_{3,23} - x_{4,5} + x_{5,25} - x_{21,25} + x_{23,24} - x_{24,25} \leq 6.$$

Substituting the solution shown in Figure 7 into the left-hand side of this inequality gives the value 20/3. We added this inequality to our LP and obtained an integral optimum solution in the next step. Based on this example, we invented a heuristic to search for violated "subdivided K_5-inequalities." One example in which this heuristic and all our further efforts failed is the fractional solution of a 5 × 5 problem, shown in Figure 8. We were unable to produce an inequality valid for CUT(G) that was violated by the solution of

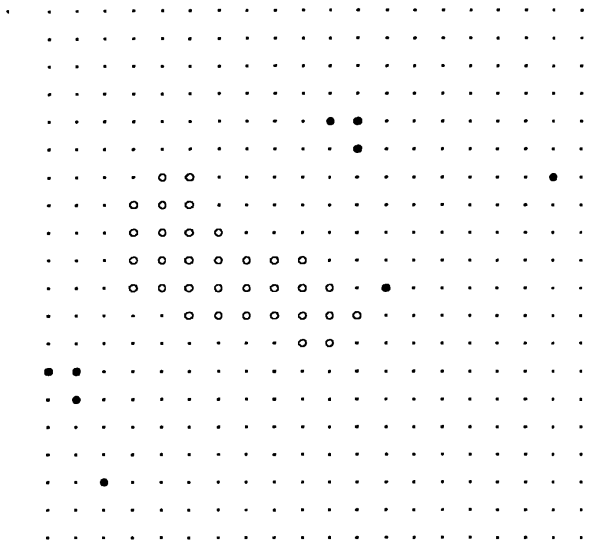

Figure 9. The effect of increasing the strength of the magnetic field on the ground state of a 20 × 20 spin glass system with ± 1 interactions.

Figure 8. But a few steps in a branch-and-bound method handles this case.

Finally, we would like to show an example of a ground state and the effect of increasing the strength of the exterior field. Given is a 20 × 20 grid on the torus with ±1 interactions. 14% of all interactions are negative. The strength of the exerior magnetic field is $h = 0.1$. Figure 9 shows a ground state of this problem. All spins represented by a "•" are pointing into the direction of the magnetic field (up). All other spins point downwards. Increasing the strength of the field to $h = 0.3$ flips a whole cluster of spins, those denoted by an open circle. Still, all "•"-spins point upward, as do all "O"-spins.

6. Final Remarks

In statistical physics, one is interested not only in calculating just one ground state; knowing all ground states or knowing certain properties of ground states (for example, the rigidity of bonds) is of equal importance. The algorithmic approach described in this paper is particularly well suited to obtain this type of information.

The computational experience described in Section 5 shows that, for all but a few ground-state problems, the optimum solution of our LP-relaxation of the max-cut problem was integral. This result puts all the tools of postoptimality analysis of linear programming at our disposal. For instance, using LP-duality we can often derive results that show that

- The ground state is unique, or that
- A certain cluster of spins will have the same relative orientation in all ground states (rigidity of the ground states).

Actually, in the examples of Section 5, we frequently observed that the ground states are unique. If the ground state is not unique, we can use reduced cost criteria to exhibit alternative ground states. We cannot produce all ground states (in reasonable time) since there may be exponentially many. Even so, LP-duality can be used to prove that certain edges have value one or zero in all ground states. From this information we can derive the fact that certain clusters of spins have the same relative orientation in all ground states. And thus, our methods enable us to determine the existence of long distance order. Let us remark that information of this type is hardly obtainable from enumerative or branch-and-bound methods.

A number of variations of the ground state problem are relevant for understanding spin glasses. Let us mention one question due to A. J. Bray and M. A. Moore (1986). Suppose a spin glass (Gaussian model) on a toroidal $k \times k$ grid without exterior magnetic field is given. Let ω be a ground state and E_g be its energy. We pick a column of spins of the grid and take an adjacent column of spins. The spins in the first column are fixed to their orientations in ω, while the spins in the second column are fixed to the orientations opposite those in ω. This fixing can be achieved by using the same trick as in via minimization to preassign pins and wire segments (i.e., add an exterior field and use $\pm M$ and zero forces). Let E_{+-} be the ground-state energy subject to this side condition. Set $\Delta E := |E_g - E_{+-}|$. It has been conjectured that $(\Delta E)^2 \sim k^\gamma$. In particular, that γ is negative. For the straightforward generalizations of this question to 3-dimensional grids, it is believed that γ is positive. Using the algorithm described in this paper, we can obtain, numerically, estimates for γ.

It is also possible to contribute to the open problem mentioned in Angles d'Auriac and Maynard, quoted earlier, by calculating ground states under the additional condition that the magnetization is zero. We can "misuse" the exterior magnetic field to formulate this problem as an integer linear program, but further

polyhedral studies are necessary before this approach can be used algorithmically.

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