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by
Michael Jünger, Giovanni Rinaldi

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Institut für Informatik
Universität zu Köln
Pohligstr. 1
50969 Köln

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Relaxations of the Max Cut Problem and Computation of Spin Glass Ground States

Michael Jünger[1] *and Giovanni Rinaldi*[2]

[1] Institut für Informatik, Universität zu Köln, GERMANY.
[2] Istituto di Analisi dei Sistemi e Informatica, CNR, Roma, ITALY.

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1 Introduction

A *cut* is the set of all the edges of a graph $G = (V, E)$ that go across the members of a partition of V in two sets. More precisely, for a subset $W \subseteq V$, which defines the partition $(W, \overline{W})$ (or, $(W, V \setminus W)$) of V, the associated cut is denoted by $\delta(W)$ and defined by

$$\delta(W) = \left\{(i,j) \in E \mid i \in W,\, j \in \overline{W}\right\},$$

where (i, j) denotes the edge with endpoints i and j. The sets W and $\overline{W}$ are called the *shores* of the cut $\delta(W)$. In the definition of a cut the case where one of the shores is the empty set and the other is the set V is *not* excluded. The cut corresponding to these two shores is the empty set and it is called the *empty cut*.

If G is connected, then for two distinct node sets A and B the edge sets $\delta(A)$ and $\delta(B)$ coincide if and only if $A = \overline{B}$. Therefore, the number of distinct cuts of G is half the number of the subsets of V, i.e., $2^{|V|-1}$.

Given a simple loop-less graph $G = (V, E)$ with $n = |V|$ nodes and $m = |E|$ edges, and a weight function $c\colon E \to \mathbb{R}$, which associates a weight c_{ij} (or c_e) with every edge $e = (i, j)$ of E, the *maximum cut problem* (*max-cut problem* for short) is to find a cut in G of maximum weight, where the weight of a cut is defined in the obvious way as the sum of the weights of its edges.

The max-cut problem is $\mathcal{NP}$-hard ([9]) and is one of the most interesting and studied problems in Combinatorial Optimization. Under some conditions on the graph G or on the weight function, max-cut is polynomially solvable, e.g., when G is planar. Since here we are interested in some computational issues concerning $\mathcal{NP}$-hard instances that occur in some relevant applications, we will not mention most of the theoretical results concerning max-cut and we will omit most of the important references to the literature. Excellent sources of information and of pointers are the book of Deza and Laurent [4] and the annotated bibliography of Laurent [10].

2 Spin glasses

A *spin glass* is an alloy of magnetic impurities (e.g., particles of iron) diluted in a "host" non-magnetic metal (e.g., gold). The magnetic impurities have a *spin*, i.e.,

a magnetic moment that can be described as a unit vector in $\mathbb{R}^3$. The magnetic field generated by the spin of a particle may interact with the spin of another. As a result, the spins of the two particles tend to be parallel and oriented in the same direction or in opposite directions. We say that there is a *positive interaction* in the first case and a *negative interaction* in the second. The magnetic moment of an impurity produces a magnetic polarization of the conduction electrons of the host which has an oscillatory behavior when the distance between impurities changes. A model of the interaction J of two particles at distance r is given, e.g., by

$$J(r) = A\frac{cos(Dr)}{Br^3},$$

where the constants A, B, and D depend on the material. Due to the random positions of the particles in the host, positive and negative interactions are equally possible. This fact makes the behavior of a spin glass particularly interesting. At relatively high temperature the thermal fluctuations make the spins chaotically oriented in all possible directions; the material reveals an anti-ferromagnetic behavior. At relatively low temperatures the effect of the interactions between impurities becomes dominant and the orientations of the spins tend to some stable ordered configurations that induce a local magnetization of the material.

This singular behavior of spin glasses has attracted a lot of interest. Fischer and Herts in a book [5] on spin glasses, an excellent reference for the interested reader, have estimated that in the 1980's more that 400 papers per year were published on spin glasses in the Physics literature. Researchers have developed several theories to explain the behavior of spin glasses. Some of these theories predict contradicting phenomena. Unfortunately it is very difficult to validate these theories by physical experiments: most of the interesting things happen when a spin glasses reaches a *ground state*, i.e., a spin configuration of minimal energy. To reach a ground state in a physical experiment the material has to be cooled towards 0^oK very slowly and a correct cooling process may take an excessive amount of time. For this reason some mathematical models have been developed to test these theories and the experiments are conducted via computer simulation.

The energy interaction between two particles i and j with spins S_i and S_j, respectively, is given by $H_{ij} = J_{ij}S_j \cdot S_j$, and so it is proportional to the interaction J_{ij} and to the scalar product of the two 3-dimensional vectors.

Consider now a spin glass having n spins in a given configuration ω (represented by n 3-dimensional vectors and suppose that the whole system is under an exterior magnetic field of strength h and orientation given by the 3-dimensional unit vector F. The energy of the system is given by the following Hamiltonian:

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

An important simplification in the study of the Hamiltonian is to assume that all the spins are parallel to each other and can only assume one of the two possible opposite orientations. This means that the 3-dimensional vector S_i that describes the orientation of spin i can now be replaced by the ± 1 variable s_i. Analogously, treating the exterior field as a spin with index 0, we can represent the orientation of the exterior field with the ± 1 variable s_0. The model that results from this simplification is called the *Ising model*.

Let us now associate a graph $G = (V, E)$ to a spin glass with n impurities. The node set is defined by $V = \{0, 1, \ldots, n\}$, while the edge set is given by all the pairs of indices that correspond to spins with nonzero mutual interaction.

A configuration is now any assignment of ± 1 values to the $(n+1)$-dimensional node-vector s, i.e., it is a partitioning of the node set V into two sets V^+ and V^-, made of all nodes with s-value $+1$, and -1, respectively. For $W \subseteq V$, let us denote by $\gamma(W)$ the set of edges of G having both the endpoints in W. Then, noticing that E can be partitioned into the three sets $\gamma(V^+)$, $\gamma(V^-)$, and $\delta(V^+)$, the Hamiltonian of the system can be written as

$$\begin{aligned} H(\omega) &= -\sum_{(i,j)\in\gamma(V^+)} J_{ij}s_is_j - \sum_{(i,j)\in\gamma(V^-)} J_{ij}s_is_j - \sum_{(i,j)\in\delta(V^+)} J_{ij}s_is_j \\ &= -\sum_{(i,j)\in\gamma(V^+)} J_{ij} - \sum_{(i,j)\in\gamma(V^-)} J_{ij} + \sum_{(i,j)\in\delta(V^+)} J_{ij} \\ &= -C + 2\sum_{(i,j)\in\delta(V^+)} J_{ij}, \end{aligned}$$

where $C = \sum_{(i,j)\in E} J_{ij}$ is a constant. Therefore, by assigning the weight $c_{ij} = -J_{ij}$ to each edge (i,j) in E, a configuration of minimal energy can be determined by computing a maximum c-weighted cut in G.

Several models of spin glasses have been considered depending on the type of interaction and on the range of the interactions. In the *Gaussian* models the values of the interactions are drawn from a Gaussian distribution with 0 mean and prescribed variance. In the $\pm J$ models the interaction may assume only the two values $\pm J$ drawn from a binary distribution. The *long range models* are those where any two spins may have a nonzero interaction; the associated graphs are dense. In the *short range models* the spins are assumed to be located at regular positions in 2- or 3-dimensional structures; a spin is supposed to interact only with its nearest neighbors. The resulting graphs are two or three dimensional grid graphs. In all cases the node corresponding to the exterior field is connected to any other node of the graph with a fixed interaction value.

When the size of the grid is not big enough to approximate a real spin glass, the behavior of the spin at the boundary of the grid may produce erratic results. For this reason often the extreme points of any line of the grid are assumed to be connected. The resulting graph is a toroidal two or three dimensional grid. These models are said to have *periodic boundary conditions.*

The only models whose ground state is known to be efficiently computable with a polynomial time algorithm for arbitrary interaction values are the 2-dimensional grid problems with no exterior magnetic field, since the associated graphs are planar. For all the other instances finding a ground state exactly is a difficult problem. For these reasons many researchers have done experiments where the max-cut problem is solved heuristically using Monte Carlo, genetic, evolutionary, and similar other methods.

A typical experiment goes along these lines: a number of instances is randomly generated; then for each instance the (approximate) ground state is computed and a corresponding physical quantity, e.g., the energy, is recorded. Finally, the average value of such a quantity and the statistical error are produced.

The results of such an experiment are affected by two kinds of errors:

- algorithmic errors, due to the fact that the energy computed is always an overestimation of the real one.

- statistical errors, due to the fact that the size of the instances produced and the number of instances analyzed are not big enough, due to the limited speed of the solution algorithms.

Therefore, the challenge for those who devise exact optimization algorithms is to find the exact optimal solution of large instances of max-cut in a reasonably short time. If this goal is reached, one can then run experiments whose results have no algorithmic errors and smaller statistical errors, because they can be based on larger instance sizes and on larger numbers of instances.

3 Formulations and relaxations of max-cut

A standard way to solve an $\mathcal{NP}$-hard combinatorial optimization problem exactly is to first formulate it as a mathematical programming problem and then to relax some of its constraints in order to solve it in polynomially time. The solution to the relaxed problem is finally used as a upper bound (in the case of maximization) in an enumeration scheme like branch-and-bound or branch-and-cut.

Depending on whether the variables of the mathematical programming problem describe the shores of a cut or its edges, we have the so called *node formulation* or the *edge formulation*, respectively.

3.1 Node formulation

This is the most natural formulation. A cut $\delta(W)$ of G is represented by a vector χ^W in $\mathbb{R}^V$, i.e., by a vector whose components are indexed by the nodes of G. For $u \in V$ the component χ^W_u associated with u is equal to 1 if $u \in W$ and is equal to -1 if $u \in \overline{W}$. Thus the solution set is quite simple, being the collection of all possible ± 1 n-dimensional vectors. However, the objective function is nonlinear: the contribution of the edge (i, j) to the objective function is 0 if $\chi^W_i = \chi^W_j$ and c_{ij} if $\chi^W_i = \chi^W_j$; therefore, if can be expressed as $c_{ij}(1 - \chi^W_i \chi^W_j)/2$.

Let $L(G, c)$ be the symmetric $n \times n$ matrix associated with G and c, whose entry ℓ_{ij} is defined by

$$\ell_{ij} = \begin{cases} -c_{ij} & \text{for } i \neq j \text{ and } (i,j) \in E \\ 0 & \text{for } i \neq j \text{ and } (i,j) \notin E \\ -\sum_{(i,k)\in\delta(\{i\})} c_{ik} & \text{for } i = j. \end{cases}$$

$L(G, c)$ is called the *Laplacian matrix*. Noticing that $(\chi^W_u)^2 = 1$ for all $u \in V$, it easy to check that the maximum cut problem can be formulated as follows:

$$\max \left\{ \frac{1}{4} x^T L(G, c) x \mid x \in \{-1, 1\}^n \right\}.$$

If we relax the feasible region to a sphere of radius $\sqrt{n}$ with origin 0, which clearly contains all the ± 1 points, the optimal value of the resulting problem can be given in closed form, once the largest eigenvalue $\lambda_{\max}$ of $L(G, c)$ has been computed. It

is actually given by $\frac{n}{4}\lambda_{\max}(L(G,c))$, which provides an upper bound to the problem that can be evaluated efficiently.

A better bound is based on the observation that if for $z \in \mathbb{R}^V$ we denote by $\mathrm{diag}(z)$ the diagonal matrix with the diagonal made of the components of the vector z and if z satisfies $e^T z = 0$, where $e \in \mathbb{R}^V$ is a vector of all 1's, then the value of a cut does not change if $\mathrm{diag}(z)$ is added to $L(G,c)$. On the other hand, the optimal value of the relaxation depends on z. Therefore one can compute the upper bound

$$\phi(G,c) = \frac{n}{4}\inf\left\{\lambda_{\max}(L(G,c) + \mathrm{diag}(z) \mid z \in \mathbb{R}^V, e^T z = 0\right\}. \qquad (1)$$

This bound can be computed quite efficiently if G is sparse, since the sparsity of the matrix $L(G,c)$ can be exploited. The bound has been computed by Poljak and Rendl [12] on graphs of sizes up to a few hundred nodes. The same authors also report on optimal solutions, obtained by inserting the computation of the bound in a branch-and-bound framework, for graphs of sizes up to 80 nodes.

3.2 Edge formulation: the semidefinite relaxation

Let x be an n-dimensional ± 1 vector that can be interpreted as a descriptor of the cut $\delta(S)$ of G, according to the node formulation of the previous section. Consider the matrix $X = xx^T$. The matrix X has the following properties that can be easily verified: (i) X is symmetric; (ii) each diagonal entry of X is equal to 1; (iii) X is positive semidefinite (psd); (iv) the entry x_{ij} of X is equal to -1 if the edge (i,j) belongs to the cut $\delta(S)$; hence the weight of $\delta(S)$ can be expressed as $\mathrm{tr}(L(G,c)X)$, where $\mathrm{tr}(A)$ is the *trace* of A, i.e., the sum of its diagonal entries; (v) X is integer.

On the other hand, any matrix X satisfying the above five conditions can be written as xx^T, where x is the descriptor of a cut. From the conditions (i) and (ii) it is clear that the the matrix X represents $\binom{n}{2}$ variables, one for each edge of a complete graph on n nodes; therefore the conditions (i)–(v) provide an edge formulation of the max-cut problem.

The optimal value of the following *semidefinite programming problem*, obtained by relaxing condition (v), gives an upper bound of the value of the maximum cut of G:

$$\psi(G,c) = \frac{1}{4}\max\left\{\mathrm{tr}(L(G,c)X) \mid X \text{ is symmetric and psd, } \mathrm{diag}(X) = e\right\}. \qquad (2)$$

Using semidefinite programming duality, Poljak and Rendl [11] proved that $\phi(G,c) = \psi(G,c)$.

Using interior point techniques a semidefinite programming problem, i.e., a problem where a matrix is constrained to be psd and its entries satisfy linear inequalities and equations, can be solved very efficiently. However it is not clear yet how the sparsity of the matrix $L(G,c)$ can be exploited. The solution of (2) is considerably faster than the solution of (1) when G is dense.

Another advantage of the bound given by (2) is that the relaxation can be strengthened by adding inequalities on the entries of the matrix X that come from the polyhedral relaxations of the max-cut problem (see the following section). Such an approach has been successfully tried by Helmberg and Rendl [7], who report on the solution of several instances with sizes up to 100 nodes to optimality.

3.3 Edge formulation: the polyhedral relaxations

With every cut $\delta(S)$ of G we associate an incidence vector $y^S \in \mathbb{R}^E$ defined to have all the components corresponding to the edges of $\delta(S)$ at value 1 and all the others at value 0. Thus a cut is represented by an m-dimensional 0–1 vector.

The convex hull of the incidence vectors of all the cuts of G is the *cut polytope* associated to G that we denote here by P_G.

If a description of P_G were known in terms of linear inequalities, the max-cut problem could be solved, in principle, by maximizing the linear function $c^T y$ over P_G using linear programming techniques.

Since a complete system of linear inequalities describing P_G for any graph G is not known, one usually considers a *polyhedral relaxation* of P_G, i.e., a polytope containing P_G whose linear system is fully described. Each inequality of this system has to be *valid* for P_G, i.e., must be satisfied by the incidence vectors of all the cuts of G.

There are two requirements that a polyhedral relaxation should satisfy. The first is that every feasible integral point should be the incidence vector of a cut. A second is that every inequality of its defining system should not be dominated by another valid inequality for P_G.

To satisfy the first requirement we should find out whether any 0–1 m-dimensional vector is the incidence vector of a cut. Since, unlike in the case of the node formulation, the answer is no, we have to find some combinatorial property that is satisfied by all the edge sets that are cuts and is violated by all the others.

Such a property fortunately exists and is very simple: the intersection of every cut of G with every cycle of G has even cardinality. Moreover, if a subset of E has an intersection of even cardinality with all the cycles of G, then it is a cut.

The translation of the above property into a system of linear inequalities is as follows:

$$\sum_{e \in F} (1 - y_e) + \sum_{e \in C \setminus F} y_e \geq 1, \quad \begin{array}{l} \text{for each cycle } C \text{ of } G \text{ and} \\ \text{for each } F \subseteq C \text{ with } |F| \text{ odd.} \end{array} \tag{3}$$

The inequalities (3) are called *cycle inequalities*. It is easy to verify that if a subset E' of E intersects a cycle of G in an odd number of edges F', the inequality defined by such a cycle and by F' is violated by the incidence vector of E'. Moreover it is easy to show that the incidence vector of any cut of G satisfies all the inequalities (3).

Finally, to make sure that y is an incidence vector, the following *trivial inequalities* have to be added to the system:

$$0 \leq y_e \leq 1 \quad \text{for each } e \in E. \tag{4}$$

The system (3)–(4) provides a polyhedral relaxation, called the *semimetric polytope* M_G, whose integral points are exactly the incidence vectors of all the cuts of G. Thus, the system (3)–(4) along with the integrality requirement on y and the objective function $c^T y$, yields an integer linear programming formulation for max-cut.

It is easy to see that if the cycle C has a chord, the corresponding inequalities (3) are dominated by a positive combination of other cycle inequalities. Moreover, if an edge e belongs to a *triangle* (a complete 3-node subgraph) of G, then the

corresponding inequalities (4) are dominated by a positive combination of cycle inequalities.

Barahona and Mahjoub in [1] did a first systematic study of the cut polytope and proved, among many other results, that the cycle inequalities defined by chord-less cycles and the trivial inequalities defined by edges that do not belong to a triangle of G define facets of P_G, which means that the system of these inequalities satisfies the second of the above two requirements.

4 Optimizing over the semimetric polytope

The typical instances that come from spin glass models have several thousand nodes. However their graph are rather sparse. For example, a toroidal 2-dimensional $k \times k$ grid with an extra node that represents the field has k^2+1 nodes but only $3k^2$ edges.

At the present state of the art neither the algorithm based on the node formulation nor those based on the semidefinite relaxation can be used to solve these kinds of instances. To the contrary, the polyhedral relaxation based on the inequalities (3)–(4), has been shown to be pretty effective on them.

How difficult is it to optimize a linear function on the semimetric polytope M_G?

A fundamental result in Polyhedral Combinatorics (see, e.g., [6]) states that one can optimize in polynomial time a linear function over a polytope P if and only if one can solve in polynomial time the following separation problem: "Given a point x, find an inequality valid for P that is violated by x, or prove that x belongs to P".

For a complete graph the system defining M_G has polynomial size, thus the separation can be carried out exhaustively. For general graphs the inequality system may have exponential size, yet a simple polynomial time algorithm is available that solves the separation problem (see, e.g., [1]).

We have integrated an efficient implementation of the separation algorithm for the semimetric polytope in a branch and cut scheme. The resulting software solves instances which are considerably larger than those solved in the literature and performs much faster than any other software. For example, using this software it was possible to carry out two experiments on a large number of instances of large size. [2] and [3] report on two experiments on 2-dimensional grids with Gaussian and $\pm J$ interactions, respectively, each based on more that $20,000$ instances on toroidal grids with sizes ranging from 5×5 to 100×100.

For 3-dimensional grids the situation is quite different: only grids of moderate sizes can be handled. To analyze larger grids a relaxation for P_G stronger than the semimetric one would be necessary.

5 Computation of the exact susceptibility

An important parameter associated with each configuration ω of a spin glass is its *magnetization* $\mu = |V^+| - |V^-|$. When the glass is subject to an exterior magnetic field of strength h, it is interesting to compute the magnetization as a function

of h. Such a function is called the *susceptibility function* of the glass, it is stepwise constant, and it takes a constant value $|V|$ for all h larger that some value $\overline{h}$.

If we compute the susceptibility function for a large number of instances and we take the average, we obtain a continuous function that can be well approximated, at least in a neighborhood of the origin, with the function $\alpha h^{\frac{1}{\delta}}$. The parameter δ plays an important role in the study of the long range model and its accurate estimation requires the exact computation of the susceptibility function.

Usually, in the literature the susceptibility is computed by solving a series of max-cut instances obtained from the same instance by taking for h the values 0, τ, 2τ, 3τ, ..., for a value τ sufficiently small. Although each instance is solved to optimality, the susceptibility obtained this way is only an approximation of the real one. The smaller the step size τ the better is the approximation but the larger is the number of instances to be solved to optimality.

Assume now that we have a polyhedral relaxation of P_G that is tight enough to provide integral optimal solutions for all the objective functions of interest and that the separation problem for this relaxation is polynomially solvable. This means that for these objective functions we can solve the max-cut problem with a *pure* cutting-plane algorithm without any recourse to enumeration, variable fixing, and all the other tricks that are usually exploited in a state-of-the-art branch-and-cut algorithm. Under this assumption, the susceptibility function can be computed exactly. We briefly describe how this can be done.

Let $Bx \leq b$ denote the finite system of inequalities describing P_G and x^* the optimal solution to the problem

$$\max\{cx \mid Bx \leq b\}. \tag{5}$$

As $Bx \leq b$ is a huge system and impossible to represent explicitly, by the assumption we can think that x^* has been obtained by a pure cutting plane procedure in a finite number of steps. From x^* we can readily compute the magnetization μ^*. We can assume that c corresponds to a spin glass instance with a given value of the field strength h. Let d be the incidence vector of the set of the edges incident to node 0, which represents the exterior field. We want to know the minimum value $\overline{\alpha}$ of α for which problem (5), with the new objective function $c + \alpha d$, yields an optimal solution different from x^*. With this new solution we can compute the value of the magnetization that immediately follows μ^* in the exact susceptibility function and the field strength $h + \overline{\alpha}$ at which the change occurs. If we can compute the value $\overline{\alpha}$, the function can be determined exactly by solving at most $|V|$ times problem (5) with different objective functions.

It is not difficult to show that the sought value for α can be computed by solving the problem

$$-t \max\left\{cx - cx^* \mid Bx \leq b,\ dx \leq dx^* + \frac{1}{t}\right\}, \tag{6}$$

where t is a scalar small enough to make x^* the only integral feasible point.

Again, problem (6) can be solved exactly in practice if the relaxation at hand is "tight enough". Quite surprisingly, this is the case for the semimetric relaxation for 2-dimensional toroidal grids and Gaussian interactions. In [13] it is reported that, using this technique, it was possible to compute the parameter δ with high accuracy. It is amazing that the computed value disagrees substantially with the value predicted by the *scaling theory* (see, e.g., [5] for details).

When the interactions are of $\pm J$ type or in the case of 3-dimensional toroidal grids, the semimetric relaxation is totally inadequate for this technique. Evidently this fact calls for stronger relaxations of P_G.

6 Beyond the semimetric relaxation

The polytope P_{K_p}, the cut polytope for a complete graph with p nodes, has been extensively studied and a number of families of valid inequalities, several of them facet defining for P_{K_p}, have been described. In addition, for some of these inequalities separation procedures have been proposed (see, e.g., [4] for a survey).

How can these results be used when the graph is not complete? A trivial way to exploit the current knowledge about P_{K_p} for the case of an arbitrary graph G, is to add the missing edges to G and assigning them a zero weight, in order to obtain an artificial complete graph. Such a technique has been successfully used for other combinatorial problems, where the sparsity of the original graph can actually be exploited to handle the artificial complete graph efficiently. This is the case, for example, for the traveling salesman problem. On the contrary, for the max-cut there is no obvious way to exploit the sparsity of the original problem. This means that if one uses the above technique, the exact solution of max-cut on sparse graphs has the same computational difficulties of the max-cut on complete graphs. Unfortunately, applications of max-cut, like the study of minimal energy configurations in spin glasses, require the exact solution of instances with several thousand nodes. Therefore, the solution of these instances is out of reach, unless the problem is solved in the original sparse graph.

On the other hand, there is no obvious way to use the description of P_{K_p} by linear inequalities to obtain an equivalent description of P_G, where G an arbitrary subgraph of $K_p = (V_p, E_P)$. Moreover, after the publication of the paper by Barahona and Mahjoub [1], very little effort was devoted to the study of P_G on arbitrary graphs.

A first step towards closing the gap of polyhedral knowledge between the max-cut problem in general and in complete graphs is made in [8] where a technique is described that we outline here.

We are given a point $\overline{x}_n \in \mathbb{R}^E$ that satisfies all the inequalities (3)–(4) but does not belong to P_G. We want to find an inequality valid for P_G (possibly facet defining) that is not satisfied by $\overline{x}_n$. To do so, we want to use the algorithmic and the structural results that are available for P_{K_p}.

First, by a sequence of operations, $\overline{x}_n$ is transformed to $\overline{x}_p \in \mathbb{R}^{E_p}$, where p is usually much smaller than n. The point $\overline{x}_p$ is guaranteed to be outside P_{K_p} but to satisfy (3)–(4). It can be seen as a fractional solution of a cutting plane algorithm applied to an max-cut instance on the complete graph K_p.

At this point all the machinery available for the max-cut on complete graphs can be used. Therefore, some separation procedures for the cut polytope on complete graphs are applied to $\overline{x}_p$ that (hopefully) generate an inequality $a_p x_p \geq \alpha$, valid for P_{K_p} and violated by $\overline{x}_p$.

Finally, a sequence of lifting procedures is applied to $a_p x_p \geq \alpha$ that transforms it to an inequality $a_n x_n \geq \beta$ valid for P_G and violated by $\overline{x}_n$.

As a by-product, one of these lifting procedures provides a simple way to generate facet defining inequalities for P_G.

In conclusion, these separation and lifting procedures enrich the description by linear inequalities of P_G on arbitrary graphs and yield a relaxation that is stronger than the semimetric polytope.

We only have very preliminary computational results with the new relaxation of P_G. For example, for 243 out of the 20 000 "Gaussian" instances examined in [2] the recurse to branching was necessary to get the optimal solution using the semimetric relaxation. With the new relaxation this happened only for one problem; in addition, it is possible to solve problem (6) also for $\pm J$ instances of moderate size and to reduce the computation time for 3-dimensional grids by a factor of ten.

References

[1] F. Barahona and A.R. Mahjoub. On the cut polytope. *Mathematical Programming*, 36:157–173, 1986.

[2] C. De Simone, M. Diehl, M. Jünger, P. Mutzel, G. Reinelt, and G. Rinaldi. Exact ground states of Ising spin glasses: New experimental results with a branch and cut algorithm. *Journal of Statistical Physics*, 80:487–496, 1995.

[3] C. De Simone, M. Diehl, M. Jünger, P. Mutzel, G. Reinelt, and G. Rinaldi. Exact ground states of $2D \pm J$ Ising spin glasses. *Journal of Statistical Physics*, 84:1363–1371, 1996.

[4] M. Deza and M. Laurent. Cut Polyhedra and Metrics. Springer, Berlin, 1997.

[5] K.H. Fischer and J.A. Hertz. *Spin Glasses.* Cambridge University Press, Cambridge, 1991.

[6] M. Grötschel, L. Lovász, and A. Schrijver. *Geometric Algorithms and Combinatorial Optimization.* Springer, Berlin, 1988.

[7] C. Helmberg and F. Rendl. Solving quadratic $(0,1)$-problems by semidefinite programs and cutting planes. To appear in *Mathematical Programming.*

[8] M. Jünger, G. Reinelt, G. Rinaldi. Lifting and separation procedures for the cut polytope. In preparation.

[9] R.M. Karp. Reducibility among combinatorial problems. In R.E. Miller and J.W. Thather, editors, *Complexity of Computer Computation*, pages 85–103. Plenum Press, New York, 1972.

[10] M. Laurent. The max-cut problem. In M. Dell'Amico, F. Maffioli, and S. Martello, editors, *Annotated Bibliographies in Combinatorial Optimization.* Wiley, Chichester, 1997.

[11] S. Poljak and F. Rendl. Nonpolyhedral relaxations of graph-bisection problems. *SIAM Journal on Optimization*, 5:467–487, 1995.

[12] S. Poljak and F. Rendl. Solving the max-cut problem using eigenvalues. *Discrete Applied Mathematics*, 62:249–278, 1995.

[13] H. Rieger, S. Santen, U. Blasum, M. Diehl, M. Jünger, and G. Rinaldi. The critical exponents of the two-dimensional Ising spin glass revisited: exact ground-state calculations and Monte Carlo simulations. *J. Phys. A: Math. Gen.* 29:3939–3950, 1996.