Mathematical Programming manuscript No.
(will be inserted by the editor)

Michael Jünger · Volker Kaibel

Box-Inequalities for Quadratic Assignment Polytopes

Received: date / Revised version: date

Abstract. Linear Programming based lower bounds have been considered both for the general as well as for the symmetric quadratic assignment problem several times in the recent years. Their quality has turned out to be quite good in practice. Investigations of the polytopes underlying the corresponding integer linear programming formulations (the non-symmetric and the symmetric quadratic assignment polytope) have been started during the last decade [34, 31, 21, 22]. They have lead to basic knowledge on these polytopes concerning questions like their dimensions, affine hulls, and trivial facets. However, no large class of (facet-defining) inequalities that could be used in cutting plane procedures had been found. We present in this paper the first such class of inequalities, the box inequalities, which have an interesting origin in some well-known hypermetric inequalities for the cut polytope. Computational experiments with a cutting plane algorithm based on these inequalities show that they are very useful with respect to the goal of solving quadratic assignment problems to optimality or to compute tight lower bounds. The most effective ones among the new inequalities turn out to be indeed facet-defining for both the non-symmetric as well as for the symmetric quadratic assignment polytope.

1. Introduction

The *quadratic assignment problem* shares (at least) one property with many interesting questions in mathematics: It can be stated very easily, but its solution is extremely hard. Koopmans and Beckmann [28] introduced this problem in order to model the situation where n objects, having flows f_{ik} between each other, have to be assigned to n locations (with distances d_{jl} between each other) by a permutation π such that the sum $\sum_{i,k} f_{ik} d_{\pi(i)\pi(k)} + \sum_i c_{i\pi(i)}$ is minimized, where c_{ij} is the *linear cost* for assigning object i to location j. The problem we will deal with is a generalization due to Lawler [29], who formulated the quadratic assignment problem as the task to minimize a polynomial of degree

Michael Jünger: Institut für Informatik, Universität zu Köln, Pohligstr. 1, 50969 Köln, Germany, mjuenger@informatik.uni-koeln.de

Volker Kaibel: MA 6–2, TU Berlin, Straße des 17. Juni 136, 10623 Berlin, Germany, kaibel@math.TU-Berlin.de

Mathematics Subject Classification (1991): 90C57, 90C27

two in the entries of the permutation matrices:

$$
\begin{aligned}
(\mathrm{QAP})_{g,h}^{(n)} \qquad & \min \sum_{\substack{i,k=1\\ i<k}}^{n} \sum_{\substack{j,l=1\\ j\neq l}}^{n} h_{ijkl} x_{ij} x_{kl} + \sum_{i=1}^{n}\sum_{j=1}^{n} g_{ij} x_{ij} \\
& \text{s.t.} \sum_{j=1}^{n} x_{ij} = 1 \qquad (i \in \{1,\dots,n\}) \\
& \sum_{i=1}^{n} x_{ij} = 1 \qquad (j \in \{1,\dots,n\}) \\
& x_{ij} \in \{0,1\} \qquad (i,j \in \{1,\dots,n\})
\end{aligned}
$$

The *symmetric quadratic assignment problem* is restricted to those instances where the coefficients in the Lawler formulation satisfy the equations $h_{ijkl} = h_{ilkj}$. For example, a Koopmans/Beckmann instance with a symmetric flow or a symmetric distance matrix leads to a symmetric quadratic assignment problem (since in this case, we have $h_{ijkl} = f_{ik}d_{jl} + f_{ki}d_{lj}$).

The most successful algorithms that have emerged from the attempts to find practical solution procedures for this $\mathcal{NP}$-hard combinatorial optimization problem during the past 40 years are branch-and-bound algorithms. Until very recently, these algorithms usually used the lower bound proposed by Gilmore [17] and Lawler [29] (for the history and bibliographic information we refer, e.g., to [32, 7, 10, 8]). By appropriate implementations for high performance parallel computers, the "world record" sizes for exactly solved instances have been pushed slightly beyond $n = 20$ in the mid 90's [12, 11, 6]. Recently, branch-and-bound codes exploiting more elaborate procedures for computing lower bounds have been successfully implemented [19, 5]. Currently, the "world record" (by Anstreicher, Brixius, Goux, and Linderoth [2]) is the solution of several instances with $n = 30$ (e.g., `nug30` from the QAPLIB, which is the commonly used set of test instances compiled by Burkard, Karisch, and Rendl [9]).

However, all these codes usually generate extremely large branch-and-bound trees. This, of course, evokes the wish for better lower bounding procedures than the ones that are currently used. One of the tightest bounding procedures that have been developed arises from an integer linear programming formulation of the quadratic assignment problem that was introduced by Adams and Johnson in the early 90's [20, 1]. They proved that the linear programming relaxation coming from their formulation yields a bound that always is at least as good as the Gilmore/Lawler bound. In fact, at that time these bounds turned out to be the best known bounds for most instances in the QAPLIB [33]. However, compared with the effort that it takes to solve the linear programs, they are still too weak. A way to improve the strength of these linear programming based bounds is to investigate the polyhedral structure of the quadratic assignment problem, as it was done successfully for many other combinatorial optimization problems, like, e.g., the *traveling salesman problem*.

The polyhedral knowledge on the quadratic assignment problem is at an early stage. Padberg and Rijal [34, 31] found answers to some very first questions concerned with the associated polytope, such as its dimension, affine hull, and trivial facets. These results had partially already been obtained in a paper of Barvinok [3], where the connection between the theory of representations of finite groups and combinatorial optimization polyhedra are considered. However, it seems that the approach of Barvinok is difficult to apply to deeper polyhedral studies, and the work of Padberg and Rijal showed that a simple "classical" polyhedral treatment of the problem yields enormous technical difficulties even for, e.g., the dimension proof. This might be the most important reason that kept the development of the polyhedral approach to the quadratic assignment problem from proceeding a major step.

In this paper, we present the first large class of facet defining inequalities (the *box inequalities*) for both the polytope that is naturally associated with the quadratic assignment problem, as well as for a polytope, which is especially associated with the symmetric quadratic assignment problem. The consideration of this latter polytope was already suggested in [34,31], since it corresponds to an integer linear programming formulation (for symmetric instances) with roughly half as many variables as the non-symmetric one has.

The paper is organized as follows. Section 2 briefly presents the necessary background on the polyhedral approach to the quadratic assignment problem. In particular, a technique (the "star-transformation") that we have developed [22] in order to overcome the technical difficulties mentioned above is reviewed. We introduce the box inequalities in Section 3 and describe their origin in some well-known *hypermetric inequalities* for the cut polytope. In Section 4 the box inequalities are investigated with respect to their meaning for the face lattices of the quadratic assignment polytopes. In particular, we prove that a large subclass of these inequalities are facet-defining for these polytopes. The computational experiments on which we report in Section 5 show that the box inequalities for the first time open up the possibility of attacking quadratic assignment problems successfully with cutting plane procedures. Our preliminary pure cutting plane algorithm is able to solve several instances from the QAPLIB to optimality and produces significantly increased lower bounds for many others. We conclude with a brief discussion of the promising directions of the further polyhedral investigations of the quadratic assignment problem in Section 6.

Throughout the paper, we denote by $\mathbb{R}^I$ (for any finite set I) the vector space $\mathbb{R}^{|I|}$, where the vectors are indexed by the elements of I.

2. Quadratic Assignment Polytopes

This section is intended to give a short introduction into some polyhedral constructions for the quadratic assignment problem. It provides the basic background that will be needed in the subsequent sections. For a detailed treatment (including the proofs of the statements in this section) we refer to [21,22].

Definitions of the Polytopes $\mathcal{QAP}_n$ and $\mathcal{SQAP}_n$. In order to profit from the convenient notions of graph theory, we formulate the quadratic assignment problem as a (hyper)graph problem. For a set M and a cardinality $\kappa \in \mathbb{N}$ we denote by $\binom{M}{\kappa}$ the set of all subsets $N \subseteq M$ with $|N| = \kappa$. Let $\mathcal{G}_n = (\mathcal{V}_n, \mathcal{E}_n)$ be the graph defined on n^2 nodes $\mathcal{V}_n = \{1, \dots, n\} \times \{1, \dots, n\}$ with edges

$$\mathcal{E}_n = \left\{ \{(i,j),(k,l)\} \in \binom{\mathcal{V}_n}{2} \middle| \, i \neq k, j \neq l \right\}.$$

The n-cliques in $\mathcal{G}_n$ correspond to the $n \times n$-permutation matrices, and thus to all possible assignments of n objects to n locations. We denote the edges of $\mathcal{G}_n$ by $[i,j,k,l] = \{(i,j),(k,l)\}$. The sets $\text{row}_i = \{(i,j) \mid 1 \leq j \leq n\}$ and $\text{col}_j = \{(i,j) \mid 1 \leq i \leq n\}$ are called the *i-th row* and the *j-th column* of $\mathcal{V}_n$, respectively. Weighting the nodes of this graph by the linear terms coefficients g_{ij} of the Lawler formulation $(\text{QAP})_{g,h}^{(n)}$ and putting the weights h_{ijkl} on the edges $[i,j,k,l]$, the quadratic assignment problem becomes equivalent to finding a minimally node- and edge-weighted n-clique in $\mathcal{G}_n$.

In the symmetric case (i.e., the equations $h_{ijkl} = h_{ilkj}$ hold), we consider a hypergraph $\hat{\mathcal{G}}_n = (\mathcal{V}_n, \hat{\mathcal{E}}_n)$ defined on the same node set $\mathcal{V}_n$, but having hyperedges

$$\hat{\mathcal{E}}_n = \left\{ \{(i,j),(k,l),(i,l),(k,j)\} \in \binom{\mathcal{V}_n}{4} \middle| \, i \neq k, j \neq l \right\}.$$

A hyperedge is denoted by $\langle i,j,k,l \rangle = \{(i,j),(k,l),(i,l),(k,j)\}$. We call the edge $[i,j,k,l]$ the *mate* of the edge $[i,l,k,j]$. Hence, the hyperedges of $\hat{\mathcal{G}}_n$ are the unions of pairs of mates of edges of $\mathcal{G}_n$. In particular, the number of edges of $\mathcal{G}_n$ is twice the number of hyperedges of $\hat{\mathcal{G}}_n$.

We call a subset $C \subset \mathcal{V}_n$ a *clique of* $\hat{\mathcal{G}}_n$ if it is a clique of $\mathcal{G}_n$, and we consider a hyperedge $\langle i,j,k,l \rangle$ *belonging* to a clique $C \subset \mathcal{V}_n$ of $\hat{\mathcal{G}}_n$ if $(i,j),(k,l) \in C$ or $(i,l),(k,j) \in C$ holds. Weighting the nodes as in the non-symmetric case and the hyperedges $\langle i,j,k,l \rangle$ by h_{ijkl} (or, equivalently, by h_{ilkj}), the quadratic assignment problem in the symmetric case is to find a minimally node- and hyperedge-weighted n-clique in $\hat{\mathcal{G}}_n$.

We fix a few notations concerned with these (hyper)graphs. For a subset $W \subseteq \mathcal{V}_n$ of nodes the set of all edges of $\mathcal{G}_n$ with both end nodes in W is denoted by $\mathcal{E}_n(W)$, and $\hat{\mathcal{E}}_n(C)$ is the set of all hyperedges of $\hat{\mathcal{G}}_n$ belonging to C. For two disjoint subsets $S, T \subseteq \mathcal{V}_n$, the set of all edges of $\mathcal{G}_n$ with one end-node in S and the other one in T is $(S : T)$. We often, also in other contexts, omit the brackets for singleton sets and write, e.g., $(v : T)$ in case of $S = \{v\}$. If $x \in \mathbb{R}^{\mathcal{V}_n}$ is a vector indexed by the nodes $\mathcal{V}_n$, and $W \subseteq \mathcal{V}_n$ is a subset of nodes, then $x(W)$ denotes the sum $\sum_{v \in W} x_v$ of all components of x that are associated with nodes in the subset W. Similarly, $y(F)$ and $z(\hat{F})$ are defined for vectors $y \in \mathbb{R}^{\mathcal{E}_n}$, $z \in \mathbb{R}^{\hat{\mathcal{E}}_n}$, and subsets $F \subseteq \mathcal{E}_n$, $\hat{F} \subseteq \hat{\mathcal{E}}_n$. For a subset $W \subseteq \mathcal{V}_n$ the *characteristic vector* $x^W \in \mathbb{R}^{\mathcal{V}_n}$ of W in $\mathcal{V}_n$ is defined via $x_v^W = 1$ for $v \in W$ and $x_v^W = 0$ for $v \notin W$. Analogously, characteristic vectors $y^F \in \mathbb{R}^{\mathcal{E}_n}$ and $z^{\hat{F}} \in \mathbb{R}^{\hat{\mathcal{E}}_n}$ are defined for subsets $F \subseteq \mathcal{E}_n$ and $\hat{F} \subseteq \hat{\mathcal{E}}_n$ of (hyper)edges.

With these definitions, we can now easily introduce the two objects that are at the center of interest in this paper. The *(non-symmetric) quadratic assignment* *polytope* is the convex hull of all characteristic vectors of n-cliques of $\mathcal{G}_n$

$$\mathcal{QAP}_n = \operatorname{conv}\left\{ (x^C, y^{\mathcal{E}_n(C)}) \,\middle|\, C \text{ is an } n\text{-clique of } \mathcal{G}_n \right\}.$$

The *symmetric quadratic assignment polytope* is the convex hull of the characteristic vectors of the n-cliques in the hypergraph $\hat{\mathcal{G}}_n$:

$$\mathcal{SQAP}_n = \operatorname{conv}\left\{ (x^C, z^{\hat{\mathcal{E}}_n(C)}) \,\middle|\, C \text{ is an } n\text{-clique of } \hat{\mathcal{G}}_n \right\}$$

There is an important relation between these two polytopes: The symmetric quadratic assignment polytope $\mathcal{SQAP}_n$ is the image of the non-symmetric one $\mathcal{QAP}_n$ under a certain linear map. Let us call an inequality $(u,v)^T(x,y) \leq \omega$ (with $(u,v) \in \mathbb{R}^{\mathcal{V}_n} \times \mathbb{R}^{\mathcal{E}_n}$) *symmetric* if the equations $v_{[i,j,k,l]} = v_{[i,l,k,j]}$ hold for all pairs of mates. Obviously, a symmetric valid inequality $(u,v)^T(x,y) \leq \omega$ for $\mathcal{QAP}_n$ immediately gives rise to a valid inequality $(u,\hat{v})^T(x,z) \leq \omega$ for $\mathcal{SQAP}_n$ by defining $\hat{v}_{\langle i,j,k,l \rangle} = v_{[i,j,k,l]}$ (or, equivalently, $\hat{v}_{\langle i,j,k,l \rangle} = v_{[i,l,k,j]}$). Furthermore, if the inequality $(u,v)^T(x,y) \leq \omega$ is facet-defining for $\mathcal{QAP}_n$ then so is the inequality $(u,\hat{v})^T(x,z) \leq \omega$ for $\mathcal{SQAP}_n$ [21]. Therefore, we are especially interested in symmetric (facet-defining) inequalities for the polytope $\mathcal{QAP}_n$, because they can immediately also be used for the symmetric case.

The Star-Transformation. The vertices of the polytopes $\mathcal{QAP}_n$ and $\mathcal{SQAP}_n$ have a coordinate structure that makes investigations with respect to questions like the dimension of the polytopes or the dimension of certain faces of them quite difficult. However, after a suitable isomorphic transformation of the polytopes the situation becomes much more convenient. For a detailed treatment see [22]. Here, we only review the transformation for the non-symmetric case, since we can reduce all questions arising in this paper that concern the symmetric quadratic assignment polytope to the non-symmetric case by exploiting the connection between these two polytopes described in the previous paragraph.

The basic observation is that the orthogonal projection of $\mathbb{R}^{\mathcal{V}_n} \times \mathbb{R}^{\mathcal{E}_n}$ onto $\mathbb{R}^{\mathcal{V}_{n-1}} \times \mathbb{R}^{\mathcal{E}_{n-1}}$ that simply "forgets" all components belonging to any nodes in the n-th row or in the n-th column or to any edges that share a node with the n-th row or with the n-th column, maps the polytope $\mathcal{QAP}_n$ isomorphically into the lower-dimensional vector space $\mathbb{R}^{\mathcal{V}_{n-1}} \times \mathbb{R}^{\mathcal{E}_{n-1}}$. With $n^\star = n-1$ we call the image of $\mathcal{SQAP}_n \subset \mathbb{R}^{\mathcal{V}_n} \times \mathbb{R}^{\mathcal{E}_n}$ under this projection $\mathcal{QAP}^\star_{n^\star} \subset \mathbb{R}^{\mathcal{V}_{n^\star}} \times \mathbb{R}^{\mathcal{E}_{n^\star}}$. The polytope $\mathcal{QAP}^\star_{n^\star}$ is the convex hull of all characteristic vectors of $n^\star$- and $(n^\star-1)$-cliques of $\mathcal{G}_{n^\star}$. Furthermore, if an inequality defining a face $\mathcal{F}$ of $\mathcal{SQAP}_n$ has only zero-coefficients on components that belong to nodes in the n-th row or in the n-th column or to edges that share a node with the n-th row or with the n-th column then the "projected inequality" defines the face $\mathcal{F}^\star$ of $\mathcal{QAP}^\star_{n^\star}$ that is isomorphic to $\mathcal{F}$ via the isomorphism between $\mathcal{QAP}_n$ and $\mathcal{QAP}^\star_{n^\star}$. This implies that an inequality with zeroes on all coefficients belonging to variables that are "projected out" defines a facet of $\mathcal{QAP}_n$ if and only if its "projection" defines a facet of $\mathcal{QAP}^\star_{n^\star}$.

In [22] it is proved that the following equation system describes the affine hull of the polytope $\mathcal{QAP}^\star_{n^\star}$:

$$x(\mathrm{row}_i \cup \mathrm{row}_k) - y(\mathrm{row}_i : \mathrm{row}_k) = 1 \qquad (i,k \in \{1,\dots,n^\star\}, i<k) \tag{1}$$

$$x(\mathrm{col}_j \cup \mathrm{col}_l) - y(\mathrm{col}_j : \mathrm{col}_l) = 1 \qquad (j,l \in \{1,\dots,n^\star\}, j<l) \tag{2}$$

Theorem 1. *The set*

$$B = \{[1,j,2,l] \in \mathcal{E}_{n^\star} \mid j<l\} \cup \{[i,1,k,2] \in \mathcal{E}_{n^\star} \mid i<k\}$$

is the index set of a basis of the equation system (1), (2)*, i.e., the submatrix of the left-hand-side coefficient matrix of this equation system which consists of the columns corresponding to B has full column rank, and this column rank equals the rank of the whole matrix. In particular, since* (1) *and* (2) *form a complete equation system for $\mathcal{QAP}^\star_{n^\star}$, the dimension of $\mathcal{QAP}^\star_{n^\star}$ is*

$$\dim\left(\mathcal{QAP}^\star_{n^\star}\right) = \dim\left(\mathbb{R}^{\mathcal{V}_{n^\star}} \times \mathbb{R}^{\mathcal{E}_{n^\star}}\right) - |B|.$$

Basic Results on the QAP-Polytopes. A simple (but, nevertheless, extremely useful) property of all three polytopes $\mathcal{QAP}_n$, $\mathcal{SQAP}_n$, and $\mathcal{QAP}^\star_{n^\star}$ is that they are each invariant under permuting the rows or the columns of the (hyper)graph.

Another issue that will be important within this paper is the connection between the (non-symmetric) quadratic assignment polytope and the *boolean quadric polytope*. The latter polytope was introduced by Padberg [30] as follows. Let $K_N = (V_N, E_N)$ denote the complete graph on N nodes. We use notations like $E_N(W)$ (for $W \subseteq V_N$) or x^W and $x(W)$ analogously to their definitions in the context of $\mathcal{G}_n$. The *boolean quadric polytope* (on the complete graph with N nodes) is defined as

$$\mathcal{BQP}_N = \mathrm{conv}\left\{ (x^C, y^{E_N(C)}) \,\middle|\, C \subseteq V_N \right\}.$$

It turns out that the canonical embedding of the polytope $\mathcal{QAP}_n$ into the vector space $R^{V_{n^2}} \times \mathbb{R}^{E_{n^2}}$ (setting all components indexed by elements of $E_{n^2} \setminus \mathcal{E}_n$ to zero) not only is contained in $\mathcal{BQP}_{n^2}$, but in fact is a face of this polytope. Moreover, De Simone [13] has shown that $\mathcal{BQP}_N$ is isomorphic to the extensively studied *cut polytope* $\mathcal{CUT}_{N+1}$, which is the convex hull

$$\mathcal{CUT}_{N+1} = \mathrm{conv}\left\{ y^{(S:V_{N+1}\setminus S)} \,\middle|\, S \subseteq V_{N+1} \right\}$$

of all characteristic vectors of cuts in the complete graph K_{N+1} on $N+1$ nodes. Thus, $\mathcal{QAP}_n$ is also isomorphic to some face of the cut polytope $\mathcal{CUT}_{n^2+1}$.

The following summarizes the basic results on the facial structures of $\mathcal{QAP}_n$ and $\mathcal{SQAP}_n$. We denote by $\Delta^{(i,j)}_{(k,j)}$ the set of all hyperedges containing both nodes (i,j) and (k,j). All proofs can be found in [21] and [22]. The results on $\mathcal{QAP}_n$ have independently been also discovered by [34,31].

1. The affine hull of $\mathcal{QAP}_n$ is described by

$$x(\text{row}_i) = 1 \qquad (i \in \{1, \dots, n\}) \tag{3}$$

$$x(\text{col}_j) = 1 \qquad (j \in \{1, \dots, n\}) \tag{4}$$

$$-x_{(i,j)} + y((i,j) : \text{row}_k) = 0 \qquad (i, j, k \in \{1, \dots, n\}, i \neq k) \tag{5}$$

$$-x_{(i,j)} + y((i,j) : \text{col}_l) = 0 \qquad (i, j, l \in \{1, \dots, n\}, j \neq l). \tag{6}$$

2. The affine hull of $\mathcal{SQAP}_n$ is described by

$$x(\text{row}_i) = 1 \qquad (i \in \{1, \dots, n\}) \tag{7}$$

$$x(\text{col}_j) = 1 \qquad (j \in \{1, \dots, n\}) \tag{8}$$

$$-x_{(i,j)} - x_{(k,j)} + z(\Delta^{(i,j)}_{(k,j)}) = 0 \qquad (i, j, k \in \{1, \dots, n\}, i \neq k) \tag{9}$$

$$-x_{(i,j)} - x_{(i,l)} + z(\Delta^{(i,j)}_{(i,l)}) = 0 \qquad (i, j, l \in \{1, \dots, n\}, j \neq l). \tag{10}$$

3. The "trivial inequalities" $y \geq 0$ define facets of $\mathcal{QAP}_n$.
4. The "trivial inequalities" $x \geq 0$ and $z \geq 0$ define facets of $\mathcal{SQAP}_n$.

Consider the relaxation polytopes

$$\mathcal{EQP}_n = \left\{(x, y) \in \mathbb{R}^{\mathcal{V}_n} \times \mathbb{R}^{\mathcal{E}_n} \mid (x, y) \text{ satisfies (3), (4), (5), (6), } (x, y) \geq 0\right\}$$

and

$$\mathcal{SEQP}_n = \left\{(x, z) \in \mathbb{R}^{\mathcal{V}_n} \times \mathbb{R}^{\hat{\mathcal{E}}_n} \mid (x, z) \text{ satisfies (7), (8), (9), (10), } (x, z) \geq 0\right\} .$$

The integer points of these relaxation polytopes are precisely the vertices of the polytopes $\mathcal{QAP}_n$ and $\mathcal{SQAP}_n$, respectively. Moreover, the lower bounds one can compute by solving the linear programs corresponding to these two relaxation polytopes (called the *(non-symmetric) equation bound* and the *symmetric equation bound*, respectively) have turned out to be of good quality in practice. Corresponding experiments were done for the non-symmetric equation bound by [33]. For symmetric instances, the symmetric equation bound cannot be better than the non-symmetric equation bound, but experiments reported in [21] have shown that the symmetric bound is not much worse than the non-symmetric one, in practice. The aim of this paper is to present and to investigate a class of inequalities that significantly tightens these relaxations.

3. The Box-Inequalities

Since the quadratic assignment polytope is a face of a boolean quadric polytope (see Section 2) the first candidates for valid inequalities for the quadratic assignment polytope are the valid inequalities that are known for the boolean quadric polytope. In this section, we follow that line by introducing the *ST-inequalities* for boolean quadric polytopes, a class of inequalities that slightly generalizes the three classes of inequalities proposed by [30]. Before we investigate them with respect to the quadratic assignment polytopes, we also show that the ST-inequalities correspond to some special *hypermetric inequalities* for the cut polytope. The *box inequalities* for the quadratic assignment polytope are finally defined to be those ST-inequalities that are symmetric, and hence are of special interest, since they define also faces of the symmetric quadratic assignment polytope.

The starting point for deriving the ST-inequalities is the observation that $(\gamma-1)\gamma \geq 0$ holds for any choice of an integer number $\gamma \in \mathbb{Z}$. Suppose, $\mathcal{S}, \mathcal{T} \subseteq V_N$ are disjoint subsets of nodes, and $\beta \in \mathbb{Z}$ is any integer number. Let $(x, y) \in \mathcal{BQP}_N$ be any vertex of $\mathcal{BQP}_N$, i.e., (x, y) is a characteristic vector of some $C \subseteq V_N$. Note that we have $x(\mathcal{R})^2 = x(\mathcal{R}) + 2y(\mathcal{R})$ for any $\mathcal{R} \subseteq V_N$ and $x(\mathcal{S})x(\mathcal{T}) = y(\mathcal{S} : \mathcal{T})$ (here we need that $\mathcal{S}$ and $\mathcal{T}$ are disjoint). The above observation yields

$$\begin{aligned}
0 &\leq (x(\mathcal{T}) - x(\mathcal{S}) - \beta)\,(x(\mathcal{T}) - x(\mathcal{S}) - (\beta - 1)) \\
&= x(\mathcal{T})^2 - 2x(\mathcal{S})x(\mathcal{T}) + x(\mathcal{S})^2 \\
&\quad + (-(\beta-1) - \beta)x(\mathcal{T}) + (\beta - 1 + \beta)x(\mathcal{S}) + \beta(\beta - 1) \\
&= 2y(\mathcal{T}) - 2y(\mathcal{S} : \mathcal{T}) + 2y(\mathcal{S}) - (2\beta - 2)x(\mathcal{T}) + 2\beta x(\mathcal{S}) + \beta(\beta - 1) \\
&= -2\left(-y(\mathcal{T}) + y(\mathcal{S} : \mathcal{T}) - y(\mathcal{S}) + (\beta - 1)x(\mathcal{T}) - \beta x(\mathcal{S}) - \frac{\beta(\beta-1)}{2}\right).
\end{aligned}$$

Hence, we have shown that the *ST-inequality*

$$-\beta x(\mathcal{S}) + (\beta - 1)x(\mathcal{T}) - y(\mathcal{S}) - y(\mathcal{T}) + y(\mathcal{S} : \mathcal{T}) \leq \frac{\beta(\beta-1)}{2} \tag{11}$$

is valid for $\mathcal{BQP}_N$. The vertices of the face of $\mathcal{BQP}_N$ defined by this inequality are precisely the characteristic vectors of subsets $C \subseteq V_N$ of nodes satisfying

$$|C \cap \mathcal{T}| - |C \cap \mathcal{S}| \in \{\beta, \beta - 1\}.$$

It turns out that the faces of $\mathcal{BQP}_N$ that are defined by ST-inequalities correspond (via the isomorphism between the boolean quadric polytope $\mathcal{BQP}_N$ and the cut polytope $\mathcal{CUT}_{N+1}$ mentioned in Section 2) to some well-known faces of $\mathcal{CUT}_{N+1}$, namely to some special *hypermetric faces.* A *hypermetric inequality* for the cut polytope $\mathcal{CUT}_{N+1}$ (on the complete graph with nodes $\{0, 1, \ldots, N\}$) is an inequality

$$\sum_{v=0}^{N} \sum_{w=v+1}^{N} \zeta_v \zeta_w z_{\{v,w\}} \leq 0$$

for some set of integer numbers $\zeta_0, \zeta_1, \ldots, \zeta_N \in \mathbb{Z}$ satisfying $\sum_{v=0}^{N} \zeta_v = 1$. The hypermetric inequalities were introduced independently by Deza [14] and Kelly [27]. The subclass of these inequalities to which the ST-inequalities correspond are those with (for some $p, q \in \mathbb{N}$)

$$\begin{aligned}
\zeta_0 &= 1 - p + q \\
\zeta_1 = \cdots = \zeta_p &= +1 \\
\zeta_{p+1} = \cdots = \zeta_{p+q} &= -1 \\
\zeta_{p+q+1} = \cdots = \zeta_N &= 0\ .
\end{aligned}$$

Hypermetric inequalities of this type are either so-called *linear* or *quasilinear* hypermetric inequalities. Deza [15] found a complete characterization of the facet defining ones among these inequalities [16]. Clearly, one can obtain from this characterization a complete characterization of the ST-inequalities defining facets of the boolean quadric polytope. Rather than doing this, we will return to the quadratic assignment polytopes and investigate the meaning the ST-inequalities have there. The considerations of the boolean quadric polytope and of the cut polytope were just intended to clarify the origin of the ST-inequalities.

Since the canonical embedding of $\mathcal{QAP}_n$ into $\mathbb{R}^{V_{n^2}} \times \mathbb{R}^{E_{n^2}}$ is a face of $\mathcal{BQP}_{n^2}$ (see Section 2) for any two disjoint subsets $\mathcal{S}, \mathcal{T} \subseteq \mathcal{V}_n$ of nodes and any integer number $\beta \in \mathbb{Z}$ the ST-inequality (11) is also valid for $\mathcal{QAP}_n$. Of course, we have $\mathcal{QAP}^\star_{n^\star} \subset \mathcal{BQP}_{n^{\star 2}}$ (in fact, $\mathcal{QAP}^\star_{n^\star}$ is also a face of $\mathcal{BQP}_{n^{\star 2}}$), and hence, the ST-inequality (11) is valid for $\mathcal{QAP}^\star_{n^\star}$, too.

With respect to the investigations of the symmetric quadratic assignment polytope $\mathcal{SQAP}_n$ it is of special interest to know which ST-inequalities are symmetric (see Section 2). Let us call an ST-inequality a *4-box inequality* (or simply a *box inequality*) if there are two disjoint subsets $P_1, P_2 \subseteq \{1, \ldots, n\}$ of row indices and two disjoint subsets $Q_1, Q_2 \subseteq \{1, \ldots, n\}$ of column indices of $\mathcal{V}_n$ such that

$$\text{(12)} \qquad \mathcal{S} = (P_1 \times Q_1) \cup (P_2 \times Q_2) \quad \text{and} \quad \mathcal{T} = (P_1 \times Q_2) \cup (P_2 \times Q_1)$$

hold (see Figure 1). A face that is defined by a 4-box inequality is a *4-box face*. We call any subset $\mathcal{R} \subseteq \mathcal{V}_n$ that can be written as $\mathcal{P} = P \times Q$ for some $P, Q \subseteq \{1, \ldots, n\}$ a *box*. Its *size* is $|P| \times |Q|$.

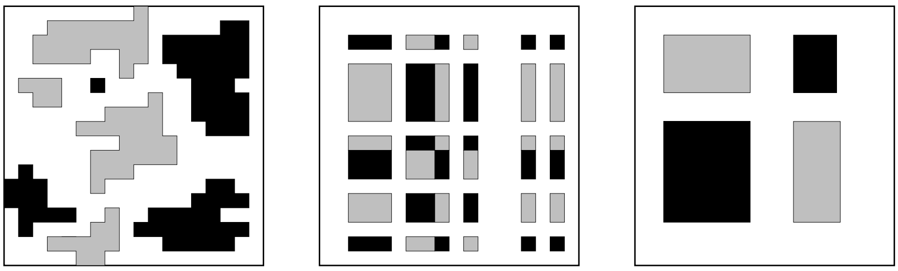

Fig. 1. The node sets of ST-inequalities in general, of 4-box inequalities and of 4-box inequalities after suitable permutations of rows and columns. The set $\mathcal{S}$ is always indicated by the gray parts, the set $\mathcal{T}$ by the black ones.

Theorem 2. *An ST-inequality is symmetric if and only if it is a 4-box inequality.*

Proof. Clearly, any 4-box inequality is symmetric. To prove the opposite direction, let $(\mathcal{S}, \mathcal{T}, \beta)$ determine a symmetric ST-inequality. We call a subset $F \subseteq \mathcal{E}_n$

of edges *symmetric* if for all pairs of mates $e, e' \in \mathcal{E}_n$ either both e and e' or none of them belong to F.

First, we show that for any subset $W \subseteq \mathcal{V}_n$ the set of edges $\mathcal{E}_n(W)$ induced by W is symmetric if and only if W is a box. To see the non-trivial direction of this claim, let P consist of all numbers i with $\text{row}_i \cap W \neq \emptyset$, and let Q contain all j with $\text{col}_j \cap W \neq \emptyset$. Clearly, we have $W \subseteq P \times Q$. Assume that there is a node $(i, j) \in (P \times Q) \setminus W$. By construction of P and Q there must be nodes $(i, l) \in W$ (with $l \neq j$) and $(k, j) \in W$ (with $k \neq i$), yielding that the edge $[i, l, k, j]$ is contained in $\mathcal{E}_n(W)$, and hence, since $\mathcal{E}_n(W)$ was supposed to be symmetric, $[i, j, k, l] \in \mathcal{E}_n(W)$ holds, contradicting $(i, j) \notin W$.

From this, since $\mathcal{E}_n(\mathcal{S} \cup \mathcal{T})$ is precisely the set of edges having non-zero coefficients in the inequality under inspection, we deduce that $\mathcal{S} \cup \mathcal{T}$ must be a box, say $\mathcal{S} \cup \mathcal{T} = \{1, \ldots, p\} \times \{1, \ldots, q\}$. By permutations of rows and columns, we can assume $(1, 1), \ldots, (1, q') \in \mathcal{S}$, $(1, q'+1), \ldots, (1, q) \in \mathcal{T}$, $(1, 1), \ldots, (p', 1) \in \mathcal{S}$, and $(p' + 1, 1), \ldots, (p, 1) \in \mathcal{T}$. Let $i \in \{2, \ldots, p'\}$ and $j \in \{2, \ldots, q'\}$. Since we have $(1, j), (i, 1) \in \mathcal{S}$, the edge $[1, j, i, 1]$ must have coefficient -1 in the inequality, hence so does the edge $[1, 1, i, j]$. By $(1, 1) \in \mathcal{S}$ this implies also $(i, j) \in \mathcal{S}$. Thus, we have $\{1, \ldots, p'\} \times \{1, \ldots, q'\} \subseteq \mathcal{S}$. Similarly, one shows $\{p' + 1, \ldots, p\} \times \{q' + 1, \ldots, q\} \subseteq \mathcal{S}$, $\{1, \ldots, p'\} \times \{q' + 1, \ldots, q\} \subseteq \mathcal{T}$ and $\{p' + 1, \ldots, p\} \times \{1, \ldots, q'\} \subseteq \mathcal{T}$. This proves the theorem.

In particular, the 4-box inequalities are precisely those ST-inequalities that yield also inequalities for $\mathcal{SQAP}_n$. We call a 4-box inequality defined by P_1, P_2, Q_1, and Q_2 as above a *2-box inequality* if (at least) one of the sets P_1, P_2, Q_1, or Q_2 is empty. If one of P_1 or P_2 and one of Q_1 or Q_2 is empty then we call the inequality a *1-box inequality*. Analogously to the 4-box case, *2-box faces* as well as *1-box faces* are defined.

4. Box-Facets

There are two main reasons to investigate a given valid inequality for a combinatorial optimization problem with respect to the question if it defines a facet of the corresponding polytope or not. The first one is that restricting ourselves to adding facet defining inequalities to the linear programs in a cutting plane procedure gives a guarantee that one does not create any redundancies during the process. The other reason is that once one knows that an inequality is facet defining for the underlying polytope one can stop all attempts to strengthen it by, e.g., "playing" with its coefficients.

These two reasons seemed to us to be very important in particular for the quadratic assignment problem, where the linear programs are quite hard to solve, and hence, to avoid redundancies and using only cutting planes that are as strong as possible is a crucial issue. Therefore, we started to investigate the faces that are defined by box inequalities (which we call *box faces*). We did this extensively for the 1-box and the 2-box inequalities, and ended up with the following characterization, which is in a certain sense complete (where we call a face *non-proper* if it is either empty or the whole polytope).

Theorem 3. *Let $n \geq 7$ hold.*

(i) For every 1-box face $\mathcal{F}$ of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$ one of the following statements is true:
(a) $\mathcal{F}$ is non-proper.
(b) $\mathcal{F}$ is contained in a trivial facet of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively.
(c) $\mathcal{F}$ is a facet of of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively.

(ii) For every 2-box face $\mathcal{F}$ of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$ one of the following statements is true:
(a) $\mathcal{F}$ is non-proper.
(b) $\mathcal{F}$ is contained in a trivial facet of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively.
(c) $\mathcal{F}$ is contained in a 1-box facet of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively.
(d) $\mathcal{F}$ is contained in a curtain facet [21] of $\mathcal{SQAP}_n$.
(e) $\mathcal{F}$ is an "inconvenient" face of $\mathcal{QAP}_n$ (see below).
(f) $\mathcal{F}$ is a facet of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively.

This means that for every 1-box face and for every 2-box face we know if it is a facet of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively, and in case it is not a facet, we even know why, since we know a facet of the respective polytope where the face is contained in. This holds in all cases but for a few non-symmetric ones, which we called *inconvenient* in the statement of the theorem. For these 2-box faces we can prove that they do not define facets of $\mathcal{QAP}_n$, but we do not know any facets where they are contained in.

Extending the results of Theorem 3 to the class of 4-box inequalities has failed up to now. The proof of Theorem 3 as well as more details on the characterization (e.g., the exact conditions on the triples $(\mathcal{S}, \mathcal{T}, \beta)$ that guarantee to define a facet) can be found in [23]. This proof is extremely technical. Rather than giving it here, we prove a simpler result that describes some sufficient conditions on a 1-box face for being a facet of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively. This seems to us to be a satisfactory compromise, since on the one hand, the proof of this simpler theorem already shows the basic principles of the proof of Theorem 3, and on the other hand, the 1-box inequalities are of particular interest, since they seem to be of special importance within a cutting plane procedure (see Section 5).

Theorem 4. *Let $n \geq 7$, let $P, Q \subseteq \{1, \ldots, n\}$ generate $\mathcal{T} = P \times Q \subseteq \mathcal{V}_n$, and let $\beta \in \mathbb{Z}$ be an integer number such that*

– $\beta \geq 2$,
– $|P|, |Q| \geq \beta + 2$,
– $|P|, |Q| \leq n - 3$, *and*
– $|P| + |Q| \leq n + \beta - 5$

hold. Then the 1-box inequality

$$(\beta - 1)x(\mathcal{T}) - y(\mathcal{T}) \leq \frac{\beta(\beta - 1)}{2}$$

defined by the triple $(\emptyset, \mathcal{T}, \beta)$ defines a facet of both $\mathcal{QAP}_n$ and $\mathcal{SQAP}_n$.

Before we prove Theorem 4 let us briefly discuss how restrictive the conditions posed there on the set $\mathcal{T}$ are. A simple observation is that for $\beta < 2$ the box inequality defined by $(\emptyset, \mathcal{T}, \beta)$ can neither define a facet of $\mathcal{QAP}_n$ nor of $\mathcal{SQAP}_n$. The reason is that if $\beta < 2$ holds then the n-cliques $C \subseteq \mathcal{V}_n$ of $\mathcal{G}_n$ or $\hat{\mathcal{G}}_n$, respectively, that correspond to vertices of the defined face satisfy $|C \cap \mathcal{T}| \in \{0, 1\}$, and hence, the 1-box face defined by $(\emptyset, \mathcal{T}, \beta)$ is strictly contained in a trivial facet of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively (provided that $\mathcal{T}$ contains at least two (hyper)edges).

Furthermore, for both $\mathcal{QAP}_n$ and $\mathcal{SQAP}_n$ the following equations hold, where we denote $\bar{\mathcal{T}} = P \times (\{1, \ldots, n\} \setminus Q)$ and $\tilde{\mathcal{T}} = (\{1, \ldots, n\} \setminus P) \times Q$ (with P and Q as in Theorem 4):

$$x(\mathcal{T}) + x(\bar{\mathcal{T}}) = |P| \tag{13}$$

$$x(\mathcal{T}) + x(\tilde{\mathcal{T}}) = |Q| \tag{14}$$

From these equations it follows that the triples $(\emptyset, \bar{\mathcal{T}}, |P| - (\beta - 1))$ and $(\emptyset, \tilde{\mathcal{T}}, |Q| - (\beta - 1))$ define the same face as $(\emptyset, \mathcal{T}, \beta)$ does. Thus, it suffices to investigate those 1-box faces that are defined by a triple $(\emptyset, \mathcal{T}, \beta)$ with $\mathcal{T} = P \times Q$ for some sets $P, Q \subseteq \mathcal{V}_n$ with $|P|, |Q| \leq \lfloor n/2 \rfloor$.

Moreover, if $|P| < \beta + 1$ or $|Q| < \beta + 1$ holds, we can deduce from the equations (13) and (14) that every vertex of the face defined by the corresponding 1-box inequality must satisfy $x(\bar{\mathcal{T}}) \in \{0, 1\}$ or $x(\tilde{\mathcal{T}}) \in \{0, 1\}$, respectively. Thus, that 1-box face is, again, properly contained in a trivial facet of $\mathcal{QAP}_n$ or $\mathcal{SQAP}_n$, respectively (note that due to $|P|, |Q| \leq \lfloor n/2 \rfloor$ and $n \geq 7$ we can assume that both $\bar{\mathcal{T}}$ and $\tilde{\mathcal{T}}$ contain at least two (hyper)edges).

Figure 2 illustrates the values of $|P|$ and $|Q|$ that satisfy the conditions of Theorem 4.

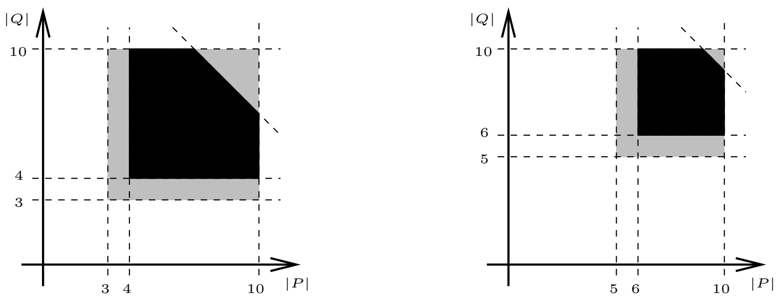

Fig. 2. The subsets (black regions) of parameter pairs $(|P|, |Q|)$ with $|P|, |Q| \leq \lfloor n/2 \rfloor$ and $|P|, |Q| \geq \beta + 1$ that satisfy the conditions of Theorem 4 (for $n = 20$ and $\beta = 2, 4$).

Proof (Proof of Theorem 4). It follows from the connections between $\mathcal{QAP}_n$ and $\mathcal{SQAP}_n$ (see Section 2) that it suffices to prove the theorem in the non-symmetric case. Furthermore, from the isomorphism between $\mathcal{QAP}_n$ and $\mathcal{QAP}^\star_{n^\star}$ (with $n^\star = n-1$, see also Section 2) we only have to prove the following:

> Let $n^\star \geq 6$, let $P, Q \subseteq \{1, \ldots, n^\star\}$ generate $\mathcal{T} = P \times Q \subseteq \mathcal{V}_{n^\star}$, and let $\beta \in \mathbb{Z}$ be an integer number such that $\beta \geq 2$, $|P|, |Q| \geq \beta + 2$, $|P|, |Q| \leq n^\star - 2$, and $|P| + |Q| \leq n^\star + \beta - 4$ hold. Then the 1-box inequality defined by the triple $(\emptyset, \mathcal{T}, \beta)$ defines a facet of $\mathcal{QAP}^\star_{n^\star}$.

Let $\mathcal{F}$ be a face of $\mathcal{QAP}^\star_{n^\star}$ which is defined by a triple $(\emptyset, \mathcal{T}, \beta)$ as above. We denote $p = |P|$ and $q = |Q|$. Since $\mathcal{QAP}^\star_{n^\star}$ is invariant under permutations of the rows and columns of $\mathcal{V}_{n^\star}$, we can assume $P = \{n^\star - p + 1, \ldots, n^\star\}$ and $Q = \{n^\star - q + 1, \ldots, n^\star\}$. We denote the set of $n^\star$- and $(n^\star - 1)$-cliques of $\mathcal{G}_{n^\star}$ that correspond to the vertices of $\mathcal{F}$ by

$$L = \Big\{ C \subset \mathcal{V}_n \Big| |C \cap \mathcal{T}| \in \{\beta - 1, \beta\}, C \text{ is an } n^\star\text{- or an } (n^\star - 1)\text{-clique of } \mathcal{G}_{n^\star} \Big\}.$$

Let

$$\Delta_L = \Big\{ (x^{C_1}, y^{\mathcal{E}_{n^\star}(C_1)}) - (x^{C_2}, y^{\mathcal{E}_{n^\star}(C_2)}) \mid C_1, C_2 \in L \Big\}$$

be the set of all difference vectors of the characteristic vectors of these cliques, i.e., the set of all differences of vertices of the face $\mathcal{F}$. Hence, Δ_L spans the linear subspace belonging to the affine subspace aff$(\mathcal{F})$. Denoting the rank of the equation system (1), (2) by ρ, we have to show that the linear dimension of Δ_L equals $\dim(\mathbb{R}^{\mathcal{V}_{n^\star}} \times \mathbb{R}^{\mathcal{E}_{n^\star}}) - \rho - 1$. Let B be the set of edges belonging to the basis of the equation system (1), (2) that we have introduced in Theorem 1. In particular, we have $|B| = \rho$. Denote by $\mathcal{B} = \{ y^e | \, e \in B\}$ the set of all canonical unit vectors belonging to B. With $e_0 = [n^\star - p + 1, n^\star - q + 1, n^\star - p + 2, n^\star - q + 2]$ (recall that $p, q \geq \beta + 2 \geq 4$ holds), it suffices to show $\text{lin}(\Delta_L \cup \mathcal{B} \cup \{y^{e_0}\}) = \mathbb{R}^{\mathcal{V}_{n^\star}} \times \mathbb{R}^{\mathcal{E}_{n^\star}}$. We will do this by successively combining all canonical unit vectors $\{x^v \mid v \in \mathcal{V}_{n^\star}\}$ and $\{y^e \mid e \in \mathcal{E}_{n^\star}\}$ of the vector space $\mathbb{R}^{\mathcal{V}_{n^\star}} \times \mathbb{R}^{\mathcal{E}_{n^\star}}$ by using just the vectors in Δ_L and $\mathcal{B} \cup \{y^{e_0}\}$. In order to abbreviate the notations, we say that an edge or a node is *combined* once the corresponding unit vector is linearly combined.

We introduce four types of vectors that will be used to combine the nodes and edges. Let $i, k, a \in \{1, \ldots, n^\star\}$ be three pairwise distinct numbers of rows of $\mathcal{V}_{n^\star}$, and let $j, l, b \in \{1, \ldots, n^\star\}$ be three pairwise distinct numbers of columns of $\mathcal{V}_{n^\star}$. We will use the following vectors (illustrated in Figure 3), where $w_1 = (i, b)$, $w_2 = (a, j)$, $w_3 = (k, b)$, $w_4 = (a, l)$, $v_0 = (a, b)$, $v_1 = (i, j)$, $v_2 = (k, j)$, $v_3 = (k, l)$, $v_4 = (i, l)$, and $C \subset \mathcal{V}_{n^\star}$ is an $n^\star$-clique of $\mathcal{G}_{n^\star}$ containing the node $w \in C$:

$$\begin{aligned}
\Theta(C, w) &= x^w + \sum_{w' \in C \setminus w} y^{\{w, w'\}} \\
\Upsilon(v_1, v_2, v_3, v_4) &= y^{[i,j,k,l]} - y^{[i,l,k,j]} \\
\Psi(v_0, v_1, v_2, v_3, v_4) &= y^{[a,b,i,j]} - y^{[a,b,k,j]} + y^{[a,b,k,l]} - y^{[a,b,i,l]} \\
\Phi(w_1, w_2, w_3, w_4) &= y^{[i,b,a,j]} - y^{[a,j,k,b]} + y^{[k,b,a,l]} - y^{[a,l,i,b]}
\end{aligned}$$

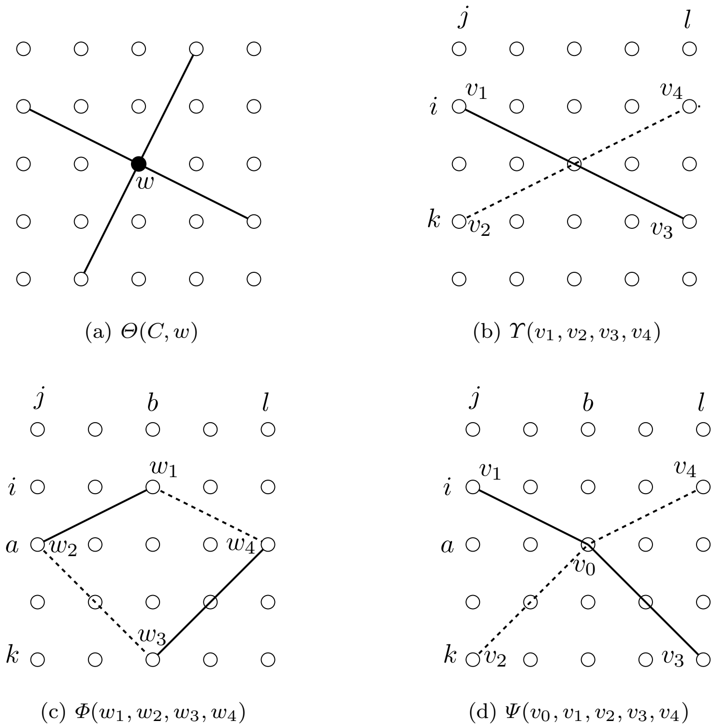

Fig. 3. The four types of vectors provided by Lemmas 1, 2, 3, and 4

The following four lemmas give sufficient conditions for these vectors to be members in $\mathrm{lin}(\Delta_L)$. We make one more notational convention. Let $W \subseteq \mathcal{V}_{n^\star}$ be a subset of nodes. We denote by $\mathcal{G}_{n^\star}/W$ the subgraph of $\mathcal{G}_{n^\star}$ that is induced by all rows and columns that do not intersect W. In order to simplify the notations, we write y^W instead of $y^{\mathcal{E}_{n^\star}(W)}$.

Lemma 1. *If for an $n^\star$-clique C' of $\mathcal{G}_{n^\star}$ and a node $w \in C'$ we have both $C' \in L$ and $C' \setminus w \in L$, then $\Theta(C', w) \in \mathrm{lin}(\Delta_L)$ holds.*

Proof. The equation $\Theta(C', w) = (x^{C'}, y^{C'}) - (x^{C' \setminus w}, y^{C' \setminus w})$ shows this.

Lemma 2. *Let $v_1, v_2, v_3, v_4 \in \mathcal{V}_{n^\star}$ be any nodes such that $\Upsilon(v_1, v_2, v_3, v_4)$ is defined. If there is an $(n^\star - 2)$-clique C' in $\mathcal{G}_{n^\star}/\{v_1, v_2, v_3, v_4\}$ such that $C' \cup \{v_1, v_3\} \in L$, $C' \cup \{v_2, v_4\} \in L$, $C' \cup \{v_1\} \in L$, $C' \cup \{v_2\} \in L$, $C' \cup \{v_3\} \in L$, and $C' \cup \{v_4\} \in L$, then $\Upsilon(v_1, v_2, v_3, v_4) \in \mathrm{lin}(\Delta_L)$ holds.*

Proof. This is due to

$$\begin{aligned}\Upsilon(v_1,v_2,v_3,v_4) =&(x^{C'\cup\{v_1,v_3\}},y^{C'\cup\{v_1,v_3\}})-(x^{C'\cup\{v_1\}},y^{C'\cup\{v_1\}})\\&-(x^{C'\cup\{v_3\}},y^{C'\cup\{v_3\}})-(x^{C'\cup\{v_2,v_4\}},y^{C'\cup\{v_2,v_4\}})\\&+(x^{C'\cup\{v_2\}},y^{C'\cup\{v_2\}})+(x^{C'\cup\{v_4\}},y^{C'\cup\{v_4\}})\ .\end{aligned}$$

Lemma 3. *Let $w_1,w_2,w_3,w_4 \in \mathcal{V}_{n^\star}$ be any nodes such that $\Phi(w_1,w_2,w_3,w_4)$ is defined. If there is an $(n^\star-3)$-clique C' in $\mathcal{G}_{n^\star}/\{w_1,w_2,w_3,w_4\}$ such that $C'\cup\{w_1,w_2\}\in L$, $C'\cup\{w_2,w_3\}\in L$, $C'\cup\{w_3,w_4\}\in L$, and $C'\cup\{w_4,w_1\}\in L$, then $\Phi(w_1,w_2,w_3,w_4)\in\operatorname{lin}(\Delta_L)$ holds.*

Proof. This is obtained from

$$\begin{aligned}\Phi(w_1,w_2,w_3,w_4) =&(x^{C'\cup\{w_1,w_2\}},y^{C'\cup\{w_1,w_2\}})-(x^{C'\cup\{w_2,w_3\}},y^{C'\cup\{w_2,w_3\}})\\&+(x^{C'\cup\{w_3,w_4\}},y^{C'\cup\{w_3,w_4\}})-(x^{C'\cup\{w_4,w_1\}},y^{C'\cup\{w_4,w_1\}})\ .\end{aligned}$$

Lemma 4. *Let $v_0,v_1,v_2,v_3,v_4 \in \mathcal{V}_{n^\star}$ be any nodes such that $\Psi(v_0,v_1,v_2,v_3,v_4)$ is defined. If there is an $(n^\star-3)$-clique C' in $\mathcal{G}_{n^\star}/\{v_0,v_1,v_2,v_3,v_4\}$ such that $C'\cup\{v_0,v_1,v_3\}\in L$, $C'\cup\{v_1,v_3\}\in L$, $C'\cup\{v_0,v_2,v_4\}\in L$, and $C'\cup\{v_2,v_4\}\in L$, then $\Psi(v_0,v_1,v_2,v_3,v_4)\in\operatorname{lin}(\Delta_L)$ holds.*

Proof. The claim follows from $\Theta(C'\cup\{v_0,v_1,v_3\},v_0),\Theta(C'\cup\{v_0,v_2,v_4\},v_0)\in\Delta_L$ (by Lemma 1), and

$$\Psi(v_0,v_1,v_2,v_3,v_4)=\Theta(C'\cup\{v_0,v_1,v_3\},v_0)-\Theta(C'\cup\{v_0,v_2,v_4\},v_0)\ .$$

Due to the combinatorial properties of the vertices of 1-box faces we need the following characterization.

Proposition 1. *Let $n'\geq 0$, $P',Q'\subseteq\{1,\dots,n'\}$, $\mathcal{T}'=P'\times Q'$, and let $\beta'\geq 0$ be any nonnegative integer number. An n'-clique $C'\subset\mathcal{V}_{n'}$ of $\mathcal{G}_{n'}$ with $|C'\cap\mathcal{T}'|=\beta'$ exists if and only if $|P'|,|Q'|\geq\beta'$ and $|P'|+|Q'|\leq n'+\beta'$ hold.*

Proof. With $p'=|P'|$ and $q'=|Q'|$ we can assume $\mathcal{T}'=\{n'-p'+1,\dots,n'\}\times\{n'-q'+1,\dots,n'\}$. Let $n''=n'-\beta'$. A clique with the desired properties exists if and only if $p',q'\geq\beta'$ holds and there exists an n''-clique $C''\subset\mathcal{V}_{n''}$ in the graph $\mathcal{G}_{n''}$ such that we have $C''\cap\mathcal{T}''=\emptyset$ for $\mathcal{T}''=\{n''-(p'-\beta'),\dots,n''\}\times\{n''-(q'-\beta')\}$. Thus, it suffices to prove that there is an n''-clique $C''\subset\mathcal{V}_{n''}$ in $\mathcal{G}_{n''}$ with $C''\cap\mathcal{T}''=\emptyset$ if and only if $p'+q'\leq n''+2\beta'$ holds.

To prove this claim, let $p''=p'-\beta'$ and $q''=q'-\beta'$, and observe that it is equivalent to the claim that in the bipartite graph G_{bip} on $n''+n''$ nodes $\{v_1,\dots,v_{n''}\}$ and $\{w_1,\dots,w_{n''}\}$ having all edges but the ones connecting nodes $\{v_1,\dots,v_{p''}\}$ with $\{w_1,\dots,w_{q''}\}$, a perfect matching exists if and only if $p''+q''\leq n''$ holds. For a subset $A\subseteq\{v_1,\dots,v_{n''}\}$ denote by $\Gamma(A)\subseteq\{w_1,\dots,w_{n''}\}$ the set of all nodes being adjacent to any node in A. Then, the König/Hall-Theorem (see any book about graph theory, e.g., the classical treatment by Berge [4]) says that a perfect matching in G_{bip} exists if and only if there is no subset $A\subseteq\{v_1,\dots,v_{n''}\}$ of nodes with $|A|>|\Gamma(A)|$, which is equivalent to $p''\leq n''-q''$, i.e., equivalent to $p'+q'\leq n''+2\beta'$.

Using Lemmas 1, 2, 3, and 4, we now exhibit those vectors that we will need for combining the nodes and edges. Let us recall that β, $p = |P|$, and $q = |Q|$ satisfy the conditions $\beta \geq 2$, $p, q \geq \beta + 2$, $p, q \leq n^\star - 2$, and $p + q \leq n^\star + \beta - 4$, implying in particular $p, q \geq 4$.

Lemma 5. *For $w_1, w_2, w_3, w_4 \in \mathcal{V}_{n^\star} \setminus \mathcal{T}$ such that $\Upsilon(w_1, w_2, w_3, w_4)$ exists, we have*

$$\Upsilon(w_1, w_2, w_3, w_4) \in \mathrm{lin}(\Delta_L) \ .$$

Proof. Let $\mathcal{G}_{n'}$ be the graph that is isomorphic to $\mathcal{G}_{n^\star}/\{w_1, w_2, w_3, w_4\}$ (i.e., the subgraph of $\mathcal{G}_{n^\star}$ arising from the removal of all rows and columns of $\mathcal{V}_{n^\star}$ that share any node with $w_1, \ldots, w_4$). The box $\mathcal{T}$ in $\mathcal{G}_{n^\star}$ of size $p \times q$ induces a box $\mathcal{T}'$ in $\mathcal{G}_{n'}$ of size $p' \times q'$. By Lemma 2 it suffices to show that for $\beta' = \beta$ the graph $\mathcal{G}_{n'}$ contains an n'-clique $C' \subset \mathcal{V}_{n'}$ with $|C' \cap \mathcal{T}'| = \beta'$. We have $n' = n^\star - 2$, $p - 2 \leq p' \leq p$, and $q - 2 \leq q' \leq q$. Thus the inequalities $p' \geq p - 2 \geq \beta = \beta'$, $q' \geq q - 2 \geq \beta = \beta'$, and $p' + q' \leq p + q \leq n^\star + \beta - 4 = n' + \beta' - 2 \leq n' + \beta'$ hold, and hence, Proposition 1 guarantees the existence of a clique C' with the desired property.

The following proofs proceed in the same way as the proof of Lemma 5. Without explicit definitions, we will always use the parameters n', p', and q' as the parameters specifying the sizes of the graph and the box after the removal of the rows and columns sharing any of the nodes which appear in the statement of the respective lemma. Thus, any of the proofs is completed by choosing an appropriate value of β' that admits to apply the right one among Lemmas 1, 2, 3, or 4, and showing the three inequalities required for the application of Proposition 1.

Lemma 6. *For $w_1, w_2, w_3, w_4 \in \mathcal{T}$ such that $\Upsilon(w_1, w_2, w_3, w_4)$ exists, we have*

$$\Upsilon(w_1, w_2, w_3, w_4) \in \mathrm{lin}(\Delta_L) \ .$$

Proof. Again, we have $n' = n^\star - 2$, but this time $p' = p - 2$ and $q' = q - 2$ hold. With $\beta' = \beta - 2$ we can apply Proposition 1 and Lemma 2: $p' = p - 2 \geq \beta = \beta' + 2 \geq \beta'$, $q' = q - 2 \geq \beta = \beta' + 2 \geq \beta'$, $p' + q' = p + q - 4 \leq n^\star + \beta - 8 = n' + \beta' - 4 \leq n' + \beta'$.

Lemma 7. *For $v_1, v_2, v_3, v_4 \in \mathcal{V}_{n^\star} \setminus \mathcal{T}$ such that $\Phi(v_1, v_2, v_3, v_4)$ exists, we have*

$$\Phi(v_1, v_2, v_3, v_4) \in \mathrm{lin}(\Delta_L) \ .$$

Proof. Here, $n' = n^\star - 3$, $p - 3 \leq p' \leq p$, and $q - 3 \leq q' \leq q$ hold. Choosing $\beta' = \beta - 1$, Proposition 1 allows to apply Lemma 3: $p' \geq p - 3 \geq \beta - 1 = \beta'$, $q' \geq q - 3 \geq \beta - 1 = \beta'$, and $p' + q' \leq p + q \leq n^\star + \beta - 4 = n' + \beta'$.

Lemma 8. *For $v_1, v_2, v_3, v_4 \in \mathcal{T}$ such that $\Phi(v_1, v_2, v_3, v_4)$ exists, we have*

$$\Phi(v_1, v_2, v_3, v_4) \in \mathrm{lin}(\Delta_L) \ .$$

Proof. This lemma will be proved together with Lemma 9.

Lemma 9. *For $v_1, v_2, v_3 \in \mathcal{T}$ and $v_4 \in \mathcal{V}_{n^\star} \setminus \mathcal{T}$ such that $\Phi(v_1, v_2, v_3, v_4)$ exists, we have*

$$\Phi(v_1, v_2, v_3, v_4) \in \operatorname{lin}(\Delta_L) \ .$$

Proof. We prove both Lemma 8 and 9. In any case we have $n' = n^\star - 3$, $p-3 \leq p' \leq p-2$, and $q-3 \leq q' \leq q-2$. If we choose $\beta' = \beta - 2$, we obtain both lemmas using Proposition 1 and Lemma 3: $p' \geq p-3 \geq \beta - 1 = \beta'$, $q' \geq q-3 \geq \beta-1 = \beta'$, and $p' + q' \leq p + q - 4 \leq n^\star + \beta - 8 = n' + \beta' - 3 \leq n' + \beta'$.

Lemma 10. *For $w_0, w_1, w_2, w_3 \in \mathcal{V}_{n^\star} \setminus \mathcal{T}$, $w_4 \in \mathcal{T}$ such that $\Psi(w_0, w_1, w_2, w_3, w_4)$ exists, we have*

$$\Psi(w_0, w_1, w_2, w_3, w_4) \in \operatorname{lin}(\Delta_L) \ .$$

Proof. We have $n' = n^\star - 3$, $p - 2 \leq p' \leq p - 1$, and $q - 2 \leq q' \leq q - 1$. If we choose $\beta' = \beta - 1$ then Proposition 1 together with Lemma 4 yields the claim: $p' \geq p - 2 \geq \beta = \beta' + 1 \geq \beta'$, $q' \geq q - 2 \geq \beta = \beta' + 1 \geq \beta'$, and $p' + q' \leq p + q - 2 \leq n^\star + \beta - 6 = n' + \beta' - 2 \leq n' + \beta'$.

Lemma 11. *For $w \in \mathcal{V}_{n^\star}$ there exists an $n^\star$-clique $C \subset \mathcal{V}_{n^\star}$ with*

$$\Theta(C, w) \in \operatorname{lin}(\Delta_L) \ .$$

Proof. We have in any case $n' = n^\star - 1$, $p - 1 \leq p' \leq p$, and $q - 1 \leq q' \leq q$. Choosing $\beta' = \beta - 1$, Proposition 1 and Lemma 1 can be applied: $p' \geq p - 1 \geq \beta + 1 = \beta' + 2 \geq \beta'$, $q' \geq q - 1 \geq \beta + 1 = \beta' + 2 \geq \beta'$, and $p' + q' \leq p + q \leq n^\star + \beta - 4 = n' + \beta' - 2 \leq n' + \beta'$.

Now we are prepared to combine all nodes and edges of $\mathcal{G}_{n^\star}$. As explained at the beginning of this proof, we start with just the edges in the set B (that constitutes a basis of the equation system (1), (2)) and the edge e_0 (see Figure 4).

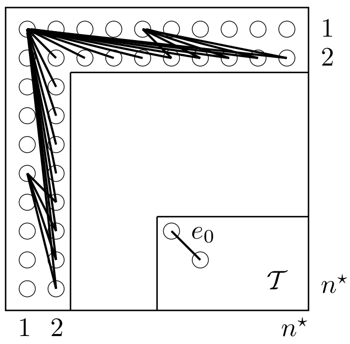

Fig. 4. The edges that are "combined" initially (where the set B is drawn just partially).

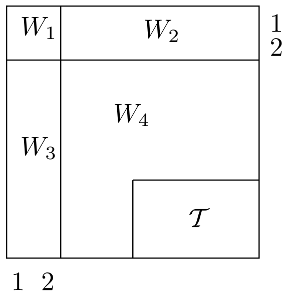

Fig. 5. Partition of the nodes $\mathcal{V}_{n^\star}$.

We partition the node set $\mathcal{V}_{n^\star}$ into five parts as indicated in Figure 5. The first observation is that by using the fact that the edges in B can be already considered combined and exploiting Lemma 5, we can combine all edges in $\mathcal{E}_{n^\star}(W_1 \cup W_2)$ as well as the ones in $\mathcal{E}_{n^\star}(W_1 \cup W_3)$. Our next goal is to combine all edges in $(W_2 : W_3)$. By suitable permutations of the rows and columns, it suffices to show how to combine an edge $[2, j, k, 2]$ for any $j, k \in \{3, \dots, n^\star\}$. Choosing $w_1 = (1, 2)$, $w_2 = (2, 1)$, $w_3 = (k, 2)$, and $w_4 = (2, j)$, we can combine this edge by applying Lemma 7, since the edges in $\mathcal{E}_{n^\star}(W_1 \cup W_2)$ and in $\mathcal{E}_{n^\star}(W_1 \cup W_3)$ are already done. But once we have combined the edges in $(W_2 : W_3)$, it is easy to combine also all edges in $(W_1 : W_4)$ by applying Lemma 5. We come to the edges in $(W_2 : W_4)$. We can assume that the edge that we want to combine is $[2, j, k, l]$ with $j, k, l \in \{3, \dots, n^\star\}$ and $(k, l) \notin \mathcal{T}$. Then, we apply Lemma 7 with $w_1 = (1, l)$, $w_2 = (2, 1)$, $w_3 = (k, l)$, and $w_4 = (2, j)$, and obtain the desired combination. Analogously, we can combine the edges in $(W_3 : W_4)$. In order to see, how one can now combine the edges in $\mathcal{E}_{n^\star}(W_4)$, let $i, j, k, l \in \{3, \dots, n^\star\}$ with $(i, j), (k, l) \notin \mathcal{T}$. This time, we choose $w_1 = (1, j)$, $w_2 = (k, 1)$, $w_3 = (i, j)$, and $w_4 = (k, l)$, and exploit, again, Lemma 7, using the fact that we have already combined all edges in $(W_1 \cup W_2 \cup W_3 : W_4)$.

Now we have combined all edges in $\mathcal{E}_{n^\star} \setminus \mathcal{T}$. The next step is to combine the edges in $(\mathcal{V}_{n^\star} \setminus \mathcal{T} : \mathcal{T})$. This can be done by applying Lemma 10. Thus, it remains to combine the edges in $\mathcal{E}_{n^\star}(\mathcal{T})$ (and all nodes). For notational convenience, let us partition the box $\mathcal{T}$ into four parts $T_1 = \{n^\star - p+1, n^\star - p+2\} \times \{n^\star - q+1, n^\star - q+2\}$, $T_2 = \{n^\star - p+1, n^\star - p+2\} \times \{n^\star - q+3, \dots, n^\star\}$, $T_3 = \{n^\star - p+3, \dots, n^\star\} \times \{n^\star - q+1, n^\star - q+2\}$, and $T_4 = \{n^\star - p+3, \dots, n^\star\} \times \{n^\star - q+3, \dots, n^\star\}$. Recall that we have the edge $e_0 = [n^\star - p + 1, n^\star - q + 1, n^\star - p + 2, n^\star - q + 2]$ in our set of "initially combined edges". By application of Lemma 9 we can use this to combine all edges in $(\{(n^\star - p+1, n^\star - q+1), (n^\star - p+2, n^\star - q+2)\} : T_2 \cup T_3)$. After this, applying Lemma 9 also enables us to combine all edges in $\mathcal{E}_{n^\star}(T_1 \cup T_2)$ and the ones in $\mathcal{E}_{n^\star}(T_1 \cup T_3)$. But then, we can proceed analogously to the combination of the edges in $\mathcal{E}_{n^\star}(\mathcal{V}_{n^\star} \setminus \mathcal{T})$ from the edges in $\mathcal{E}_{n^\star}(W_1 \cup W_2)$ and $\mathcal{E}_{n^\star}(W_1 \cup W_3)$; we just have to apply Lemma 6 instead of Lemma 5 and Lemma 8 instead of Lemma 7.

Now we have combined all edges, and thus, exploiting Lemma 11, we can immediately complete the proof of Theorem 4 by combining also all nodes.

5. Computational Results

We implemented a simple cutting plane procedure using a straightforward separation heuristic for the box inequalities. In order to find violated box inequalities for a fixed β, we first guess initial sets $\mathcal{S}$ and $\mathcal{T}$, i.e., we guess two disjoint sets P_1 and P_2 of rows as well as two disjoint sets Q_1 and Q_2 of columns defining $\mathcal{S} = (P_1 \times Q_1) \cup (P_2 \times Q_2)$ and $\mathcal{T} = (P_1 \times Q_2) \cup (P_2 \times Q_1)$. Our goal is to find $\mathcal{S}$ and $\mathcal{T}$ such that the left-hand-side value of the corresponding ST-inequality becomes as large as possible (in particular, greater than $\frac{\beta(\beta-1)}{2}$). In order to approach this goal we try to improve that left-hand-side value by local changes on the sets $\mathcal{S}$ and $\mathcal{T}$, i.e., we try to increase that value by iterated operations like adding some row to P_1 or P_2 or removing some row from P_1 or P_2 and the analogous operations for the column sets Q_1 and Q_2. Although this separation procedure is quite primitive, it usually detects many (i.e., hundreds) of violated inequalities if it is run several hundred times. This leads to another point where our implementation is quite preliminary. The criterion by which we select among the many detected violated inequalities a suitably small subset that should be added to the current linear program, is also very primitive. We simply take those inequalities that are violated the most (regardless of any scaling or similar normalization).

However, this is not yet intended to be a sound computational study on the box inequalities. Such a study will need to involve extensive experiments with all kinds of parameters like the maximal number of violated inequalities that are added to the linear programs at one iteration, the number of runs of the separation procedure, the values of β for which one searches violated inequalities, the criteria for selecting among the detected violated inequalities, different versions of the separation heuristic itself, and so on.

Initial computational experiments showed that restricting the search in our separation heuristic to 2-box inequalities mostly yielded better results than searching among all 4-box inequalities, and, restricting the search to the 1-box inequalities improved the results even more. Thus, we decided to do the preliminary computational experiments with restricting to 1-box inequalities. Furthermore, we just considered $\beta \in \{2, 3\}$. Finding good strategies for mixing 1-box, 2-box, and 4-box inequalities and for the choice of the values β to be considered is one of the tasks for a thorough experimental study.

In our tests, the (maximal) number of added inequalities per cutting plane iteration was chosen to be 0.4 or 0.2 times the number of equations in the system yielding the symmetric equation bound, where we took the factor 0.4 for the smaller instances ($n \leq 16$) and the factor 0.2 for the larger ones ($n \geq 17$). The linear programs become harder to solve as soon as that many inequalities are added. For example, for instances with $n = 20$ yielding 7640 equations we added up to 1518 inequalities per iteration that are also denser than the equations.

Although we removed after each iteration the inequalities that were not satisfied with equality by the optimum solution to the last linear program, this led to very difficult linear programs. We could not succeed in solving the linear programs by the CPLEX simplex method. Hence, we solved at every iteration the linear program from the scratch using the CPLEX barrier optimizer.

The number of iterations that we run the cutting plane code varies from about 15 for the small instances ($n = 12$) to just two or three iterations for the large instances ($n = 20$). Our runs were usually stopped (unless the bounding procedure had yielded the optimum solution value) by the queuing system of the machine due to reaching some time limit, which was, due to problems with the queuing system, not always the same.

We have used as test set the instances of the QAPLIB of sizes $n \leq 20$. They are all symmetric. The experiments were carried out on a Silicon Graphics Power Challenge machine. All linear programs were solved by the CPLEX 4.0 parallel barrier solver using four processors.

Tables 1, 2, and 3 show the results. *SEQB* stands for the symmetric equation bound, while the columns titled *1-box* contain the statistics for using 1-box inequalities as cutting planes. The absolute value of the respective bound is denoted by *bound*, *qual* is the ratio of that bound and the optimal solution value (which is available from the literature for all instances of the QAPLIB of sizes up to $n = 20$), *iter* gives the number of linear programs solved, and *time* is the time our cutting plane procedure has run (in seconds). The final column, titled *gap reduced* reports the part of the gap between the symmetric equation bound and the optimal solution value that could be closed by cutting planes. Figure 6 illustrates this.

name	SEQB		1-box				gap
	bound	qual	bound	qual	iter	time	reduced
chr12a	9552.0	1.000	9552.0	1.000	1	16.3	1.000
chr12b	9742.0	1.000	9742.0	1.000	1	16.1	1.000
chr12c	11156.0	1.000	11156.0	1.000	1	21.9	1.000
had12	1618.2	0.980	1652.0	1.000	3	435.2	1.000
nug12	520.6	0.901	576.3	0.997	13	23981.3	0.971
rou12	222212.0	0.943	235277.1	0.999	18	26541.8	0.981
scr12	29557.2	0.941	31410.0	1.000	5	1326.5	1.000
tai12a	220018.7	0.980	224416.0	1.000	3	371.9	1.000
tai12b	30581824.5	0.775	39464925.0	1.000	4	761.6	1.000
had14	2659.9	0.976	2724.0	1.000	4	2781.5	1.000
chr15a	9370.3	0.947	9896.0	1.000	7	25036.9	1.000
chr15b	7894.1	0.988	7990.0	1.000	3	2838.1	1.000
chr15c	9504.0	1.000	9504.0	1.000	1	105.5	1.000
nug15	1030.6	0.896	1129.4	0.982	6	19906.0	0.827
rou15	322944.5	0.912	340469.3	0.961	7	25315.5	0.561
scr15	48816.5	0.955	51140.0	1.000	4	5083.3	1.000
tai15a	351289.6	0.905	366465.9	0.944	7	25449.3	0.411
tai15b	51528935.0	0.995	51765268.0	1.000	7	17909.5	1.000

Table 1. Bounds for the instances with $12 \leq n \leq 15$ obtained using 1-box inequalities.

name	SEQB		1-box				gap
	bound	qual	bound	qual	iter	time	reduced
esc16a	48.0	0.706	66.0	0.971	14	32797.2	0.900
esc16b	278.0	0.952	292.0	1.000	2	762.7	1.000
esc16c	118.0	0.738	160.0	1.000	4	4929.7	1.000
esc16d	4.0	0.250	16.0	1.000	6	3832.3	1.000
esc16e	14.0	0.500	28.0	1.000	5	4674.1	1.000
esc16g	14.0	0.538	26.0	1.000	2	847.8	1.000
esc16h	704.0	0.707	996.0	1.000	4	4886.0	1.000
esc16i	0.0	0.000	14.0	1.000	4	2987.5	1.000
esc16j	2.0	0.250	8.0	1.000	2	824.2	1.000
had16	3548.1	0.954	3716.8	0.999	8	23381.4	0.982
nug16a	1413.5	0.878	1567.0	0.973	8	19296.5	0.781
nug16b	1080.0	0.871	1208.2	0.974	5	16512.0	0.801
nug17	1490.8	0.861	1643.5	0.949	4	16007.2	0.633
tai17a	440094.4	0.895	454625.1	0.924	5	25606.4	0.281

Table 2. Bounds for the instances with $16 \leq n \leq 17$ obtained using 1-box inequalities.

name	SEQB		1-box				gap
	bound	qual	bound	qual	iter	time	reduced
chr18a	10738.5	0.968	10947.1	0.986	5	22335.8	0.580
chr18b	1534.0	1.000	1534.0	1.000	1	507.5	1.000
had18	5071.1	0.946	5299.1	0.989	5	23367.8	0.795
nug18	1649.7	0.855	1809.3	0.937	5	19390.1	0.569
els19	16502856.8	0.959	17074680.9	0.992	3	17440.9	0.806
chr20a	2169.7	0.990	2172.4	0.991	2	22488.7	0.121
chr20b	2287.0	0.995	2294.8	0.999	2	13645.8	0.710
chr20c	14006.7	0.990	14033.2	0.992	2	14794.3	0.196
had20	6559.4	0.948	6731.6	0.972	2	22783.2	0.475
lipa20a	3683.0	1.000	3683.0	1.000	1	1145.0	1.000
lipa20b	27076.0	1.000	27076.0	1.000	1	935.5	1.000
nug20	2165.0	0.842	2313.5	0.900	3	17845.8	0.367
rou20	639678.3	0.882	649747.8	0.896	3	13143.1	0.117
scr20	94557.1	0.859	96561.8	0.878	3	15122.7	0.130
tai20a	614849.2	0.874	625941.4	0.890	3	34135.2	0.125
tai20b	84501939.9	0.690	104534175.0	0.854	2	10143.7	0.528

Table 3. Bounds for the instances with $18 \leq n \leq 20$ obtained using 1-box inequalities.

The results show that the 1-box inequalities have the potential to improve the symmetric equation bound a lot towards the optimum solution value. For the smaller instances, where the time limits allowed several iterations, the 1-box inequalities often even yield the optimum solution value. The most impressive gain of the bound quality is reached for the `esc16` instances. While they are the instances with by far the worst (symmetric) equation bounds, even a few iterations with 1-box cutting planes sufficed to obtain the optimum solution value (for all instances except `esc16a`). The running times of our preliminary implementation for these instances are mostly within the same order of magnitude of those needed by Clausen and Perregard [12], when they solved these instances for the first time using a parallel system with 16 Intel i860 processors.

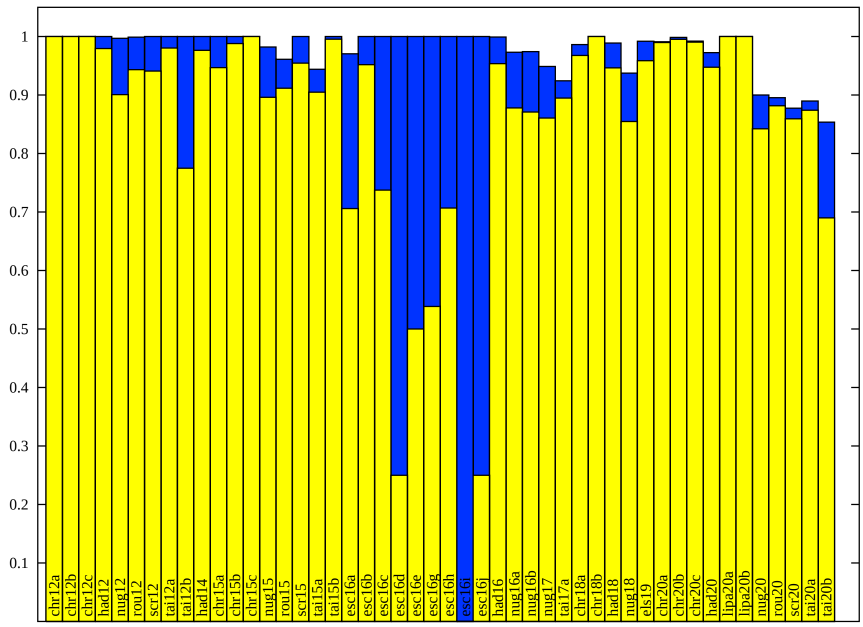

Fig. 6. The qualities of the symmetric equation bounds with (black boxes) and without (gray boxes) adding some 1-box inequalities.

Concerning the running times of our cutting plane procedure one should notice that there are bounding procedures that yield bounds of similar quality like EQP or SEQB faster than by solving the corresponding LP's [1,18,26]. However, the principal advantage of the polyhedral approach is that it offers possibilities to tighten EQB and SEQB further and further by finding more inequalities for the respective polytopes. The experiments reported in this section are just intended to demonstrate that such a tightening is indeed achieved by the insight into the polyhedral structure of the QAP described in this paper.

6. Conclusion

The most important conclusion one can draw from the results in this paper is, in our opinion, that cutting plane algorithms, based on polyhedral investigations, indeed can significantly contribute to the capability of solving quadratic assignment problems to optimality. From the theoretical point of view, the present investigation of the box inequalities shows that the techniques provided by the star-transformation allow to do deeper investigations of the quadratic assignment polytopes in a similar way as it was very successful for other $\mathcal{NP}$-hard combinatorial optimization problems, like, e.g., the traveling salesman problem.

From the practical point of view, we have continued our work into two directions between the submission of this paper and the preparation of the revised version. It turned out that a special adaption of the cutting plane code (built upon the results presented in this paper) for instances where the number of objects actually is much less than the number of locations works very effectively for several instances from the QAPLIB that have this property [24]. Another line we followed is to exploit the fact that many instances have very sparse objective functions because usually there are lots of pairs of objects that do not have any flow between them. If one exploits this by working only in the space defined by the nonzero coefficients in the objective function one can speed up the running times of the cutting plane algorithm significantly. Experimental results obtained this way are reported in [25].

References

1. W. P. Adams and T. A. Johnson, *Improved linear programming-based lower bounds for the quadratic assignment problem*, Quadratic Assignment and Related Problems (P. M. Pardalos and H. Wolkowicz, eds.), DIMACS Series in Discrete Mathematics and Theoretical Computer Science, 1994, pp. 43–75.
2. K. M. Anstreicher, N. W. Brixius, J.-P. Goux, and J. Linderoth, *Solving large quadratic assignment problems on computational grids*, Tech. report, Dept. of Computer Science, University of Iowa, October 2000, to appear in: Math. Program. Ser. B.
3. A. I. Barvinok, *Combinatorial complexity of orbits in representations of the symmetric group*, Advances in Soviet Mathematics **9** (1992), 161–182.
4. C. Berge, *Graphs*, Elsevier Science Publishers, 1991.
5. N. W. Brixius and K. M. Anstreicher, *Solving quadratic assignment problems using convex quadratic programming relaxations*, Tech. report, Dept. of Computer Science, University of Iowa, March 2000, to appear in: Optim. Methods Softw.
6. A. Bruengger, A. Marzetta, J. Clausen, and M. Perregaard, *Solving large-scale QAP problems in parallel with the search library ZRAM*, J. Parallel Distrib. Comput. **50** (1998), no. 1-2, 157–169.
7. R. E. Burkard and E. Çela, *Quadratic and three-dimensional assignments*, Annotated bibliographies in combinatorial optimization (M. et al. Dell'Amico, ed.), Wiley, Chichester, 1997, pp. 373–391.
8. R. E. Burkard, E. Çela, P. M. Pardalos, and L. S. Pitsoulis, *The quadratic assignment problem*, Handbook of Combinatorial Optimization (P. M. Pardalos and D.-Z. Du, eds.), Kluwer Academic Publishers, 1998, pp. 241–338.
9. R. E. Burkard, S. E. Karisch, and F. Rendl, *QAPLIB - A Quadratic Assignment Problem Library*, J. Glob. Optim. **10** (1997), no. 4, 391–403.
10. E. Çela, *The quadratic assignment problem. Theory and algorithms*, Kluwer Academic Publishers, 1998.
11. J. Clausen, S. E. Karisch, M. Perregard, and F. Rendl, *On the applicability of lower bounds for solving rectilinear quadratic assignment problems in parallel*, Comput. Optim. Appl. **10** (1998), no. 2, 127–147.
12. J. Clausen and M. Perregaard, *Solving large quadratic assignment problems in parallel*, Comput. Optim. Appl. **8** (1997), no. 2, 111–127.
13. C. De Simone, *The cut polytope and the boolean quadric polytope*, Discrete Math. **79** (1989), 71–75.
14. M. Deza, *On the hamming geometry of unitary cubes*, Dokl. Akad. Nauk SSR (1960), 1037–1040, English translation in: Soviet Physics Doklady 5 (1961) 940–943.
15. ———, *Matrices de formes quadratique non négative pour des arguments binaires*, Comptes Rendus de l'Académie des Sciences de Paris **277** (1973), 873–875.
16. M. M. Deza and M. Laurent, *Geometry of cuts and metrics*, Springer Verlag, 1997.
17. P. C. Gilmore, *Optimal and suboptimal algorithms for the quadratic assignment problem*, SIAM J. Appl. Math. **10** (1962), 305–313.
18. P. Hahn and T. Grant, *Lower bounds for the quadratic assignment problem based upon a dual formulation*, Oper. Res. **46** (1998), 912–922.

19. P. Hahn, T. Grant, and N. Hall, *A branch-and-bound algorithm for the quadratic assignment problem based on the Hungarian method*, Eur. J. Oper. Res. **108** (1998), no. 3, 629–640.
20. T. A. Johnson, *New linear-programming based solution procedures for the quadratic assignment problem*, Ph.D. thesis, Graduate School of Clemson University, 1992.
21. M. Jünger and V. Kaibel, *On the SQAP-polytope*, SIAM J. Opt. **11** (2001), no. 2, 444–468.
22. ———, *The QAP-polytope and the star-transformation*, Discrete Appl. Math. **111** (2001), no. 3, 283–306.
23. V. Kaibel, *Polyhedral combinatorics of the quadratic assignment problem*, Ph.D. thesis, Universität zu Köln, 1997.
24. V. Kaibel, *Polyhedral combinatorics of QAPs with less objects than locations*, Sixth Conference on Integer Programming and Combinatorial Optimization, Houston, Texas (R. E. Bixby, E. A. Boyd, and R. Z. Ríos-Mercado, eds.), Lecture Notes in Computer Science, vol. 1412, Springer Verlag, 1998, pp. 409–422.
25. V. Kaibel, *Polyhedral Methods for the QAP*, Nonlinear Assignment Problems: Algorithms and Applications (P. Pardalos and L. Pitsoulis, eds.), Kluwer Academic Publishers, 2000, pp. 109–141.
26. S. E. Karisch, J. Clausen, E. Çela, and T. Espersen, *A dual framework for lower bounds of the quadratic assignment problem based on linearization*, Computing **63** (1999), 351–403.
27. J. B. Kelly, *Hypermetric spaces*, Springer, Berlin, 1975.
28. T. C. Koopmans and M. J. Beckmann, *Assignment problems and the location of economic activities*, Econometrica **25** (1957), 53–76.
29. E. L. Lawler, *The quadratic assignment problem*, Manage. Sci. **9** (1963), 586–599.
30. M. Padberg, *The boolean quadric polytope: Some characteristics and facets*, Math. Program. **45–1** (1989), 139–172.
31. M. Padberg and M. P. Rijal, *Location, scheduling, design and integer programming*, Kluwer Academic Publishers, 1996.
32. P. M. Pardalos, F. Rendl, and H. Wolkowicz, *The quadratic assignment problem: A survey and recent developments*, Quadratic Assignment and Related Problems (P. M. Pardalos and H. Wolkowicz, eds.), DIMACS Series in Discrete Mathematics and Theoretical Computer Science, 1994, pp. 1–42.
33. M. G. C. Resende, K. G. Ramakrishnan, and Z. Drezner, *Computing lower bounds for the quadratic assignment problem with an interior point solver for linear programming*, Oper. Res. **43** (1995), 781–791.
34. M. P. Rijal, *Scheduling, design and assignment problems with quadratic costs*, Ph.D. thesis, New York University, 1995.