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Exploiting group symmetry in semidefinite programming relaxations of the quadratic assignment problem

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Abstract We consider semidefinite programming relaxations of the quadratic assignment problem, and show how to exploit group symmetry in the problem data. Thus we are able to compute the best known lower bounds for several instances of quadratic assignment problems from the problem library: (Burkard et al. in J Global Optim 10:291–403, 1997).

Keywords Quadratic assignment problem · Semidefinite programming · Group symmetry

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1 Introduction

We study the quadratic assignment problem (QAP) in the following form:

$$\min_{X \in \Pi_n} \operatorname{trace}(AX^T BX)$$

where A and B are given symmetric $n \times n$ matrices, and Π_n is the set of $n \times n$ permutation matrices.

It is well-known that the QAP contains the traveling salesman problem as a special case and is therefore NP-hard in the strong sense. Moreover, experience has shown that

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instances with $n = 30$ are already very hard to solve in practice. Thus it is typically necessary to use massive parallel computing to solve even moderately sized QAP instances; see [2].

For a detailed survey on recent developments surrounding the QAP problem, see Anstreicher [1], and the references therein.

The successful computational work in [2] employed convex relaxation of the QAP in a branch and bound setting. One class of convex relaxations that has been suggested for the QAP is via semidefinite programming (SDP); see [20,28]. These SDP relaxations turn out to be quite strong in practice, but involve matrix variables of size $(n^2 + 1) \times (n^2 + 1)$, and are therefore hard to solve by interior point algorithms.

This has led to the application of bundle methods [20] and augmented Lagrangian methods [4] to certain SDP relaxations of the QAP. Concerning one SDP relaxation (that we will consider in this paper), the authors of [20] write that '... the relaxation ... cannot be solved straightforward[ly] by interior point methods for interesting instances ($n \geq 15$).'

This statement is undoubtedly true in general, but we will show that if the QAP data matrices have sufficiently large automorphism groups, one may solve such SDP relaxations by interior point methods, sometimes for values as large as $n = 128$. We will also show that several instances in the QAP library [6] involve matrices with large automorphism groups. (This fact has already been exploited in a branch and bound framework to reduce the size of the branching tree; see [1], Sect. 4, but not in the context of solving SDP relaxations.)

As a result we are able to compute the best known lower bounds on the optimal values of real-world instances by Eschermann and Wunderlich [5] from the QAP library; these instances stem from an application in computer science, namely the testing of self-testable sequential circuits, where the amount of additional hardware for the testing should be minimized.

Our work is in the spirit of work by Schrijver [21,22], Gatermann and Parrilo [11], De Klerk et al. [7], De Klerk, Pasechnik and Schrijver [8], and others, who have shown how 'group symmetric' SDP problems may be reduced in size using representation theory.

Notation

The space of $p \times q$ real matrices is denoted by $\mathbb{R}^{p \times q}$, the space of $k \times k$ symmetric matrices is denoted by $\mathcal{S}_k$, and the space of $k \times k$ symmetric positive semidefinite matrices by $\mathcal{S}_k^+$. We will sometimes also use the notation $X \succeq 0$ instead of $X \in \mathcal{S}_k^+$, if the order of the matrix is clear from the context.

We use I_n to denote the identity matrix of order n. Similarly, J_n and e_n denote the $n \times n$ all-ones matrix and all ones n-vector respectively, and $0_{n \times n}$ is the zero matrix of order n. We will omit the subscript if the order is clear from the context.

The vec operator stacks the columns of a matrix, while the diag operator maps an $n \times n$ matrix to the n-vector given by its diagonal. The ith column of a matrix is denoted by $\text{col}_i(\cdot)$.

The *Kronecker product* $A \otimes B$ of matrices $A \in \mathbb{R}^{p\times q}$ and $B \in \mathbb{R}^{r\times s}$ is defined as the $pr \times qs$ matrix composed of pq blocks of size $r \times s$, with block ij given by $A_{ij}B$ $(i = 1, \dots, p)$, $(j = 1, \dots, q)$.

The following properties of the Kronecker product will be used in the paper, see e.g. [14] (we assume that the dimensions of the matrices appearing in these identities are such that all expressions are well-defined):

$$(A \otimes B)^T = A^T \otimes B^T, \tag{1}$$

$$(A \otimes B)(C \otimes D) = AC \otimes BD, \tag{2}$$

$$(A \otimes B)\mathrm{vec}(X) = \mathrm{vec}\left(BXA^T\right), \tag{3}$$

$$\mathrm{trace}(A \otimes B) = \mathrm{trace}(A)\,\mathrm{trace}(B). \tag{4}$$

2 SDP relaxation of the QAP problem

We associate with a matrix $X \in \Pi_n$ a matrix $Y_X \in \mathcal{S}^+_{n^2+1}$ given by

$$Y_X := \begin{pmatrix} 1 \\ \mathrm{vec}(X) \end{pmatrix} \begin{pmatrix} 1 \\ \mathrm{vec}(X) \end{pmatrix}^T. \tag{5}$$

Note that Y_X is a rank-1, component-wise nonnegative block matrix of the form

$$Y_X = \begin{pmatrix} 1 & \left(y^{(1)}\right)^T & \cdots & \left(y^{(n)}\right)^T \\ y^{(1)} & Y^{(11)} & \cdots & Y^{(1n)} \\ \vdots & \vdots & \ddots & \vdots \\ y^{(n)} & Y^{(n1)} & \cdots & Y^{(nn)} \end{pmatrix} \tag{6}$$

where

$$Y^{(ij)} := \mathrm{col}_i(X)\mathrm{col}_j(X)^T \quad (i, j = 1, \dots, n), \tag{7}$$

and $y^{(i)} = \mathrm{col}_i(X)$ $(i = 1, \dots, n)$. We will denote

$$y := \left(\left(y^{(1)}\right)^T \cdots \left(y^{(n)}\right)^T\right)^T,$$

and

$$Y := \begin{pmatrix} Y^{(11)} & \cdots & Y^{(1n)} \\ \vdots & \ddots & \vdots \\ Y^{(n1)} & \cdots & Y^{(nn)} \end{pmatrix},$$

so that the block form (6) may be written as

$$Y_X = \begin{pmatrix} 1 & y^T \\ y & Y \end{pmatrix}.$$

Letting

$$T := \begin{pmatrix} -e & I_n \otimes e^T \\ -e & e^T \otimes I_n \end{pmatrix},$$

the condition (satisfied by any $X \in \Pi_n$)

$$Xe = X^T e = e$$

is equivalent to

$$T \begin{pmatrix} 1 \\ \mathrm{vec}(X) \end{pmatrix} = 0, \tag{8}$$

since

$$T \begin{pmatrix} 1 \\ \mathrm{vec}(X) \end{pmatrix} \equiv \begin{pmatrix} -e + X^T e \\ -e + Xe \end{pmatrix}$$

where the equality follows from (3). Note that condition (8) may be rewritten as

$$\mathrm{trace}\left(T^T T Y_X\right) = 0. \tag{9}$$

Moreover, one has

$$T^T T = \begin{pmatrix} 2n & -2e^T \\ -2e & I \otimes J + J \otimes I \end{pmatrix}. \tag{10}$$

The matrix Y_X has the following sparsity pattern:

- The off-diagonal entries of the blocks $Y^{(ii)}$ $(i = 1, \ldots, n)$ are zero;
- The diagonal entries of the blocks $Y^{(ij)}$ $(i \neq j)$ are zero.

An arbitrary nonnegative matrix $Y \geq 0$ has the same sparsity pattern if and only if

$$\mathrm{trace}((I \otimes (J - I))Y + ((J - I) \otimes I)Y) = 0. \tag{11}$$

(This is sometimes called the gangster constraint; see *e.g.* [28].)

If $Y \geq 0$ satisfies (11) then, in view of (10), one has

$$\begin{aligned} \mathrm{trace}\left(T^T T \begin{pmatrix} 1 & y^T \\ y & Y \end{pmatrix}\right) &\equiv \mathrm{trace}\left(\begin{pmatrix} 2n & -2e^T \\ -2e & I \otimes J + J \otimes I \end{pmatrix} \begin{pmatrix} 1 & y^T \\ y & Y \end{pmatrix}\right) \\ &= 2n - 4e^T y + 2\,\mathrm{trace}(Y). \end{aligned}$$

Thus the condition

$$\mathrm{trace}\left(T^T T \begin{pmatrix} 1 & y^T \\ y & Y \end{pmatrix}\right) = 0 \tag{12}$$

becomes

$$\mathrm{trace}(Y) - 2e^T y = -n.$$

SDP relaxation of QAP

We obtain an SDP relxation of (QAP) by relaxing the condition $Y_X = \mathrm{vec}(X)\mathrm{vec}(X)^T$ (see (5)) to $Y_X \in \mathcal{S}^+_{n^2+1}$:

$$\left.\begin{array}{rl} \min & \mathrm{trace}(A \otimes B)Y \\ \text{subject to} & \\ & \mathrm{trace}((I \otimes (J-I))Y + ((J-I) \otimes I)Y) = 0 \\ & \mathrm{trace}(Y) - 2e^T y = -n \\ & \begin{pmatrix} 1 & y^T \\ y & Y \end{pmatrix} \succeq 0, \quad Y \geq 0. \end{array}\right\} \tag{13}$$

To obtain the objective function in (13) from the QAP objective function $\mathrm{trace}(AX^T BX)$, we used the fact that

$$\begin{aligned} \mathrm{trace}(AX^T BX) &= \mathrm{trace}(X^T BXA) \\ &= \mathrm{vec}(X)^T \mathrm{vec}(BXA) \\ &= \mathrm{vec}(X)^T (A \otimes B)\mathrm{vec}(X) \qquad \text{(by (3))} \\ &= \mathrm{trace}\left((A \otimes B)\mathrm{vec}(X)\mathrm{vec}(X)^T\right). \end{aligned}$$

The SDP relaxation (13) is equivalent to the one solved by Rendl and Sotirov [20] using bundle methods (called (QAP_{R_3}) in that paper). It is also the same as the so-called $N^+(K)$-relaxation of Lovász and Schrijver [17] applied to the QAP, as studied by Burer and Vandenbussche [4]. The equivalence between the two relaxations was recently shown by Povh and Rendl [19].

3 Valid inequalities for the SDP relaxation

The following theorem from [28] shows that several valid (in)equalities are implied by the constraints of the SDP problem (13).

Theorem 3.1 (cf. [28], Lemma 3.1) *Assume $y \in \mathbb{R}^{n^2}$ and $Y \in \mathcal{S}_{n^2}$ are such that*

$$\begin{pmatrix} 1 & y^T \\ y & Y \end{pmatrix} \succeq 0,$$

and that the matrix in the last expression has the block form (6) and satisfies (12). Then one has:

1. $\left(y^{(j)}\right)^T = e^T Y^{(ij)} \quad (i, j = 1, \ldots, n)$;
2. $\sum_{i=1}^n Y^{(ij)} = e\left(y^{(j)}\right)^T \quad (j = 1, \ldots, n)$;
3. $\sum_{i=1}^n \mathrm{diag}\left(Y^{(ij)}\right) = y^{(j)} \quad (j = 1, \ldots, n)$.

The fact that these are valid equalities easily follows from (5) and (7).

The third condition in the theorem for $i = j$, together with the gangster constraint, implies that

$$\operatorname{diag}(Y) = y.$$

By the Schur complement theorem, this in turn implies the following.

Corollary 3.1 *Assume that y and Y meet the conditions of Theorem 3.1, and that $Y \geq 0$. Then $Y \succeq \operatorname{diag}(Y)\operatorname{diag}(Y)^T$.*

Triangle inequalities

The fact that Y_X is generated by $\{0, 1\}$-vectors gives rise to the so-called *triangle inequalities*:

$$0 \leq Y_{rs} \leq Y_{rr}, \tag{14}$$
$$Y_{rr} + Y_{ss} - Y_{rs} \leq 1, \tag{15}$$
$$-Y_{tt} - Y_{rs} + Y_{rt} + Y_{st} \leq 0, \tag{16}$$
$$Y_{tt} + Y_{rr} + Y_{ss} - Y_{rs} - Y_{rt} - Y_{st} \leq 1, \tag{17}$$

which hold for all distinct triples (r, s, t). Note that there are $O(n^6)$ triangle inequalities.

A useful observation is the following.

Lemma 3.1 *If an optimal solution Y, y of (13) has a constant diagonal, then all the triangle inequalities (14)–(17) are satisfied.*

Proof Since the pair (y, Y) satisfies $\operatorname{trace}(Y) - 2e^T y = -n$, and $\operatorname{diag}(Y) = y$ is a multiple of the all-ones vector, one has $\operatorname{diag}(Y) = y = \frac{1}{n}e_{n^2}$. Thus (15) and (17) are implied, since $Y \geq 0$.

The condition $\left(y^{(j)}\right)^T = e^T Y^{(ij)} \quad (i, j = 1, \ldots, n)$ implies that the row sum of any block $Y^{(ij)}$ equals $\frac{1}{n}e_n^T$. In particular, all entries in $Y^{(ij)}$ are at most $1/n$, since $Y^{(ij)} \geq 0$. Thus (14) is implied.

Finally, we verify that (16) holds. This may be done by showing that:

$$\frac{1}{n} = \max(Y_{st} + Y_{rt} - Y_{rs})$$

subject to

$$\begin{pmatrix} \frac{1}{n} & Y_{rs} & Y_{rt} \\ Y_{rs} & \frac{1}{n} & Y_{st} \\ Y_{rt} & Y_{st} & \frac{1}{n} \end{pmatrix} \succeq 0, \quad Y_{rs} \geq 0, \quad Y_{rt} \geq 0, \quad Y_{st} \geq 0.$$

Indeed, it is straightforward to verify, using duality theory, that an optimal solution is given by $Y_{rs} = Y_{rt} = Y_{st} = 1/n$, which concludes the proof. □

As noted in [20], the size of the SDP problem (13) is too large for its solution by using interior point methods if $n \geq 15$.

We will therefore focus on a subclass of QAP instances where the data matrices have suitable algebraic symmetry. In the next section we first review the general theory of group symmetric SDP problems.

4 Group symmetric SDP problems

In this section we will give only a brief review of group symmetric SDP's, and we will state results without proofs. More details may be found in the survey by Parrilo and Gatermann [11].

Assume that the following semidefinite programming problem is given

$$p^* := \min_{X \succeq 0,\ X \geq 0} \left\{ \operatorname{trace}(A_0 X) \ : \ \operatorname{trace}(A_k X) = b_k, \quad k = 1, \ldots, m \right\}, \tag{18}$$

where $A_i \in \mathcal{S}_n$ $(i = 0, \ldots, m)$ are given. We also assume that this problem has an optimal solution.

Assumption 1 (Group symmetry) *We assume that there is a nontrivial, finite, multiplicative group of orthogonal matrices $\mathcal{G}$ such that*

$$A_k P = P A_k \quad \forall\ P \in \mathcal{G},\ k = 0, \ldots, m.$$

The *commutant* (or centralizer ring) of $\mathcal{G}$ is defined as

$$\mathcal{A}_{\mathcal{G}} := \{X \in \mathbb{R}^{n \times n} \ : \ XP = PX \quad \forall\ P \in \mathcal{G}\}.$$

In other words, in Assumption 1 we assume that the data matrices A_k $(k = 0, \ldots, m)$ lie in the commutant of $\mathcal{G}$.

The commutant is a matrix $*$-algebra over $\mathbb{R}$, i.e. a subspace of $\mathbb{R}^{n \times n}$ that is closed under matrix multiplication and taking transposes.

An alternative, equivalent definition of the commutant is

$$\mathcal{A}_{\mathcal{G}} = \{X \in \mathbb{R}^{n \times n} \ : \ R_{\mathcal{G}}(X) = X\},$$

where

$$R_{\mathcal{G}}(X) := \frac{1}{|\mathcal{G}|} \sum_{P \in \mathcal{G}} P X P^T,\ X \in \mathbb{R}^{n \times n}$$

is called the *Reynolds operator* (or group average) of $\mathcal{G}$. Thus $R_{\mathcal{G}}$ is the orthogonal projection onto the commutant. Orthonormal eigenvectors of $R_{\mathcal{G}}$ corresponding to the eigenvalue 1 form an orthonormal basis of $\mathcal{A}_{\mathcal{G}}$ (seen as a vector space).

This basis, say $B_1, \ldots, B_d$, has the following properties:

- $B_i \in \{0, 1\}^{n\times n} \quad (i = 1, \ldots, d)$;
- $\sum_{i=1}^{d} B_i = J$.
- For any $i \in \{1, \ldots, d\}$, one has $B_i^T = B_j$ for some $j \in \{1, \ldots, d\}$ (possibly $i = j$).

A basis of a matrix $*$-algebra with these properties is sometimes called a *non-commutative association scheme*; it is called an *association scheme* if the B_i's also commute.

One may also obtain the basis $B_1, \ldots, B_d$ by examining the image of the standard basis of $\mathbb{R}^{n\times n}$ under $R_{\mathcal{G}}$. In particular, if $e_1, \ldots, e_n$ denotes the standard basis of $\mathbb{R}^n$ then the $\{0, 1\}$ matrix with the same support as $R_{\mathcal{G}}(e_i e_j^T)$ is a basis matrix of the commutant, for any $i, j \in \{1, \ldots, n\}$.

Another way of viewing this is to consider the orbit of the pair of indices (i, j) (also called 2-orbit) under the action of $\mathcal{G}$. This 2-orbit of (i, j) is defined as

$$\{(Pe_i, Pe_j) \ : \ P \in \mathcal{G}\}.$$

The corresponding basis matrix has an entry 1 at position (k, l) if (e_k, e_l) belongs to the 2-orbit, and is zero otherwise.

A well-known, and immediate consequence of Assumption 1 is that we may restrict the feasible set of the optimization problem to its intersection with the commutant of $\mathcal{G}$.

Theorem 4.1 *Under Assumption* 1, *problem* (18) *has an optimal solution in the commutant of* $\mathcal{G}$.

Proof If X is an optimal solution of problem (18), then so is $R_{\mathcal{G}}(X)$, by Assumption 1. □

Assume we have a basis $B_1, \ldots, B_d$ of the commutant $\mathcal{A}_{\mathcal{G}}$. One may write $X = \sum_{i=1}^{d} x_i B_i$. Moreover, the nonnegativity condition $X \geq 0$ is equivalent to $x \geq 0$, by the properties of the basis.

Thus the SDP problem (18) reduces to

$$\min_{\sum_{i=1}^{d} x_i B_i \succeq 0} \left\{ \sum_{i=1}^{d} x_i \operatorname{trace}(A_0 B_i) : \sum_{i=1}^{d} x_i \operatorname{trace}(A_k B_i) = b_k, \quad k = 1, \ldots, m, \ x \geq 0 \right\}. \tag{19}$$

Note that the values $\operatorname{trace}(A_k B_i)$ $(i = 1, \ldots, d)$, $(k = 0, \ldots, m)$ may be computed beforehand.

The next step in reducing the SDP (19) is to block diagonalize the commutant $\mathcal{A}_{\mathcal{G}}$, i.e. block diagonalize its basis $B_1, \ldots, B_d$. To this end, we review some general theory on block diagonalization of matrix algebras in the next section.

The motivation for block diagonalization is that interior point solvers (e.g. CSDP [3] and SeDuMi [24]) can exploit such structure in SDP data matrices, since a block diagonal matrix is positive semidefinite if and only if each of its diagonal blocks is positive semidefinite.

5 Matrix algebras and their block factorizations

In this section we review the general theory of block diagonalization of matrix $*$-algebras, and introduce a heuristic to compute such a decomposition.

5.1 The canonical decomposition of a matrix $*$-algebra

The following theorem shows that a matrix $*$-algebra over $\mathbb{R}$ may be 'block diagonalized' in a canonical way via an orthogonal transformation. The theorem is due to Wedderburn [25] in a more general setting; the result as stated here follows from Theorem 5(ii) in Chap. X of [26].

Before stating the result, recall that a matrix $*$-algebra $\mathcal{A}$ is called simple if its only ideals are $\{0\}$ and $\mathcal{A}$ itself.

Theorem 5.1 (Wedderburn [25]) *Assume $\mathcal{A} \subset \mathbb{R}^{n\times n}$ is a matrix *-algebra over $\mathbb{R}$ that contains the identity I. Then there is an orthogonal matrix Q and some integer s such that*

$$Q^T \mathcal{A} Q = \begin{pmatrix} \mathcal{A}_1 & 0 & \cdots & 0 \\ 0 & \mathcal{A}_2 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \mathcal{A}_s \end{pmatrix},$$

where each $\mathcal{A}_t$ $(t = 1, \ldots, s)$ is a simple matrix $*$-algebra over $\mathbb{R}$. This decomposition is unique up to a permutation of the blocks.

Simple matrix $*$-algebras over $\mathbb{R}$ are completely classified and one can give a more detailed statement of the above theorem.

However, we will not need these details in the current paper, and will only illustrate the theorem with an example that we will need for some of the QAP instances to be considered later (see the *esc* instances in Sect. 8). The example concerns the so-called Bose–Mesner algebra of the Hamming scheme, and was first used in the context of SDP by Schrijver [21]. A more detailed exposition than given here may be found in the thesis of Gijswijt [12]; see Sects. 3.1 and 4.1 there.

Example 5.1 Consider the matrix A with 2^n rows indexed by all elements of $\{0, 1\}^n$, and A_{ij} given by the Hamming distance between $i \in \{0, 1\}^n$ and $j \in \{0, 1\}^n$.

The automorphism group of A arises as follows. Any permutation π of the index set $\{1, \ldots, n\}$ induces an isomorphism of A that maps row (resp. column) i of A to row (resp. column) $\pi(i)$ for all i. There are $n!$ such permutations. Moreover, there are an additional 2^n permutations that act on $\{0, 1\}^n$ by either 'flipping' a given component from zero to one (and vice versa), or not.

Thus $\mathrm{aut}(A)$ has order $n!2^n$. The centralizer ring of $\mathrm{aut}(A)$ is a commutative matrix $*$-algebra over $\mathbb{R}$ and is known as the Bose-Mesner algebra of the Hamming scheme.

A basis for the centralizer ring may be derived from the 2-orbits of $\mathrm{aut}(A)$ and are given by

$$B^{(k)}_{ij} = \begin{cases} 1 & \text{if Hamming}(i, j) = k; \\ 0 & \text{else} \end{cases} \qquad (k = 0, \ldots, n),$$

where $\mathrm{Hamming}(i, j)$ is the Hamming distance between i and j. The basis matrices $B^{(k)}$ are simultaneously diagonalized by the orthogonal matrix Q defined by

$$Q_{ij} = 2^{-\frac{n}{2}}(-1)^{i^T j} \quad i, j \in \{0, 1\}^n.$$

The distinct elements of the matrix $Q^T B^{(k)} Q$ equal $K_j(k)$ $(j = 0, \ldots, n)$ where

$$K_j(x) := \sum_{k=0}^{j} (-1)^k \binom{x}{k}\binom{n-x}{j-k}, \quad j = 0, \ldots, n,$$

are called Krawtchouk polynomials. Thus a linear matrix inequality of the form

$$\sum_{k=0}^{n} x_k B^{(k)} \succeq 0$$

is equivalent to the system of linear inequalities

$$\sum_{k=0}^{n} x_k K_j(k) \geq 0 \quad (j = 0, \ldots, n),$$

since

$$\sum_{k=0}^{n} x_k B^{(k)} \succeq 0 \Longleftrightarrow \sum_{k=0}^{n} x_k Q^T B^{(k)} Q \succeq 0.$$

5.2 A heuristic for computing a block diagonalization

Let $\mathcal{G}$ be a multiplicative group of orthogonal matrices with commutant $\mathcal{A}_{\mathcal{G}}$. Assume that $B_1, \ldots, B_d$ span $\mathcal{A}_{\mathcal{G}}$.

Our goal is to block-diagonalize the basis $B_1, \ldots, B_d$. The proof of Theorem 5.1 is constructive, and can in principle be used to compute the canonical block diagonalization of $\mathcal{A}_{\mathcal{G}}$. Alternatively, group representation theory may be used for the same goal.

However, we will employ a simple heuristic that may in general compute a coarser block diagonalization of $\mathcal{A}_{\mathcal{G}}$ than described in Theorem 5.1). This coarser factorization is sufficient for our (computational) purposes.

Block diagonalization heuristic

1. Choose a random symmetric element, say Z, from span$\{P : P \in \mathcal{G}\}$;
2. Compute the spectral decomposition of Z, and let Q be an orthogonal matrix with columns given by a set of orthonormal eigenvectors of Z.
3. Block diagonalize the basis $B_1, \ldots, B_d$ by computing $Q^T B_1 Q, \ldots, Q^T B_d Q$.

The heuristic is motivated by the following (well-known) observation.

Theorem 5.2 *Let q be an eigenvector of some $Z \in$ span$\{P : P \in \mathcal{G}\}$ and let $\lambda \in \mathbb{R}$ be the associated eigenvalue. Then Xq is an eigenvector of Z with eigenvalue λ for each $X \in \mathcal{A}_{\mathcal{G}}$.*

Proof Note that

$$Z(Xq) = XZq = \lambda Xq,$$

by the definition of the commutant. □

Thus if we form a matrix $Q = [q_1 \ \cdots \ q_n]$ where the q_i's form an orthogonal set of eigenvectors of Z, then $Q^T B_i Q$ is a block diagonal matrix for all i. Note that the sizes of the blocks are given by the multiplicities of the eigenvalues of Z.

6 Tensor products of groups and their commutants

The following theorem shows that, if one has two multiplicative groups of orthogonal matrices, then one may obtain a third group using Kronecker products. In representation theory this construction is known as the *tensor product* of the groups.

Theorem 6.1 (cf. Serre [23], Sect. 1.5) *Let $\mathcal{G}_p$ and $\mathcal{G}_s$ be two multiplicative groups of orthogonal matrices given by p_i $(i = 1, \ldots, |\mathcal{G}_p|)$ and s_j $(j = 1, \ldots, |\mathcal{G}_s|)$, respectively.*

Then the matrices

$$P_{ij} := p_i \otimes s_j \quad i = 1, \ldots, |\mathcal{G}_p|, \quad j = 1, \ldots, |\mathcal{G}_s|$$

form a multiplicative group of orthogonal matrices. This group is denoted by $\mathcal{G}_p \otimes \mathcal{G}_s$.

Proof Let $\mathcal{G} := \mathcal{G}_p \otimes \mathcal{G}_s$ and let indices $i, i', \hat{i}, j, j', \hat{j} \in \{1, \ldots, |\mathcal{G}|\}$ be given such that $p_i p_{i'} = p_{\hat{i}}$ and $s_j s_{j'} = s_{\hat{j}}$. Note that

$$\begin{aligned} P_{ij} P_{i'j'} &= (p_i \otimes s_j)(p_{i'} \otimes s_{j'}) \\ &= (p_i p_{i'}) \otimes (s_j s_{j'}) \\ &= p_{\hat{i}} \otimes s_{\hat{j}} \equiv P_{\hat{i}\hat{j}}. \end{aligned}$$

Moreover, note that the matrices P_{ij} are orthogonal, since the p_i and s_j's are. □

In the next theorem we show how to construct a basis for the commutant of the tensor product of groups. We note that this result is also well-known, but we again supply a proof for completeness.

Theorem 6.2 *Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two multiplicative groups of $n \times n$ orthogonal matrices with respective commutants $\mathcal{A}_1$ and $\mathcal{A}_2$. Let B_i^1 $(i = 1, \ldots, n_1)$ be a basis for $\mathcal{A}_1$ and B_j^2 $(j = 1, \ldots, n_2)$ a basis for $\mathcal{A}_2$. Then a basis for the commutant of $\mathcal{G}_1 \otimes \mathcal{G}_2$ is given by*

$$\left\{B_i^1 \otimes B_j^2 : i = 1, \ldots, n_1, \quad j = 1, \ldots, n_2\right\}.$$

Proof Letting e_i $(i = 1, \ldots, n)$ denote the standard unit vectors in $\mathbb{R}^n$, a basis for $\mathbb{R}^{n^2 \times n^2}$ is given by

$$e_i e_j^T \otimes e_k e_l^T \quad (i, j, k, l = 1, \ldots, n).$$

A basis for the commutant of $\mathcal{G} := \mathcal{G}_1 \otimes \mathcal{G}_2$ is obtained by taking the image of this basis under the Reynolds operator $R_{\mathcal{G}}$ of $\mathcal{G}$. Note that

$$\begin{aligned}
R_{\mathcal{G}}(e_i e_j^T \otimes e_k e_l^T) &:= \frac{1}{|\mathcal{G}|} \sum_{P_1 \in \mathcal{G}_1, P_2 \in \mathcal{G}_2} P_1 \otimes P_2 (e_i e_j^T \otimes e_k e_l^T) P_1^T \otimes P_2^T \\
&= \frac{1}{|\mathcal{G}_1||\mathcal{G}_2|} \sum_{P_1 \in \mathcal{G}_1, P_2 \in \mathcal{G}_2} P_1 e_i e_j^T P_1^T \otimes P_2 e_k e_l^T P_2^T \\
&= \frac{1}{|\mathcal{G}_1|} \sum_{P_1 \in \mathcal{G}_1} P_1 e_i e_j^T P_1^T \otimes \frac{1}{|\mathcal{G}_2|} \sum_{P_2 \in \mathcal{G}_2} P_2 e_k e_l^T P_2^T \\
&\equiv R_{\mathcal{G}_1}(e_i e_j^T) \otimes R_{\mathcal{G}_2}(e_k e_l^T),
\end{aligned}$$

where we have used the properties (1) and (2) of the Kronecker product. The required result follows. □

7 The symmetry of the SDP relaxation of the QAP

We now apply the theory described in the last sections to the SDP relaxation (13) of the QAP.

7.1 Symmetry reduction of (13)

Let A and B be the data matrices that define an instance of the QAP. We define the automorphism group of a matrix $Z \in \mathbb{R}^{n \times n}$ as

$$\mathrm{aut}(Z) = \{P \in \Pi_n \ : \ PZP^T = Z\}.$$

Theorem 7.1 *Define the multiplicative matrix group*

$$\mathcal{G}_{QAP} := \left\{ \begin{pmatrix} 1 & 0^T \\ 0 & P_A \otimes P_B \end{pmatrix} \; : \; P_A \in aut(A), \;\; P_B \in aut(B) \right\}, \tag{20}$$

Then the SDP problem (13) *satisfies Assumption* 1 *with respect to the* $\mathcal{G}_{QAP}$.

Proof If we view problem (13) as an SDP problem in the form (18), then the data matrices are given by:

$$A_0 := \begin{pmatrix} 0 & 0^T \\ 0 & A \otimes B \end{pmatrix}, \quad A_1 := \begin{pmatrix} 0 & 0^T \\ 0 & I \otimes (J-I) + (J-I) \otimes I \end{pmatrix},$$

$$A_2 := \begin{pmatrix} 0 & -e^T \\ -e & I \end{pmatrix}, \quad \text{and} \quad A_3 := \begin{pmatrix} 1 & 0^T \\ 0 & 0_{n^2 \times n^2} \end{pmatrix}.$$

Let $P_A \in \text{aut}(A)$ and $P_B \in \text{aut}(B)$. We have to verify that

$$\begin{pmatrix} 1 & 0^T \\ 0 & P_A \otimes P_B \end{pmatrix}^T A_i \begin{pmatrix} 1 & 0^T \\ 0 & P_A \otimes P_B \end{pmatrix} = A_i, \qquad (i = 0, \ldots, 3),$$

and this may easily be done using only the definitions of the A_i's and the properties of the Kronecker product. For example,

$$\begin{aligned} \begin{pmatrix} 1 & 0^T \\ 0 & P_A \otimes P_B \end{pmatrix}^T A_0 \begin{pmatrix} 1 & 0^T \\ 0 & P_A \otimes P_B \end{pmatrix} &= \begin{pmatrix} 0 & 0^T \\ 0 & (P_A^T \otimes P_B^T)(A \otimes B)(P_A \otimes P_B) \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0^T \\ 0 & P_A^T A P_A \otimes P_B^T B P_B \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0^T \\ 0 & A \otimes B \end{pmatrix} \equiv A_0. \end{aligned}$$

□

We may construct a basis for the commutant of $\mathcal{G}_{QAP}$ from the bases of the commutants of aut(A) and aut(B) respectively, as is shown in the following theorem.

Theorem 7.2 *The commutant of* $\mathcal{G}_{QAP}$ *is spanned by all matrices of the form*

$$\begin{pmatrix} 1 & 0^T \\ 0 & 0_{n^2 \times n^2} \end{pmatrix}, \begin{pmatrix} 0 & 0^T \\ 0 & B_i^A \otimes B_j^B \end{pmatrix},$$
$$\begin{pmatrix} 0 & \text{diag}(B_i^A \otimes B_j^B)^T \\ 0 & 0_{n^2 \times n^2} \end{pmatrix}, \begin{pmatrix} 0 & 0^T \\ \text{diag}(B_i^A \otimes B_j^B) & 0_{n^2 \times n^2} \end{pmatrix}$$

where B_i^A (*resp.* B_j^B) *is an element of the basis of the commutant of aut*(A) (*resp. aut*(B)).

Proof Let

$$\begin{pmatrix} a & b^T \\ c & Z \end{pmatrix}$$

denote a matrix from the commutant of $\mathcal{G}_{QAP}$, where $a \in \mathbb{R}$, $b, c \in \mathbb{R}^{n^2}$ and $Z \in \mathbb{R}^{n^2 \times n^2}$. For any $P_A \in \text{aut}(A)$ and $P_B \in \text{aut}(B)$ one therefore has

$$\begin{pmatrix} a & b^T \\ c & Z \end{pmatrix} \begin{pmatrix} 1 & 0^T \\ 0 & P_A \otimes P_B \end{pmatrix} = \begin{pmatrix} 1 & 0^T \\ 0 & P_A \otimes P_B \end{pmatrix} \begin{pmatrix} a & b^T \\ c & Z \end{pmatrix}$$

by the definition of the commutant. This implies that

$$Z(P_A \otimes P_B) = (P_A \otimes P_B)Z, \ (P_A \otimes P_B)b = b, \ (P_A \otimes P_B)c = c, \tag{21}$$

for all $P_A \in \text{aut}(A)$ and $P_B \in \text{aut}(B)$.

This implies that Z lies in the commutant of $\text{aut}(A) \otimes \text{aut}(B)$. Thus we may write

$$Z \in \text{span}_{i,j}\{B_i^A \otimes B_j^B\}$$

if the B_i^A's and B_j^B's form bases for the commutants of $\text{aut}(A)$ and $\text{aut}(B)$, respectively, by Theorem 6.2.

Moreover, (21) implies that b and c are linear combinations of incidence vectors of orbits of $\text{aut}(A) \otimes \text{aut}(B)$. These incidence vectors are obtained by taking the Kronecker products of incidence vectors of orbits of $\text{aut}(A)$ and $\text{aut}(B)$. We may also obtain these incidence vectors as the diagonal vectors of the basis of the commutant of $\text{aut}(A) \otimes \text{aut}(B)$, i.e. from the vectors $\text{diag}(B_i^A \otimes B_j^B)$. This completes the proof. □

We may now simplify the SDP relaxation (13) using the basis of the commutant of $\mathcal{G}_A \otimes \mathcal{G}_B$. In particular, we may assume that

$$Y = \sum_{i,j} y_{ij} B_i^A \otimes B_j^B,$$

where $y_{ij} \geq 0$.

This implies, with reference to the SDP (13), that

$$\begin{aligned} \text{trace}(I \otimes (J - I)Y) &= \sum_{i,j} y_{ij} \,\text{trace}(I \otimes (J - I)B_i^A \otimes B_j^B) \\ &= \sum_{i,j} y_{ij} \,\text{trace}(B_i^A \otimes (J - I)B_j^B) \\ &= \sum_{i,j} y_{ij} \,\text{trace}\, B_i^A \,\text{trace}(J - I)B_j^B, \end{aligned}$$

where we have used the identities (2) and (4) of the Kronecker product. Notice that trace B_i^A is simply the length of an orbit of $\mathrm{aut}(A)$ (indexed by i). Similarly, $\mathrm{trace}(J - I)B_j^B$ equals the length of a 2-orbit of $\mathrm{aut}(B)$. Note that we consider 2-orbits to be orbits of pairs of nonidentical indices, i.e. we view the orbit of (1, 1) as a (one) orbit and not as a 2-orbit.

Thus it is convenient to introduce notation for sets of orbits and 2-orbits: O_A^1 will denote the set of orbits of $\mathrm{aut}(A)$, O_A^2 the set of 2-orbits, etc. The length (i.e. cardinality) of an orbit will be denoted by $\ell(\cdot)$.

Using this notation we may rewrite the constraint:

$$\mathrm{trace}((I \otimes (J - I))Y + ((J - I) \otimes I)Y) = 0$$

as

$$\sum_{i \in O_A^1, j \in O_B^2} y_{ij}\ell(i)\ell(j) + \sum_{i \in O_A^2, j \in O_B^1} y_{ij}\ell(i)\ell(j) = 0.$$

Together with $y_{ij} \geq 0$, this implies that we may set all variables y_{ij} $(i \in O_A^1,\ j \in O_B^2)$ and y_{ij} $(i \in O_A^2,\ j \in O_B^1)$ to zero.

Moreover, we can use the fact that the first row and column (without the upper left corner) equals the diagonal, to reduce the constraint

$$\mathrm{trace}(Y) - 2e^T y = -n$$

to $\mathrm{trace}(Y) = n$ by using $\mathrm{diag}(Y) = y$, which in turn becomes

$$\sum_{i \in O_A^1,\ j \in O_B^1} y_{ij}\ell(i)\ell(j) = n.$$

Proceeding in this vein, we obtain the SDP reformulation:

$$\min \sum_{i \in O_A^2,\ j \in O_B^2} y_{ij}\,\mathrm{trace}(AB_i^A)\,\mathrm{trace}(BB_j^B) + \sum_{i \in O_A^1,\ j \in O_B^1} y_{ij}\,\mathrm{trace}(AB_i^A)\,\mathrm{trace}(BB_j^B)$$

subject to

$$\begin{aligned}
&\sum_{i \in O_A^1,\ j \in O_B^1} y_{ij}\ell(i)\ell(j) = n \\
&\begin{pmatrix} 1 & 0^T \\ 0 & 0_{n^2 \times n^2} \end{pmatrix} + \sum_{i \in O_A^1,\ j \in O_B^1} y_{ij} \begin{pmatrix} 0 & \mathrm{diag}(B_i^A \otimes B_j^B)^T \\ \mathrm{diag}(B_i^A \otimes B_j^B) & B_i^A \otimes B_j^B \end{pmatrix} \\
&\quad + \sum_{i \in O_A^2\ j \in O_B^2} y_{ij} \begin{pmatrix} 0 & 0^T \\ 0 & B_i^A \otimes B_j^B \end{pmatrix} \succeq 0 \qquad (22)\\
&y_{ij} \geq 0\ \forall i, j.
\end{aligned}$$

As mentioned before, the numbers trace(AB_i^A) and trace(BB_j^B) in the objective function may be computed beforehand. Note that the number of scalar variables y_{ij} is

$$|O_A^1||O_B^1| + |O_A^2||O_B^2|,$$

that may be much smaller than the $\binom{n^2+2}{2}$ independent entries in a symmetric $(n^2+1) \times (n^2+1)$ matrix, depending on the symmetry groups. This number may be further reduced, since the matrices appearing in the linear matrix inequality (22) should be symmetric. Recall that for every i (resp. j) there is an $i*$ (resp. $j*$) such that $(B_i^A)^T = B_{i*}^A$ (resp. $(B_j^B)^T = B_{j*}^B$).

Thus one has $y_{ij} = y_{i*j*}\ \forall\ i, j$. Letting $O_A^{2,sym}$ (resp. $O_B^{2,sym}$) denote the symmetric 2-orbits of aut(A) (resp. aut(B)), the final number of scalar variables becomes

$$|O_A^1||O_B^1| + \frac{1}{2}\left(|O_A^2||O_B^2| + |O_A^{2,sym}||O_B^{2,sym}|\right).$$

7.2 Block diagonalization

The size of the SDP can be further reduced by block diagonalizing the data matrices in (22) via block diagonalization of the matrices B_i^A and B_j^B.

Assume, to this end, that we know real, orthogonal matrices Q_A and Q_B that give some block-diagonalization of the commutants of aut(A) and aut(B) respectively. Defining the orthogonal matrix

$$Q := \begin{pmatrix} 1 & 0^T \\ 0 & Q_A \otimes Q_B \end{pmatrix},$$

one has, with reference to the LMI (22):

$$Q^T \begin{pmatrix} 0 & 0^T \\ 0 & B_i^A \otimes B_j^B \end{pmatrix} Q = \begin{pmatrix} 0 & 0^T \\ 0 & Q_A^T B_i^A Q_A \otimes Q_B^T B_j^B Q_B \end{pmatrix},$$

and

$$Q^T \begin{pmatrix} 0 & \operatorname{diag}(B_i^A \otimes B_j^B)^T \\ \operatorname{diag}(B_i^A \otimes B_j^B) & B_i^A \otimes B_j^B \end{pmatrix} Q$$
$$= \begin{pmatrix} 0 & (Q_A^T \operatorname{diag}(B_i^A) \otimes Q_B^T \operatorname{diag}(B_j^B))^T \\ Q_A^T \operatorname{diag}(B_i^A) \otimes Q_B^T \operatorname{diag}(B_j^B) & Q_A^T B_i^A Q_A \otimes Q_B^T B_j^B Q_B \end{pmatrix}.$$

These matrices all have a chordal sparsity pattern, so that the LMI (22) involving these matrices may be simplified by using the following theorem.

Theorem 7.3 (see e.g. [15]) *Assume matrices $A_0, \ldots, A_m \in \mathcal{S}_n$ are given and define the graph $G = (V, E)$ with $V = \{1, \ldots, n\}$ and $\{i, j\} \in E$ if $(A_k)_{ij} \neq 0$ for some $k \in \{0, \ldots, m\}$.*

If the graph G is chordal[1] *and its maximal cliques are denoted by $K_1, \ldots, K_d$, then the following two statements are equivalent for a given vector $y \in \mathbb{R}^m$:*

1.
$$A_0 - \sum_{i=1}^{m} y_i A_i \succeq 0,$$

2.
$$(A_0)_{K_i,K_i} - \sum_{j=1}^{m} y_i (A_j)_{K_i,K_i} \succeq 0, \ \forall \ \ i = 1, \ldots, d,$$

where $(A_j)_{K_i,K_i}$ denotes the principal submatrix of A_j formed by the rows and columns corresponding to K_i.

We may apply the theorem to the LMI (22), after performing the orthogonal transformation $Q^T(\cdot)Q$. The size of the resulting system of LMI's is determined by the sizes and number of blocks of the commutants of $\mathrm{aut}(A)$ and $\mathrm{aut}(B)$ respectively.

7.3 Triangle inequalities

The number of triangle inequalities (14)–(17) may also be reduced in number in an obvious way by exploiting the algebraic symmetry. We omit the details, and only state one result, by way of example.

Theorem 7.4 *If both $\mathrm{aut}(A)$ and $\mathrm{aut}(B)$ are transitive, then all triangle inequalities* (14)–(17) *are implied in the final SDP relaxation.*

Proof If both $\mathrm{aut}(A)$ and $\mathrm{aut}(B)$ are transitive, then every matrix in the commutant of $\mathcal{G}_{QAP}$ [see (20)] has a constant diagonal, since $\mathcal{G}_{QAP}$ only has one orbit. The required result now follows from Lemma 3.1. □

8 Numerical results

In Table 1 we give the numbers of orbits and 2-orbits of $\mathrm{aut}(A)$ and $\mathrm{aut}(B)$ for several instances from the QAPLIB library [6]. (The value of n for each instance is clear from the name of the instance, *e.g.* for esc16a, $n = 16$.)

We also give the number of scalar variables in our final SDP relaxation (see Sect. 7.1).

The automorphism groups of the matrices A and B were computed using the computational algebra software GAP [10]. The same package was used to compute the 2-orbits of these groups.

[1] A graph is called chordal, if it does not contain a cycle of length four or more as an induced subgraph.

Table 1 Symmetry information on selected QAPLIB instances

Instance	$\|O_A^1\|, \|O_B^1\|$	$\|O_A^2\|, \|O_B^2\|$	$\|O_A^{2,sym}\|, \|O_B^{2,sym}\|$	# y_{ij}'s
esc16a	6, 1	42, 4	6, 4	102
esc16b	7, 1	45, 4	3, 4	103
esc16c	12, 1	135, 4	3, 4	288
esc16d	12, 1	135, 4	3, 4	288
esc16e	6, 1	37, 4	5, 4	90
esc16f	1, 1	1, 4	1, 4	5
esc16g	9, 1	73, 4	1, 4	157
esc16h	5, 1	23, 4	3, 4	57
esc16i	10, 1	91, 4	1, 4	194
esc16j	7, 1	44, 4	2, 4	99
esc32a	26, 1	651, 5	1, 5	1,656
esc32b	2, 1	18, 5	10, 5	72
esc32c	10, 1	96, 5	6, 5	265
esc32d	9, 1	86, 5	10, 5	249
esc32g	7, 1	44, 5	2, 5	122
esc32h	14, 1	188, 5	6, 5	499
esc64a	13, 1	163, 6	5, 6	517
esc128	16, 1	253, 7	9, 7	933
nug20	6, 20	98, 380	14, 0	18,740
nug21	8, 21	117, 420	13, 0	24,738
nug22	6, 22	116, 462	16, 0	26,928
nug24	6, 24	138, 552	18, 0	38,232
nug25	6, 25	85, 600	13, 0	25,650
nug30	9, 30	225, 870	21, 0	98,145
scr20	20, 6	380, 98	0, 14	18,740
sko42	12, 42	438, 1,722	30, 0	377,622
sko49	10, 49	315, 2,352	27, 0	370,930
ste36a	35, 10	1191, 318	1, 26	189,732
ste36b	10, 35	318, 1,191	26, 1	189,732
ste36c	10, 35	318, 1,191	26, 1	189,732
tho30	10, 30	240, 870	20, 0	104,700
tho40	12, 40	404, 1,560	28, 0	315,600
wil50	15, 50	635, 2,450	35, 0	778,625
wil100	15, 100	1,260, 9,900	60, 0	6,238,500

Note that the 'esc' instances [5] are particularly suited to our approach.[2] Here the automorphism group of B is the automorphism group of the Hamming graph described

[2] We do not present results for the QAPLIB instances esc32e and esc32f in this paper, since these instances have identical data on the QAPLIB website, and moreover the bounds we obtain are not consistent with the reported optimal values for these instances. We have contacted the QAPLIB moderator concerning this, but it remains unclear what the correct data is.

Table 2 Block sizes after (heuristic) block diagonalization of the centralizer ring of aut(A) for selected esc instances. For the esc instances the centralizer ring of aut(B) could be diagonalized

Instance	Block sizes of commutant of aut(A)	Largest block in final SDP
esc32a	1, 3, 28	29
esc32b	5, 7, 8, 12	13
esc32c	1, 2, 29	30
esc32d	1, 2, 4, 25	26
esc32g	1, 31	32
esc32h	1, 31	32
esc64a	1, 63	64
esc128	1 (82 times), 2 (14 times), 18	19

Table 3 Block sizes after (heuristic) block diagonalization of the commutant of aut(A) or aut(B) for selected QAPLIB instances. For these instances either A or B had a nontrivial automorphism group, but not both

Instance	Matrix	Block sizes of commutant of aut(Matrix)	Largest block in final SDP
nug20	A	2,4, 6, 6	121
nug21	A	3, 4, 6, 8	169
nug22	A	5, 5, 6, 6	133
nug24	A	6, 6, 6, 6	145
nug25	A	1, 3, 3, 6, 6, 6	151
nug30	A	6, 6, 9, 9	271
scr20	B	4, 4, 6, 6	121
sko42	A	9, 9, 12, 12	505
sko49	A	3, 6, 6, 10, 12, 12	589
ste36a	B	8, 8, 10, 10	361
ste36b	A	8, 8, 10, 10	361
ste36c	A	8, 8, 10, 10	361
tho30	A	5, 5, 10, 10	301
tho40	A	8, 8, 12, 12	481
wil50	A	10, 10, 15, 15	751
wil100	A	10, 10, 15, 15, 25, 25	2, 501

in Example 5.1. Consequently the commutant of aut(B) may be diagonalized, and its dimension is small.

The other block sizes of the commutants of aut(A) and aut(B) that were computed using the heuristic of Sect. 5.2 are shown in Tables 2 and 3 for selected QAPLIB instances. The size of the largest block appearing in the final SDP formulation for each instance is also shown.

Note that the QAPLIP instances other than the esc instances are still too large to solve by interior point methods. The reason is that a linear system of the same size as the number of scalar variables has to be solved at each iteration of the interior point method. Thus the practical limit for the number of scalar variables is of the order of a few thousand. Note however, that a significant reduction in size is obtained for many

Table 4 Optimal values and solution times for the esc16 instances

Instance	SDP l.b. (13)	Opt.	Time(s)
esc16a	$64 \equiv \lceil 63.2756 \rceil$	68	0.75
esc16b	$290 \equiv \lceil 289.8817 \rceil$	292	1.04
esc16c	$154 \equiv \lceil 153.8242 \rceil$	160	1.78
esc16d	$13 \equiv \lceil 13.0000 \rceil$	16	0.89
esc16e	$27 \equiv \lceil 26.3368 \rceil$	28	0.51
esc16f	0	0	0.14
esc16g	$25 \equiv \lceil 24.7403 \rceil$	26	0.51
esc16h	$977 \equiv \lceil 976.2244 \rceil$	996	0.79
esc16i	$12 \equiv \lceil 11.3749 \rceil$	14	0.73
esc16j	$8 \equiv \lceil 7.7942 \rceil$	8	0.42

Table 5 Optimal values and solution times for the larger esc instances

Instance	Previous l.b.	SDP l.b. (13)	Best known u.b.	Time (s)
esc32a	103 ([4])	$104 \equiv \lceil 103.3194 \rceil$	130 (best known)	114.8750
esc32b	132 ([4])	$132 \equiv \lceil 131.8718 \rceil$	168 (best known)	5.5780
esc32c	616 ([4])	$616 \equiv \lceil 615.1400 \rceil$	642 (best known)	3.7030
esc32d	191 ([4])	$191 \equiv \lceil 190.2266 \rceil$	200 (best known)	2.0940
esc32g	6 (opt.)	$6 \equiv \lceil 5.8330 \rceil$	6 (opt.)	1.7970
esc32h	424 ([4])	$425 \equiv \lceil 424.3382 \rceil$	438 (best known)	7.1560
esc64a	47	$98 \equiv \lceil 97.7499 \rceil$	116 (best known)	12.9850
esc128	2	$54 \equiv \lceil 53.0844 \rceil$	64 (best known)	140.3590

instances. Thus, for example, the final SDP relaxation of nug25 involves 'only' 25,650 scalar variables, and the largest blocks appearing in the LMI's have size 151×151.

The final SDP problems were solved by the interior point software SeDuMi [24] using the Yalmip interface [27] and Matlab 6.5, running on a PC with Pentium IV 3.4 GHz dual-core processor and 3GB of memory.

In Tables 4 and 5 we give computational results for the esc16 and esc32 (as well as esc64a and esc128) instances respectively.

The optimal solutions are known for the ecs16 instances but most of the esc32 instances as well as esc64a and esc128 remain unsolved.

In [4] the optimal value of the SDP relaxation (13) was approximately computed for several instances of the QAPLIB library using an augmented Lagragian method. These values, rounded up, are given in the column 'previous l.b.' in Table 5 for the esc instances, except for esc64a and esc128 which were too large even for the augmented Lagragian approach. The lower bounds for esc64a and esc128 given in Table 5 are taken from the QAPLIB web page, and are given by the Gilmore-Lawler [13, 16] bound.

Note that values from [4] do not always give the same bound as we obtained, and we can improve their lower bound by 1 for esc32a and esc32h. The reason for the difference is that the augmented Lagrangian method does not always solve the SDP relaxation (13) to optimality. Moreover, as one would expect, the interior point method is about three to four orders of magnitude faster than the the augmented Lagrangian method, as is clear from comparison with computational times reported in [4]. In particular, in [4], Table 6 the authors report solution times of order 10^3 s for the esc16 instances, and order 10^5 s for the esc32 instances; this computation was done on a 2.4 GHz Pentium IV processor, which is less than a factor two slower than the processor that we used.

For the instances esc64a and esc128 we obtained a significant improvement over the best known lower bounds, namely from 47 to 98 for esc64a (upper bound 116), and from 2 to 54 for esc128 (upper bound 64).

We observed that, for all the esc instances, the optimal solution of the SDP relaxation had a constant diagonal. By Lemma 3.1, this means that none of the triangle inequalities was violated by the optimal solution, i.e. we could not improve the lower bounds in Tables 4 and 5 by adding triangle inequalities.

9 Concluding remarks

We may conclude from our computational results that the SDP relaxation from [28] is solvable by interior point methods for QAP instances where the distance matrix is from an association scheme and n is up to 128. This was the case with the esc instances [5] (where the distance matrices were Hamming distance matrices). Another example of QAP instances where the distance matrix is a Hamming distance matrix was recently given by Peng et al. [18], for a problem arising from channel coding in communications.

One more example is the QAP reformulation of the symmetric traveling salesman problem (TSP), where one of the QAP data matrices is a symmetric circulant matrix. In a subsequent work to this paper, De Klerk et al. [9] worked out the details of the reduced SDP relaxation of the QAP formulation of TSP. The result is an interesting new SDP relaxation of TSP.

These observations show that the approach presented here has both computational and theoretical implications.

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