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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: [R.E. Burkard, S.E. Karisch, F. Rendl. QAPLIB — a quadratic assignment problem library. *Journal on Global Optimization*, **10**: 291–403, 1997].

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1 Introduction

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

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

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 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].

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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 [26, 18]. These SDP relaxations turn out to be quite strong in practice, but involve matrix variables of size n^4, and are therefore hard to solve by interior point algorithms.

This has led to the application of bundle methods [18] 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 [18] 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 $n = 64$. 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], §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 [19], Gatermann and Parrilo [10], 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 if 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. [12] (we assume that the dimensions of the matrices appearing in these identities are such that all expressions are well-defined):

$$\begin{aligned}(A \otimes B)^T &= A^T \otimes B^T, &(1)\\ (A \otimes B)(C \otimes D) &= AC \otimes BD, &(2)\\ A \otimes B\mathrm{vec}(X) &= \mathrm{vec}\left(BXA^T\right), &(3)\\ \mathrm{trace}(A \otimes B) &= \mathrm{trace}(A)\,\mathrm{trace}(B). &(4)\end{aligned}$$

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 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

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

and $y^{(i)} = \mathrm{col}_i(X)$ $(i = 1,\ldots,n)$.

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

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

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

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

More over, 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.)

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 $Y_X \in \mathcal{S}^+_{n^2+1}$:

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

This SDP relaxation is equivalent to the one solved by Rendl and Sotirov [18] 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 [16] applied to the QAP, as studied by Burer and Vandenbussche [4]. The equivalence between the two relaxations was recently shown by Povh and Rendl [17].

3 Valid inequalities for the SDP relaxation

The following theorem from [26] shows that several valid (in)equalities are implied by the constraints of the SDP problem (13).

Theorem 3.1 (*cf.* [26], 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. $\sum_{i=1}^n \operatorname{diag}\left(Y^{(ij)}\right) = y^{(j)} \quad (j = 1, \ldots, n).$

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*:

$$\begin{aligned} 0 \leq Y_{rs} &\leq Y_{rr}, && (14)\\ Y_{rr} + Y_{ss} - Y_{rs} &\leq 1, && (15)\\ -Y_{tt} - Y_{rs} + Y_{rt} + Y_{st} &\leq 0, && (16)\\ Y_{tt} + Y_{rr} + Y_{ss} - Y_{rs} - Y_{rt} - Y_{st} &\leq 1, && (17) \end{aligned}$$

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 $\mathrm{trace}(Y) - 2e^T y = -n$, and $\mathrm{diag}(Y) = y$ is a multiple of the all-ones vector, one has $\mathrm{diag}(Y) = y = \frac{1}{n}e_{n^2}$. 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

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

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 [18], it is not possible to solve the SDP problem (13) in general using interior point methods if $n \geq 15$ — let alone when the triangle inequalities have been added to the formulation.

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

Assume that the following semidefinite programming problem is given

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

where $A_i \in \mathcal{S}_n$ $(i = 0, \ldots, m)$ are given. The associated dual problem is

$$p^* = \max_{y \in \mathbb{R}^m} \{ b^T y \ : \ A_0 - \sum_{i=1}^m y_i A_i \succeq 0 \}. \tag{19}$$

We assume that both problems satisfy the Slater condition so that both problems have optimal solutions with identical optimal values.

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

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

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_i $(i = 0, \ldots, m)$ lie in the commutant of $\mathcal{G}$.

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

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

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

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 a orthonormal basis of $\mathcal{A}_{\mathcal{G}}$ (seen as a vector space).

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

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

One may also obtain the basis 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 $R_{\mathcal{G}}(e_ie_j^T)$ 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, both problem (18) and its dual have optimal points 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. The proof for the dual problem is similar. $\square$

Assume we have a basis $B_1, \ldots, B_d$ of the commutant $\mathcal{A}_\mathcal{G}$. One may write $X = \sum_{i=1}^d x_i B_i$ so that the SDP problem (18) reduces to

$$\min_{\sum_{i=1}^d x_i B_i \succeq 0} \left\{ \sum_{i=1}^d x_i \operatorname{trace}(A_0 B_i) \ : \ \sum_{i=1}^d x_i \operatorname{trace}(A_k B_i) = b_k, \quad k = 1, \ldots, m \right\}. \quad (20)$$

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 (20) 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.

5 Matrix algebras and their block factorizations

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

5.1 The completely reduced representation of a matrix C^*-algebra

The center of an algebra is a specific commutative sub-algebra of it, defined as follows.

Definition 5.1 (Center of an algebra)**.** *Let $\mathcal{A}$ be an algebra. The center of $\mathcal{A}$ is defined as*

$$\textit{center}(\mathcal{A}) = \{X \in \mathcal{A} \ : \ XY = YX \ \ \forall Y \in \mathcal{A}\}.$$

Note that the center is a commutative sub-algebra of $\mathcal{A}$. Moreover, if $\mathcal{A}$ is a C^*-algebra, then so is its center.

The center of a C^*-algebra that contains the identity possess a special basis (as a vector space), namely a basis of self-adjoint, minimal, central idempotents (see e.g. [11]), defined as follows.

Definition 5.2 (Minimal idempotent)**.** *Let $X = X^2$ be an idempotent in an algebra $\mathcal{A}$. We call X a minimal idempotent if it cannot be written as a sum of other idempotents.*

We will also use the notation

$$\mathcal{A}X := \{YX \ : \ Y \in \mathcal{A}\}.$$

Note that $\mathcal{A}X$ is a sub-algebra of $\mathcal{A}$.

We are now in a position to state the basic result on decomposition of matrix C^*-algebras.

Theorem 5.1 (Wedderburn [23])**.** *Let $\mathcal{A}$ be a finite dimensional C^* matrix algebra that contains the identity matrix. Denote the basis of minimal, nonzero, self-adjoint, central idempotents of the center of $\mathcal{A}$ by*

$$\min \mathcal{A} := \left\{X \in \textit{center}(\mathcal{A}) \ : \ X = X^2 \neq 0 \textit{ is minimal}, \ X^* = X\right\}.$$

Then

$$\mathcal{A} = \bigoplus_{X \in \min \mathcal{A}} \mathcal{A}X.$$

Moreover, each of the C^**-algebras* $\mathcal{A}X$ $(X \in \min \mathcal{A})$ *is isomorphic to* $\mathbb{C}^{r_X \times r_X}$ *for some integer value* r_X*.*

The theorem may be used to find a block diagonalization of a real matrix C^*-algebra as follows:

1. Find a minimal idempotent in the center of $\mathcal{A}$;
2. Let Q be a orthogonal matrix with columns given by a set of orthogonal eigenvectors of this idempotent.
3. Perform the block diagonalization $Q^T \mathcal{A} Q$.

Indeed, note that if X is a central idempotent of $\mathcal{A}$, then

$$\mathcal{A}X = \mathcal{A}X^2 = X\mathcal{A}X.$$

Letting $X = Q\Lambda Q^T$ with Q orthogonal and Λ a zero-one diagonal matrix, one has:

$$Q^T \mathcal{A} X Q = Q^T X \mathcal{A} X Q = Q^T Q \Lambda Q^T \mathcal{A} Q \Lambda Q^T Q = \Lambda Q^T \mathcal{A} Q \Lambda.$$

Note that the final expression is (isomorphic to) the algebra obtained by taking the principal sub-matrices, defined by the nonzero entries of Λ, of all elements of the algebra $Q^T \mathcal{A} Q$. Thus

$$Q^T \mathcal{A} Q = \bigoplus_{X \in \min \mathcal{A}} Q^T \mathcal{A} X Q$$

is an algebra of block diagonal matrices, with each block isomorphic to the full algebra of the same size. This decomposition is sometimes called the *completely reduced representation* of $\mathcal{A}$, since the blocks cannot be further reduced.

We end with an example that is also relevant for some of the QAP instances to be considered later.

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 aut(A) *has order* $n!2^n$*. The centralizer ring of aut*(A) *is a commutative* C^**-algebra (also called an association scheme) 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 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 Hamming(i,j) *is the Hamming distance between* i *and* j*. The basis matrices* $B^{(k)}$ *are simultaneously diagonalized by the matrix* Q *defined by*

$$Q_{ij} = (-1)^{|i \cap j|} \quad i, j \in \{0,1\}^n,$$

where $|i \cap j|$ *is the number of positions where both* i *and* j *have an entry* 1.

5.2 A heuristic for computing the 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 $\mathcal{A}_{\mathcal{G}}$.

In order to compute the completely reduced representation of the commutant of $\mathcal{A}$, one requires a minimal, nonzero, central idempotent of the commutant, as seen in the previous subsection. Such an idempotent may be difficult to obtain in practice.

We will therefore use a heuristic approach to block diagonalize $\mathcal{A}_{\mathcal{G}}$, where we select a random matrix from the commutant of the commutant, as opposed to the center of the commutant. Notice that the commutant of the commutant is the algebra $\text{span}\{P \,:\, P \in \mathcal{G}\}$, and that the center of $\mathcal{A}_{\mathcal{G}}$ is a sub-algebra thereof.

Block diagonalization heuristic

1. Choose a random symmetric element, say Z, from $\text{span}\{P \,:\, P \in \mathcal{G}\}$;
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 $Q^T B_1 Q$,…, $Q^T B_d Q$.

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

Theorem 5.2. *Let* q *be an eigenvector of some* $Z \in \text{span}\{P \,:\, P \in \mathcal{G}\}$ *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.

Finally, note that the heuristic will not in general produce the completely reduced representation of the commutant, but may lead to a coarser block factorization. This coarser factorization is usually sufficient for our (computational) purposes.

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. *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

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

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

Proof: Let 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.

Theorem 6.2. *Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be two multiplicative groups of 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*

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

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 group*

$$\mathcal{G}_A := \left\{ \begin{pmatrix} 1 & 0^T \\ 0 & P \end{pmatrix} \ : \ P \in aut(A) \right\}$$

and define $\mathcal{G}_B$ analogously.

Then the SDP problem (13) satisfies Assumption 1 with respect to the group $\mathcal{G}_A \otimes \mathcal{G}_B$.

Proof. Direct verification. □

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

Theorem 7.2. *The commutant of of $\mathcal{G}_A \otimes \mathcal{G}_B$ is spanned by all matrices of the form*

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

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

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 $\mathcal{G}_A \otimes \mathcal{G}_B$, where $a \in \mathbb{R}$, $b, c \in \mathbb{R}^{n^2}$ and $Z \in \mathbb{R}^{n^2\times n^2}$. For any $P_A \in \mathrm{aut}(A)$ and $P_B \in \mathrm{aut}(B)$ 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

$$Z(P_A \otimes P_B) = (P_A \otimes P_B)Z, \ (P_A \otimes P_B)b = b, \ (P_A \otimes P_B)c = c, \qquad (21)$$

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

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

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

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

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

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

where we have use the identities (2) and (4) of the Kronecker product. Notice that $\mathrm{trace}\,B_i^A$ 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 $\mathrm{aut}(B)$.

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., where we view 2-orbits of 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.

Using this notation we may rewrite the constraint:

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

as

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

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

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

Proceeding in this vein, we obtain the SDP reformulation:

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

subject to

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

As mentioned before, the numbers $\mathrm{trace}(AB_i^A)$ and $\mathrm{trace}(BB_j^B)$ 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 $\binom{n^2+1}{2}$ independent entries in a symmetric $n^2 \times n^2$ 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 number of symmetric 2-orbits of $\mathrm{aut}(A)$ (resp. $\mathrm{aut}(B)$), 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 orthogonal matrices Q_A and Q_B that block-diagonalize the commutants of $\mathrm{aut}(A)$ and $\mathrm{aut}(B)$ respectively. Defining the orthogonal matrix

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

one has

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

which is block-diagonal, since the Kronecker product of block-diagonal matrices is again block-diagonal. Also note that the size of the largest block is the product of the largest sizes of blocks appearing in the factorization of the commutants of $\mathrm{aut}(A)$ and $\mathrm{aut}(B)$.

On the other hand,

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

$$\begin{pmatrix} 0 & (Q_A^T \,\mathrm{diag}(B_i^A) \otimes Q_B^T \,\mathrm{diag}(B_j^B))^T \\ Q_A^T \,\mathrm{diag}(B_i^A) \otimes Q_B^T \,\mathrm{diag}(B_j^B) & Q_A^T B_i^A Q_A \otimes Q_B^T B_j^B Q_B \end{pmatrix},$$

that is not block-diagonal, but has a so-called chordal sparsity structure, that may be exploited as described in the following lemma.

Lemma 7.1 (see *e.g.* [13])**.** *Let $x_i \in R^k$ and $X_i \in \mathcal{S}_k$ $(i = 1, \ldots, n)$ be given. One has*

$$\begin{bmatrix} 1 & x_1^T & \cdots & x_n^T \\ x_1 & X_1 & & 0_{k\times k} \\ \vdots & & \ddots & \vdots \\ x_n & 0_{k\times k} & \cdots & X_n \end{bmatrix} \succeq 0,$$

if and only if

$$\begin{bmatrix} 1 & x_i^T \\ x_i & X_{ii} \end{bmatrix} \succeq 0 \quad (i = 1, \ldots, n).$$

We may therefore apply the lemma in an obvious way to the linear matrix inequality (22), after performing the orthogonal transformation $Q^T(\cdot)Q$. Thus we still obtain a 'block diagonalization' of (22), where the blocks are obtained by adding one more row and column to the blocks of $Q_A^T B_i^A Q_A \otimes Q_B^T B_j^B Q_B$.

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 7.3. *If both aut(A) and aut(B) are transitive, then all triangle inequalities (14) – (17) are implied in the final SDP relaxation.*

Proof. If both aut(A) and aut(B) are transitive, then every matrix in the commutant of $\mathcal{G}_A \otimes \mathcal{G}_B$ has a constant diagonal, since $\mathcal{G}_A \otimes \mathcal{G}_B$ only has one orbit. The required result now follows from Lemma 3. □

8 Numerical results

In Table 1 we give the numbers of orbits and 2-orbits of aut(A) and 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.

The automorphism groups of the matrices A and B were computed using the computational algebra software GAP [9]. The same package was used to compute the 2-orbits of these groups.

Note that the 'esc' instances [5] are particularly suited to our approach.[1] Here the automorphism group of B is the automorphism group of the Hamming graph described in Example 5.1. Consequently the commutant of aut(B) may be diagonalized, and its dimension is small.

On the other hand, all the other instances in the table are still to 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 instances.

With one exception, the final SDP problems were solved by the interior point software SeDuMi [22] using the Yalmip interface [25] and Matlab 6.5, running on a PC with Pentium IV 3.4 GHz dual-core processor and 3GB of memory.

The exception was the (large) instance esc64a that was solved in parallel on a distributed memory cluster with 32 processors, using the parallel implementation of the solver CSDP (see [3]) described in [14]. Each node of the cluster has two 64bit AMD Opteron 2.4 GHz CPU's, running ClusterVisionOS Linux, and has 4 GB memory.

As already mentioned, we diagonalized the commutant of aut(B) for the esc instances as described in Example 5.1. The commutant of aut(A) was block diagonalized using the heuristic described in Section 5.2. The sizes of the blocks that we thus obtained for the esc32 and esc64a instances are shown in Table 2.

In Tables 3 and 4 we give computational results for the esc16 and esc32 (and esc64a) instances respectively.

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

In [4] the optimal value of the SDP relaxation (13) was approximately computed using an augmented Lagragian method. These values, rounded up, are given in the

[1] 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.

instance	$\lvert O_A^1\rvert$, $\lvert O_B^1\rvert$	$\lvert O_A^2\rvert$, $\lvert O_B^2\rvert$	$\lvert O_A^{2,sym}\rvert$, $\lvert O_B^{2,sym}\rvert$	# 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	1656
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
nug20	6, 20	98, 380	15, 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, 1722	30, 0	377,622
sko49	10, 49	315, 2352	27, 0	370,930
ste36a	35, 10	1191, 318	1, 26	189,732
ste36b	10, 35	318, 1191	26, 1	189,732
ste36c	10, 35	318, 1191	26, 1	189,732
tho30	10, 30	240, 870	20, 0	104,700
tho40	12, 40	404, 1560	28, 0	315,600
wil50	15, 50	635, 2450	35, 0	778,625
wil100	15, 100	1260, 9900	60, 0	6,238,500

Table 1: Symmetry information on selected QAPLIB instances.

instance	block sizes
esc32a	1, 3, 28
esc32b	5, 7, 8, 12
esc32c	1, 2, 29
esc32d	1, 2, 4, 25
esc32g	1, 31
esc32h	1, 31
esc64a	1, 63

Table 2: Block sizes after block diagonalization of aut(A) for the esc32 and esc64 instances.

instance	SDP l.b. (13)	opt.	time(s)
esc16a	63.2756	68	47.4
esc16b	289.8817	292	41.2
esc16c	153.8242	160	51.6
esc16d	13.0000	16	22.1
esc16e	26.3368	28	26.9
esc16f	0	0	8.8
esc16g	24.7403	26	29.9
esc16h	976.2244	996	43.5
esc16i	11.3749	14	33.1
esc16j	7.7942	8	26.9

Table 3: Optimal values and solution times for the esc16 instances.

instance	previous l.b.	SDP l.b. (13)	best known u.b.	time(s)
esc32a	103 ([4])	103.3194	130 (best known)	4,084
esc32b	132 ([4])	131.8718	168 (best known)	3,872
esc32c	616 ([4])	615.1400	642 (best known)	2,807
esc32d	191 ([4])	190.2266	200 (best known)	2,304
esc32g	6 (opt.)	5.8330	6 (opt.)	2,950
esc32h	424 ([4])	424.3382	438 (best known)	3,621
esc64a	47	97.7499	116	23,828

Table 4: Optimal values and solution times for the esc32 and esc64 instances.

column ”previous l.b.” in Table 4. Note that values from [4] do not always give the same bound as we obtained, and we can improve the 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 two 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 seconds for the esc16 instances, and order 10^5 seconds for the esc32 instances; this computation was done on a 2.4GHz Pentium IV processor, which is less than a factor two slower than the processor that we used.

The SDP relaxation (13) of the instance esc64a was too large even for the augmented Lagrangian method, and here we obtain a significant improvement over the best known lower bound, namely from 47 to 98 (upper bound 116).

We observed that, for all the esc instances, the optimal solution of the SDP relaxation had a constant diagonal. By Lemma 3, 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 3 and 4 by adding triangle inequalities.

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