Symmetry in RLT-type relaxations for the quadratic assignment and standard quadratic optimization problems

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Abstract

The *reformulation-linearization technique* (RLT), introduced in [H.D. Sherali and W.P. Adams. A Hierarchy of Relaxations Between the Continuous and Convex Hull Representations for Zero-One Programming Problems, *SIAM Journal on Discrete Mathematics*, 3(3):411–430, 1990], provides a way to compute a hierarchy of linear programming bounds on the optimal values of NP-hard combinatorial optimization problems. In this paper we show that, in the presence of suitable algebraic symmetry in the original problem data, it is sometimes possible to compute level two RLT bounds with additional linear matrix inequality constraints. As an illustration of our methodology, we compute the best-known bounds for certain graph partitioning problems on strongly regular graphs.

Keywords: reformulation-linearization technique, Sherali-Adams hierarchy, quadratic assignment problem, standard quadratic optimization, semidefinite programming.

AMS subject classification: 90C22, 90C27

1 Introduction

The term *reformulation-linearization technique* (RLT) was coined by Sherali and Adams in the seminal paper [40] (see also [41]). Thus a hierarchy of linear programming relaxations was introduced, based on a linearization technique studied earlier by these authors in [3] (see also [4]); the subsequent development of the RLT-technique is contained in their monograph [42].

The main idea is the following: if there are two valid linear inequalities for a given set $S \subset \mathbb{R}^n$, for example if $l_1 \le v_1^\top x$ and $l_2 \le v_2^\top x$ for all $x \in S$, then their product also yields the valid inequality:

$$(v_1^\top x)(v_2^\top x) - l_2 v_1^\top x - l_1 v_2^\top x \ge -l_1 l_2 \quad \forall x \in S.$$

Introducing new variables X_{ij} corresponding to $x_i x_j$, we can linearize the last inequality:

$$\sum_{i,j} v_{1i} v_{2j} X_{ij} - \sum_i (l_2 v_{1i} + l_1 v_{2i}) x_i \ge -l_1 l_2. \tag{1}$$

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An inequality of this type is known as a first-level *RLT cut* in the variables x and X. This process may be repeated to obtain level two RLT cuts, etc. This type of method has become known as a *lift-and-project* strategy: the 'lifting' refers to the addition of new variables, and the 'projection' to projecting the optimal values of the new variables to a feasible point in $\mathbb{R}^n$ of the original problem; see Laurent [28] for a comparison of the RLT with related schemes.

In this paper we will study the RLT for two specific problems, namely the standard quadratic program and the quadratic assignment problem (QAP). The first level RLT formulation of the QAP was previously studied in [2] and [21]. Adams, Guignard, Hahn and Hightower [1] considered the second level RLT formulation of the QAP. Numerical results presented in [1] show that the second level RLT relaxation of the QAP often provides significantly better bounds than the first level RLT relaxation, but that it is computationally very expensive to solve. Recently, the third level RLT relaxation of the QAP was also investigated in [19]. The numerical results show that this relaxation empirically provides tight bounds for medium-sized instances (where it is still possible to solve the third level relaxation).

In this paper, we show how one may solve the second level RLT relaxation with additional semidefinite programming (SDP) constraints in the presence of suitable algebraic symmetry in the problem data. As a result we are able to compute the best known bounds for certain graph partitioning problems involving strongly regular graphs. (These graph partitioning problems have QAP reformulations.) Our results are in the spirit of the recent papers [39, 29, 16, 26, 27] where improved semidefinite programming bounds were obtained for various combinatorial problems by exploiting algebraic symmetry. Our results may also be seen as an extension of recent results by Ostrowski [34], who studied symmetry in (pure) linear programming RLT relaxations of symmetric binary integer programs.

Scope and organization of this paper

We start by describing RLT relaxations of the standard quadratic optimization problem in Section 2, and of the QAP in Section 3. In these sections we also present new results on how the resulting RLT relaxations relate to known relaxations from the literature. This is followed by background material on exploiting algebraic symmetry in the data of SDP problems in Section 4. We apply this methodology to the standard quadratic programming problem in Section 5, and to the QAP in Section 6. Finally, we present numerical results to illustrate the complete approach in Section 7. Throughout, the main (computational) focus is on the QAP, and our treatment of the standard quadratic program serves as a relatively easy introduction to the more complicated analysis of the QAP.

2 RLT cuts for the standard quadratic programming problem

We will use the notation from Sherali and Adams [42, §7.1] (see also [44] for RLT in the context of continuous polynomial programs):

$$\left[\prod_{i\in\mathcal{J}} x_i\right]_L = X_{\mathcal{J}},$$

where $\mathcal{J}$ is an index set with elements from $\{1,\ldots,n\}$ where repetition of elements is allowed. Thus, for example, $[x_1^2x_2]_L = X_{\{1,1,2\}}$ or X_{112}, for short. In other words, $[.]_L$ is a "linearization operator" that maps a monomial to a new variable. This operator may be extended to a linear map from general polynomials to linear ones by simply replacing each monomial by its linearization.

The standard quadratic program ($stQP$) is defined as

$$\min_{x\in\Delta} x^{\mathsf{T}}Qx$$

where $\Delta = \{x \in \mathbb{R}^n \mid \sum_i x_i = 1,\ x \geq 0\}$ is the *standard simplex* in $\mathbb{R}^n$, and $Q = Q^{\mathsf{T}} \in \mathbb{R}^{n\times n}$ is given.

It is easy to verify (see e.g. [43] or §8.3 in [42]) that the first level RLT relaxation of ($stQP$) takes the form

$$\min_{X=X^{\mathsf{T}}\in\mathbb{R}^{n\times n}} \{\langle Q, X\rangle \mid \langle J, X\rangle = 1,\ X \geq 0\}$$

where $\langle Q, X\rangle = \mathrm{trace}(QX)$, $[x_i x_j]_L = X_{ij}$ $(i, j = 1, \ldots, n)$, and J is the all-ones matrix. Since X corresponds to the positive semidefinite matrix xx^{T}, we may also add the constraint that X should be symmetric positive semidefinite, denoted by $X \succeq 0$, to obtain the stronger relaxation:

$$\min_{X\in D_n} \{\langle Q, X\rangle \mid \langle J, X\rangle = 1\}, \qquad (stQP_{SDP+RLT-1})$$

where $D_n \subset \mathbb{R}^{n\times n}$ is the doubly nonnegative cone, i.e. the cone of $n \times n$ symmetric positive semidefinite matrices that are also entrywise nonnegative.

Note that we have removed the original variable x from the formulation; it is worth noting that this will not be possible for the quadratic assignment problem studied in Section 3. The second level RLT relaxation involves the new matrix variables

$$Y^{(k)} = (Y^{(k)})^{\mathsf{T}} = [x_k X]_L \quad (k = 1, \ldots, n).$$

Since $Y^{(k)}_{ij}$ corresponds to $x_i x_j x_k$, one has the relations

$$Y^{(k)}_{ij} = Y^{(i)}_{jk} = Y^{(j)}_{ik} \quad i, j, k = 1, \ldots, n.$$

In other words, $Y^{(k)}_{ij}$ $(i, j, k = 1, \ldots, n)$ may be viewed as a *fully symmetric 3-tensor*, i.e. $Y^{(k)}_{ij}$ is invariant under all permutations of i, j, k.

The second level RLT relaxation with SDP constraints becomes

$$\min_{Y^{(1)},\ldots,Y^{(n)}\in D_n, X\in\mathbb{R}^{n\times n}} \left\{\langle Q, X\rangle \mid \langle J, X\rangle = 1, \sum_{k=1}^{n} Y^{(k)} = X,\ Y^{(k)}_{ij} \text{ fully symmetric}\right\}. \qquad (stQP_{SDP+RLT-2})$$

Note that $X \in D_n$ is implied by $Y^{(1)}, \ldots, Y^{(n)} \in D_n$ and $\sum_{k=1}^{n} Y^{(k)} = X$.

The $(t-1)$-level RLT relaxation is

$$\min\left\{ \sum_{i_1,\ldots,i_t=1}^{n} Q_{i_1 i_2} Z_{i_1\ldots i_t} \;\middle|\; \sum_{i_1,\ldots,i_t=1}^{n} Z_{i_1\ldots i_t} = 1, Z \geq 0, Z \text{ is fully symmetric}\right\}.$$

Since the variable $Z_{i_1\ldots i_t}$ corresponds to the product $x_{i_1}\ldots x_{i_t}$, the matrix $(Z_{i_1\ldots i_t})^{n}_{i_r,i_s=1}$ corresponds to the matrix $\left(\prod_{\substack{j=1\\ j\neq r,s}}^{t} x_{i_j}\right) xx^T$, and we can require its positive semidefiniteness. In other words, any matrix obtained from the tensor Z by fixing $(t-2)$ coordinates has to be positive semidefinite. Therefore it is natural to define ($stQP_{SDP+RLT-t}$) by adding these linear matrix inequality constraints to the level t RLT relaxation of ($stQP$).

2.1 Related semidefinite programming relaxations

We may rewrite problem ($stQP_{SDP+RLT-2}$) as the conic linear program

$$\min_{X\in\mathcal{C}} \{\langle Q,X\rangle \mid \langle J,X\rangle = 1\} = \max_{t\in\mathbb{R}} \{t \mid Q - tJ \in \mathcal{C}^*\}, \tag{2}$$

where $\mathcal{C}$ is the following convex cone:

$$\mathcal{C} := \left\{ X \in \mathbb{R}^{n\times n} \mid X = \sum_{k=1}^{n} Y^{(k)},\ Y^{(k)} \in D_n,\ Y^{(k)}_{ij} = Y^{(i)}_{jk} = Y^{(j)}_{ik}\ (1 \le i,j,k \le n) \right\}, \tag{3}$$

$\mathcal{C}^*$ is its dual cone, and the equality in (2) is due to the conic duality theorem. In a similar way, one may define RLT relaxations of any order, by generalizing the definition of the cone $\mathcal{C}$. We will argue that these generalized cones coincide with a hierarchy of cones introduced by Dong [14]. In Dong's notation, $\mathcal{M}^r_n$ denotes the set of tensors of order r and dimension n, and $\mathcal{S}^r_n$ is the set of fully symmetric tensors. Furthermore, for $r > 0, \beta \in \{1,\ldots,n\}^r$ and $T \in \mathcal{M}^{r+2}_n$, $T[\beta,:,:]$ denotes the ordinary matrix obtained by fixing the first r indices of T to β, and the set of such matrices is $\mathrm{Slice}(T)$. The operator $\mathrm{Collapse}(T)$ is defined as the sum of the slices of the tensor T, that is

$$\mathrm{Collapse}(T)[i,j] = \sum_{\beta\in\{1,\ldots,n\}^r} T[\beta,i,j] = \sum_{P\in\mathrm{Slice}(T)} P_{i,j}.$$

Now one may define the following cones:

$$\mathcal{TD}^r_n = \{X :\ \exists Y \in \mathcal{S}^{r+2}_n, \mathrm{Slice}(Y) \subset D_n, X = \mathrm{Collapse(Y)}\}, \tag{4}$$

where D_n is the cone of doubly nonnegative $n\times n$ matrices, as before. Dong [14] proved that the cones $\mathcal{TD}^r_n$ are dual to cones defined earlier by Peña et al. [36] (called $\mathcal{Q}^r_n$ there). The cones $\mathcal{TD}^r_n$ are precisely the generalization of the cone $\mathcal{C}$ in (3). In particular, the values $Y^{(i)}_{jk}$ in (3) correspond to a fully symmetric 3-tensor, and the $Y^{(k)}$ to slices of this tensor. This leads us to the following theorem.

Theorem 1. *The level t RLT bound with semidefinite constraints ($stQP_{SDP+RLT-t}$) for the standard quadratic program is given by*

$$\min_{X\in\mathcal{TD}^{t-1}_n} \{\langle Q,X\rangle \mid \langle J,X\rangle = 1\} = \max\{t \mid Q - tJ \in \mathcal{Q}^{t-1}_n\} \quad (t = 1,2,\ldots), \tag{5}$$

where the cones $\mathcal{TD}^{t-1}_n$ are defined in (4), and $\mathcal{Q}^{t-1}_n$ are the corresponding dual cones ($t = 1,2,\ldots$).

Proof. The proof is by induction, and is omitted since it is straightforward. ■

We conclude this section with a brief comparison of the ($stQP_{SDP+RLT-t}$) bound to other bounds from the literature. These bounds are related to sufficient conditions for matrix copositivity due to Parrilo [35] (recall that a matrix M is copositive if $x^\top Mx \ge 0$ for all nonnegative vectors x).

To explain these bounds, note that

$$\begin{aligned}\min_{x\in\Delta} x^{\mathsf T}Qx &= \max\{t \mid x^{\mathsf T}Qx \geq t, \quad \forall x\in\Delta\}\\ &= \max\{t \mid x^{\mathsf T}(Q-tJ)x \geq 0, \quad \forall x\in\Delta\}\\ &= \max\{t \mid Q-tJ \text{ is a copositive matrix}\}.\end{aligned}$$

Parrilo [35] introduced the following hierarchy of sufficient conditions for a matrix M to be copositive, namely

$$\left(\sum_{i,j} M_{ij}x_i^2x_j^2\right)\left(\sum_{i=1}^n x_i^2\right)^r \text{ is a sum of squared polynomials,}$$

for some integer $r \geq 0$.

The cone of matrices that satisfy this sufficient condition for a given r is denoted by $\mathcal{K}_n^{(r)}$. Bomze and De Klerk [9] studied the following lower bounds for the standard quadratic optimization problem:

$$p^{(r)} := \max\{t \mid Q-tJ \in \mathcal{K}_n^{(r)}\} = \min_{X\in\mathcal{K}_n^{*(r)}} \{\langle Q,X\rangle \mid \langle J,X\rangle = 1\} \quad (r=0,1,\dots) \tag{6}$$

Since it is known that $\mathcal{Q}_n^r \subseteq \mathcal{K}_n^{(r)}$ $(r=0,1,\dots)$ and equality (only) holds for $r=0,1$ [36], we have the following result.

Theorem 2. *The bound $p^{(t-1)}$ in* (6) *is at least as tight as the bound from ($stQP_{SDP+RLT-t}$) in* (5) *for $t=1,2,\dots$, and the two bounds (only) coincide for $t=1,2$.*

3 RLT cuts for the quadratic assignment problem

Given two symmetric $n\times n$ matrices A and B, the quadratic assignment problem (QAP) is defined as:

$$\min_{\pi\in\mathcal{S}_n} \sum_{i,j=1}^n A_{ij}B_{\pi(i),\pi(j)} = \min_{P\in\Pi_n} \operatorname{trace}(AP^{\mathsf T}BP), \tag{QAP}$$

where $\mathcal{S}_n$ is the symmetric group on $\{1,\dots,n\}$, and Π_n is the set of $n\times n$ permutation matrices.

The QAP may be rewritten as

$$\begin{aligned}\min \quad & \sum_{i,j,k,l} a_{ik}b_{jl}x_{ij}x_{kl}\\ s.t. \quad & \sum_{i=1}^n x_{ij} = 1, \quad j=1,\dots,n,\\ & \sum_{j=1}^n x_{ij} = 1, \quad i=1,\dots,n,\\ & x_{ij}\in\{0,1\}, \quad i,j=1,\dots,n.\end{aligned} \tag{7}$$

Writing the integrality constraints as $x_{ij}^2 = x_{ij}$ $(i, j = 1, \ldots, n)$, and introducing new variables $X_{ijkl} = [x_{ij}x_{kl}]_L$ $(i, j, k, l = 1, \ldots, n)$ as before, the first-level RLT relaxation of QAP is the following linear program:

$$
\begin{aligned}
\min \quad & \sum_{i,j,k,l} a_{ik} b_{jl} X_{ijkl} \\
s.t. \quad & \sum_{i=1}^{n} x_{ij} = 1, \quad j = 1, \ldots, n, \\
& \sum_{j=1}^{n} x_{ij} = 1, \quad i = 1, \ldots, n, \\
& \sum_{i=1}^{n} X_{ijkl} = x_{kl}, \quad j, k, l = 1, \ldots, n, \\
& \sum_{j=1}^{n} X_{ijkl} = x_{kl}, \quad i, k, l = 1, \ldots, n, \\
& x \geq 0, \\
& X_{ijij} = x_{ij}, \quad i, j = 1, \ldots, n, \\
& X_{ijkl} = X_{klij} \geq 0, \quad i, j, k, l = 1, \ldots, n.
\end{aligned}
\tag{QAP_{RLT-1}}
$$

3.1 Related semidefinite programming relaxations

Povh and Rendl [37] studied a semidefinite programming (SDP) relaxation for the QAP problem (the resulting lower bound coincides with an earlier bound studied in [48]). We will show that this relaxation may be viewed as a first level RLT relaxation of the QAP with positive semidefiniteness constraints added.

In stating and analyzing this SDP relaxation, we will need several properties of the Kronecker product. Recall that the Kronecker product $A \otimes B$ of matrices $A = (a_{ij}) \in \mathbb{R}^{m \times n}$ and $B = (b_{ij}) \in \mathbb{R}^{r \times s}$ is the $mr \times ns$ block matrix with block (i, j) given by $a_{ij}B$ $(i = 1, \ldots, m,\ j = 1, \ldots, n)$. We will often use the properties that, for $A, B, C, D \in \mathbb{R}^{n \times n}$, $(A \otimes B)(C \otimes D) = AC \otimes BD$, and $\operatorname{trace}(A \otimes B) = \operatorname{trace}(A)\operatorname{trace}(B)$.

The Povh-Rendl [37] relaxation takes the form:

$$
\begin{aligned}
\min \ & \langle A \otimes B, Y \rangle \\
s.t. \ & \langle I_n \otimes E_{ii}, Y \rangle = 1, \ \langle E_{ii} \otimes I_n, Y \rangle = 1, \quad i = 1, \ldots, n, \\
& \langle I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n, Y \rangle = 0, \\
& \langle J_n \otimes J_n, Y \rangle = n^2, \\
& Y \in D_{n^2},
\end{aligned}
\tag{QAP_{SDP}}
$$

where I_n and J_n are the identity and all-ones matrices of order n respectively, and E_{ii} is the $n \times n$ diagonal matrix with 1 in position (i, i) and zeros elsewhere.

If we define $\operatorname{vec}(\cdot)$ as the operator that maps an $n \times n$ matrix to an n^2-vector by stacking its columns, then we may view the matrix variable Y as a relaxation of $\operatorname{vec}(X)\operatorname{vec}(X)^\mathsf{T}$ for $X \in \Pi_n$.

Consequently, we may view Y as having the following block structure:

$$Y := \begin{pmatrix} Y^{(11)} & \dots & Y^{(1n)} \\ \vdots & \ddots & \vdots \\ Y^{(n1)} & \dots & Y^{(nn)} \end{pmatrix}, \tag{8}$$

where $Y^{(ij)} \in \mathbb{R}^{n\times n}$ $(1 \le i, j \le n)$. Thus $Y^{(jl)}_{ik} = [x_{ij}x_{kl}]_L$, and $Y^{(jl)}_{ik}$ therefore corresponds to the variable X_{ijkl} in (QAP_{RLT-1}).

Theorem 3 ([37]). *A doubly nonnegative matrix Y is feasible for (QAP_{SDP}) if and only if Y satisfies*

(i) $\langle I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n, Y\rangle = 0$,

(ii) $\mathrm{trace}(Y^{(ii)}) = 1 \quad \forall\, i, \qquad \sum_{i=1}^n diag(Y^{(ii)}) = e$,

(iii) $Y^{(ij)}e = diag(Y^{(ii)}) \quad \forall\, i, j$,

(iv) $\sum_{i=1}^n Y^{(ij)} = e\, diag(Y^{(jj)})^\mathsf{T} \quad \forall\, j$,

where e denotes the all-ones vector, and the $diag(\cdot)$ operator maps the diagonal entries of a matrix to a vector in the obvious way.

We may use Theorem 3 to show that the Povh-Rendl relaxation (QAP_{SDP}) coincides with the first-level RLT relaxation (QAP_{RLT-1}) with positive semidefiniteness constraints added.

Theorem 4. *If Y is feasible for (QAP_{SDP}), then $X_{ijkl} = Y^{(jl)}_{ik}$ and $x_{ij} = Y^{(jj)}_{ii}$ $(1 \le i, j, k, l \le n)$ is feasible for (QAP_{RLT-1}) with the same objective value. Conversely, if a feasible solution X_{ijkl} of (QAP_{RLT-1}) corresponds to a positive definite matrix Y of the form (8) where $Y^{(jl)}_{ik} := X_{ijkl}$ $(1 \le i, j, k, l \le n)$, then the matrix Y is feasible for (QAP_{SDP}) with the same objective value.*

Proof. By Theorem 3, for every feasible solution Y of (QAP_{SDP}) one has:

$$Y^{(jl)}e = diag(Y^{(ll)}) \quad \Longrightarrow \quad \sum_i Y^{(jl)}_{ik} = Y^{(ll)}_{kk} \quad \forall\, j, k, l,$$

$$\sum_j Y^{(jl)} = e\, diag(Y^{(ll)})^\mathsf{T} \quad \Longrightarrow \quad \sum_j Y^{(jl)}_{ik} = Y^{(ll)}_{kk} \quad \forall\, i, k, l.$$

Recalling that $Y^{(jl)}_{ik}$ corresponds to X_{ijkl} in (QAP_{RLT-1}), it is now straightforward to verify that $X_{ijkl} = Y^{(jl)}_{ik}$ and $x_{ij} = Y^{(jj)}_{ii}$ satisfy all the constraints of (QAP_{RLT-1}), and that the two objective values are the same. The converse proof is similar and therefore omitted. ∎

For the second-level RLT reformulation we introduce the new variable $Z^{[ij](lq)}_{(kp)} = [x_{ij}x_{kl}x_{pq}]_L$.

Thus we obtain the second level RLT relaxation:

$$
\begin{aligned}
\min\ & \langle A \otimes B, Y\rangle \\
s.t.\ & \langle I_n \otimes E_{ii}, Y\rangle = 1,\ \langle E_{ii} \otimes I_n, Y\rangle = 1 \ \ i = 1,\dots,n, \\
& \langle I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n, Y\rangle = 0, \\
& \langle J_n \otimes J_n, Y\rangle = n^2, \\
& \sum_i Z^{[ij]} = Y \ \ j = 1,\dots,n, \\
& \sum_j Z^{[ij]} = Y \ \ i = 1,\dots,n, \\
& Z^{[ij]} \in D_{n^2} \ \ i,j = 1,\dots,n, \\
& Z^{[ij](lq)}_{(kp)} = Z^{[kl](jq)}_{(ip)} = Z^{[pq](jl)}_{(ik)} \ \ i,j,k,l,p,q = 1,\dots,n.
\end{aligned}
\qquad (QAP_{SDP+RLT-2})
$$

As before, note that $Y \in D_{n^2}$ is implied by $Z^{[ij]} \in D_{n^2}$ and $\sum_j Z^{[ij]} = Y$.

Since the level 2 RLT bound is stronger that the level 1 bound, we have the following corollary of Theorem 4.

Corollary 5. *The bound from ($QAP_{SDP+RLT-2}$) is at least as tight as the Povh-Rendl bound (QAP_{SDP}).*

4 Background on symmetry-induced reduction

In what follows we will show how the RLT relaxations may be reduced in size if the data of the underlying optimization problem exhibits suitable algebraic symmetry. This approach is called *symmetry-induced reduction*, or *symmetry reduction*, for short. We will review some basic concepts first.

Let $\mathcal{S}_n$ denote the symmetric group on $\{1,\dots,n\}$. We consider a fixed permutation group $\mathcal{G} \subset \mathcal{S}_n$. With each permutation $\pi \in \mathcal{G}$, we associate an $n \times n$ permutation matrix $P_\pi \in \Pi_n$, defined by

$$
(P_\pi)_{ij} = \begin{cases} 1 & \text{if } \pi(j) = i \\ 0 & \text{else} \end{cases} \qquad (i,j = 1,\dots,n)
$$

Thus $\pi(j) = i$ if and only if $P_\pi e_j = e_i$ if e_i denotes the ith standard unit vector in $\mathbb{R}^n$. Moreover, for any $X \in \mathbb{R}^{n\times n}$ one has

$$
\left(P_\pi^{\mathsf{T}} X P_\pi\right)_{ij} = X_{\pi(i),\pi(j)} \qquad (i,j = 1,\dots,n).
$$

We call $\{P_\pi \mid \pi \in \mathcal{G}\}$ the permutation matrix representation of $\mathcal{G}$.

The centralizer ring (or commutant) of $\mathcal{G}$ is the set

$$
\mathcal{A}_\mathcal{G} := \{X \in \mathbb{C}^{n\times n} \mid P_\pi^{\mathsf{T}} X P_\pi = X \ \forall \pi \in \mathcal{G}\}.
$$

In words, $\mathcal{A}_\mathcal{G}$ is the set of matrices that are invariant under the row and column permutations in $\mathcal{G}$. The centralizer ring $\mathcal{A}_\mathcal{G}$ is a matrix *-algebra, i.e. a linear subspace of $\mathbb{C}^{n\times n}$ that is also closed under matrix multiplication and under taking the complex conjugate transpose.

A centralizer ring $\mathcal{A}_\mathcal{G} \subset \mathbb{C}^{n\times n}$ has a basis of 0-1 matrices, say $A_1, \ldots, A_d \in \{0,1\}^{n\times n}$, where $d = \dim(\mathcal{A}_\mathcal{G})$. In addition, one may assume that $\sum_{i=1}^d A_i = J$, and that $\mathcal{A}_\mathcal{G}$ contains the identity. The basis $A_1, \ldots, A_d$ corresponds to the orbits of pairs (also called 2-*orbits* or *orbitals*) of indices under the action of $\mathcal{G}$, and forms a *coherent configuration*; see [11] for the formal definition of, and more information on, coherent configurations. In particular, the basis $A_1, \ldots, A_d$ is given by the set of 0-1 matrices with support

$$\{(\pi(i), \pi(j)) \mid \pi \in \mathcal{G}\}$$

for some $i, j \in \{1, \ldots, n\}$.

The orthogonal projection of a matrix $X \in \mathbb{C}^{n\times n}$ onto $\mathcal{A}_\mathcal{G}$ is given by

$$\begin{aligned} \mathcal{P}_{\mathcal{A}_\mathcal{G}}(X) &= \sum_{i=1}^d \frac{\langle A_i, X\rangle}{\|A_i\|^2} A_i \\ &= \frac{1}{|\mathcal{G}|} \sum_{\pi\in\mathcal{G}} P_\pi^\mathsf{T} X P_\pi, \end{aligned}$$

where $\|A_i\|^2 = \langle A_i, A_i\rangle = \mathrm{trace}(A_i^2) = \langle A_i, J\rangle$, i.e. the norm in question is the Frobenius norm.

The projection operator is known as the Reynolds operator of $\mathcal{G}$ and the projection is also called the barycenter of the orbit.

For an integer k, the stabilizer subgroup $\mathcal{G}[k] \subset \mathcal{G}$ is defined as the group

$$\mathcal{G}[k] = \{\pi \in \mathcal{G} \mid \pi(k) = k\},$$

and we will denote the centralizer ring of $\mathcal{G}[k]$ by $\mathcal{A}_{\mathcal{G}[k]}$.

If $\mathcal{A}$ and $\mathcal{A}'$ are two matrix *-algebras, then a linear map $\phi : \mathcal{A} \mapsto \mathcal{A}'$ is called an algebra *-isomorphism if it is one-to-one,

$$\phi(XY) = \phi(X)\phi(Y) \quad \forall X, Y \in \mathcal{A}$$

and

$$\phi(X^*) = (\phi(X))^* \quad \forall X \in \mathcal{A}.$$

Each matrix *-algebra that contains the identity is isomorphic to a direct sum of full matrix algebras, in the following sense.

Theorem 6 (Wedderburn, cf. [47])**.** *Let $\mathcal{A} \subset \mathbb{C}^{n\times n}$ be a matrix *-algebra that contains the identity. Then there exists an algebra *-isomorphism ϕ such that*

$$\phi(\mathcal{A}) = \oplus_i \mathbb{C}^{n_i \times n_i}$$

for some integers n_i that satisfy $\sum_i n_i^2 = dim(\mathcal{A})$.

The image of $\mathcal{A}$ under the isomorphism ϕ is called the Wedderburn (or canonical) decomposition of $\mathcal{A}$, or the (canonical) block-diagonalization of $\mathcal{A}$. An accessible proof of the Wedderburn decomposition theorem is given in [15, Chapter 2]. Moreover, this proof is constructive, and shows how to obtain ϕ.

The following result relates matrix *-isomorphisms to symmetry reduction for SDP.

Theorem 7 (see e.g. Theorem 4 in [24])**.** *Assume that $\mathcal{A}$ and $\mathcal{A}'$ are two matrix *-algebras and $\phi : \mathcal{A} \mapsto \mathcal{A}'$ a matrix *-isomorphism. Moreover assume that symmetric matrices $M_0, \ldots, M_k \in \mathcal{A}$ and a vector $y \in \mathbb{R}^k$ are given. One now has*

$$M_0 + \sum_{i=1}^{k} y_i M_i \succeq 0 \Longleftrightarrow \phi(M_0) + \sum_{i=1}^{k} y_i \phi(M_i) \succeq 0,$$

where '$\succeq 0$' means 'Hermitian positive semidefinite'.

In practice, this means that we may often replace the matrices M_i by block diagonal matrices $\phi(M_i)$ with block sizes much smaller than the size of M_i. This block-diagonal structure may in turn be exploited by interior point solvers.

The following example illustrates the definitions above, and will be used later on.

Example 8. *Consider the complete k-partite graph $K_{m,\ldots,m}$ with $n = mk$, and let $\mathcal{G} = Aut(K_{m,\ldots,m})$ be the automorphism group of $K_{m,\ldots,m}$. The centralizer ring of $\mathcal{G}[1]$ is a 12-dimensional subspace of $\mathbb{C}^{n\times n}$ and has the following basis. (The matrices $A_6, \ldots, A_{12}$ all have the same block structure, and subscripts that indicate size are therefore only indicated in full for A_1 to A_6.)*

$$A_1 = \begin{pmatrix} 1 & 0_{1\times n-1} \\ 0_{n-1\times 1} & 0_{n-1\times n-1} \end{pmatrix}, \; A_2 = \begin{pmatrix} 0 & 1_{1\times m-1} & 0_{1\times (k-1)m} \\ 0_{n-1\times 1} & 0_{n-1\times m-1} & 0_{n-1\times (k-1)m} \end{pmatrix} = A_3^{\mathsf{T}},$$

$$A_4 = \begin{pmatrix} 0 & 0_{1\times m-1} & 1_{1\times (k-1)m} \\ 0_{n-1\times 1} & 0_{n-1\times m-1} & 0_{n-1\times (k-1)m} \end{pmatrix} = A_5^{\mathsf{T}},$$

$$A_6 = \begin{pmatrix} 0 & 0_{1\times m-1} & 0_{1\times m} \\ 0_{m-1\times 1} & I_{m-1} & 0_{m-1\times m} \\ 0_{(k-1)m\times 1} & 0_{(k-1)m\times m-1} & 0_{(k-1)m\times (k-1)m} \end{pmatrix},$$

$$A_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & J-I & 0 \\ 0 & 0 & 0 \end{pmatrix}, \; A_8 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & e^{\mathsf{T}} \otimes J \\ 0 & 0 & 0 \end{pmatrix} = A_9^{\mathsf{T}},$$

$$A_{10} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I\otimes I \end{pmatrix}, \; A_{11} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I\otimes (J-I) \end{pmatrix}, \; A_{12} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & (J-I)\otimes J \end{pmatrix}.$$

The centralizer ring $\mathcal{A}_{\mathcal{G}}$ is isomorphic to $\mathbb{C} \oplus \mathbb{C} \oplus \mathbb{C} \oplus \mathbb{C}^{3\times 3}$, and the associated algebra $*$-isomorphism ϕ satisfies:

$$\phi(A_1) = \begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & 0 & & & \\ & & & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & 0 & 0 & 1 \end{pmatrix}, \; \phi(A_2) = \sqrt{m-1} \begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & 0 & & & \\ & & & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & 1 & 0 & 0 \end{pmatrix} = \phi(A_3)^{\mathsf{T}},$$

$$\phi(A_4) = \sqrt{(k-1)m} \begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & 0 & & & \\ & & & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & 0 & -1 & 0 \end{pmatrix} = \phi(A_5)^{\mathsf{T}}, \; \phi(A_6) = \begin{pmatrix} 1 & & & & & \\ & 0 & & & & \\ & & 0 & & & \\ & & & 1 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \end{pmatrix},$$

$$\phi(A_7) = \begin{pmatrix} -1 & & & & & \\ & 0 & & & & \\ & & 0 & & & \\ & & & m-2 & 0 & 0 \\ & & & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \end{pmatrix}, \; \phi(A_8) = \sqrt{(k-1)m(m-1)} \begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & 0 & & & \\ & & & 0 & -1 & 0 \\ & & & 0 & 0 & 0 \\ & & & 0 & 0 & 0 \end{pmatrix} = \phi(A_9)^{\mathsf{T}},$$

$$\phi(A_{10}) = \begin{pmatrix} 0 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 0 & 0 & 0 \\ & & & 0 & 1 & 0 \\ & & & 0 & 0 & 0 \end{pmatrix}, \ \phi(A_{11}) = \begin{pmatrix} 0 & & & & & \\ & -1 & & & & \\ & & m-1 & & & \\ & & & 0 & 0 & 0 \\ & & & 0 & m-1 & 0 \\ & & & 0 & 0 & 0 \end{pmatrix},$$

$$\phi(A_{12}) = m \begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & -1 & & & \\ & & & 0 & 0 & 0 \\ & & & 0 & k-2 & 0 \\ & & & 0 & 0 & 0 \end{pmatrix}.$$

Finally, the following lemma will be crucial for the symmetry reduction in the following section. We supply a proof, since we could not find this result in the required form in the literature.

Lemma 9. *Assume that the permutation group $\mathcal{G} \subset \mathcal{S}_n$ acts transitively on $\{1, \ldots, n\}$, and that its centralizer ring $\mathcal{A}_\mathcal{G}$ has a 0-1 basis $A_1, \ldots, A_d$. Assume, moreover, that the centralizer ring of the stabilizer subgroup $\mathcal{G}[1]$ has a 0-1 basis $A'_1, \ldots, A'_{d'}$. Finally, let $\pi_k \in \mathcal{G}$ be such that $\pi_k(k) = 1$ $(k = 1, \ldots, n)$. Then, for any $t \in \{1, \ldots, d'\}$, there exists an $f(t) \in \{1, \ldots, d\}$ such that*

$$\sum_{k=1}^{n} P_{\pi_k}^{\mathsf{T}} A'_t P_{\pi_k} = \frac{n\langle A'_t, J\rangle}{\langle A_{f(t)}, J\rangle} A_{f(t)}.$$

Moreover, $f(t) \in \{1, \ldots, d\}$ is the unique value such that

$$\operatorname{support}(A'_t) \subseteq \operatorname{support}(A_{f(t)}). \tag{9}$$

Proof. If we define the following subsets of $\mathcal{G}$,

$$\mathcal{G}_i = \{\pi \in \mathcal{G} \mid \pi(i) = 1\} \quad (i = 1, \ldots, n),$$

then we have that $\pi_i \in \mathcal{G}_i$ $(i = 1, \ldots, n)$. Moreover, $\mathcal{G}_1 = \mathcal{G}[1]$, $\mathcal{G}_i = \mathcal{G}[1] \circ \pi_i$ $(i = 1, \ldots, n)$, where '$\circ$' denotes the composition operation, and

$$\mathcal{G} = \bigcup_{i=1}^{n} \mathcal{G}_i, \quad \mathcal{G}_i \cap \mathcal{G}_j = \emptyset \text{ if } i \neq j. \tag{10}$$

Fix $t \in \{1, \ldots, d'\}$, and consider the projection of A'_t onto $\mathcal{A}_\mathcal{G}$:

$$\begin{aligned}
\mathcal{P}_{\mathcal{A}_\mathcal{G}}(A'_t) &= \frac{1}{|\mathcal{G}|} \sum_{\pi \in \mathcal{G}} P_\pi^{\mathsf{T}} A'_t P_\pi \\
&= \frac{1}{|\mathcal{G}|} \sum_{i=1}^{n} \sum_{\sigma \in \mathcal{G}_i} P_\sigma^{\mathsf{T}} A'_t P_\sigma \quad \text{(by (10))} \\
&= \frac{1}{|\mathcal{G}|} \sum_{i=1}^{n} \sum_{\rho \in \mathcal{G}_1} (P_\rho P_{\pi_i})^{\mathsf{T}} A'_t P_\rho P_{\pi_i} \quad (\text{since } \mathcal{G}_i = \mathcal{G}_1 \circ \pi_i) \\
&= \frac{1}{|\mathcal{G}|} \sum_{i=1}^{n} P_{\pi_i}^{\mathsf{T}} \left(\sum_{\rho \in \mathcal{G}[1]} P_\rho^{\mathsf{T}} A'_t P_\rho \right) P_{\pi_i} \quad (\text{since } \mathcal{G}_1 = \mathcal{G}[1]) \\
&= \frac{|\mathcal{G}[1]|}{|\mathcal{G}|} \sum_{i=1}^{n} P_{\pi_i}^{\mathsf{T}} A'_t P_{\pi_i} \quad (\text{since } A'_t \in \mathcal{A}_{\mathcal{G}[1]}) \\
&= \frac{1}{n} \sum_{i=1}^{n} P_{\pi_i}^{\mathsf{T}} A'_t P_{\pi_i} \quad (\text{since } |\mathcal{G}| = n|\mathcal{G}[1]|).
\end{aligned}$$

On the other hand, since $\{A_1/\|A_1\|, \ldots, A_d/\|A_d\|\}$ is an orthonormal basis of $\mathcal{A}_{\mathcal{G}}$, one has

$$\begin{aligned} \mathcal{P}_{\mathcal{A}_{\mathcal{G}}}(A'_t) &= \sum_{i=1}^{d} \frac{\langle A'_t, A_i\rangle}{\|A_i\|^2} A_i \\ &= \frac{\langle A'_t, J\rangle}{\langle A_{f(t)}, J\rangle} A_{f(t)}, \end{aligned}$$

if $f(t) \in \{1, \ldots, d\}$ is the unique value such that (9) holds. (The uniqueness of $f(t)$ follows from the fact that $\mathcal{G}[1]$ is a subgroup of $\mathcal{G}$, and therefore each orbital of $\mathcal{G}[1]$ is a subset of some (unique) orbital of $\mathcal{G}$.) This completes the proof. ■

5 Symmetry reduction of ($stQP_{SDP+RLT-2}$)

We may eliminate the matrix variable $X = \sum_k Y^{(k)}$ from the second level RLT relaxation of (stQP) with SDP constraints to obtain:

$$\min_{Y^{(1)},\ldots,Y^{(n)} \in D_n} \left\{ \sum_{k=1}^{n} \langle Q, Y^{(k)}\rangle \mid \sum_{k=1}^{n} \langle J, Y^{(k)}\rangle = 1,\ Y^{(k)}_{ij} \text{ fully symmetric} \right\}. \quad (stQP_{SDP+RLT-2})$$

Let $\mathcal{G}$ be the automorphism group of the matrix Q, i.e.

$$\mathcal{G} = \mathrm{Aut}(Q) \equiv \left\{\pi \in \mathcal{S}_n \mid Q_{ij} = Q_{\pi(i),\pi(j)}\ \forall i, j \in \{1, \ldots, n\}\right\}. \quad (11)$$

Lemma 10. *Assume that $Y^{(k)}$ $(k = 1, \ldots, n)$ are optimal for ($stQP_{SDP+RLT-2}$). Then*

$$\bar{Y}^{(k)} = \frac{1}{|\mathcal{G}|} \sum_{\pi \in \mathcal{G}} P_\pi^{\mathsf{T}} Y^{(\pi(k))} P_\pi \quad (k = 1, \ldots, n)$$

are also optimal.

Proof. Assume that $Y^{(k)}$ and $\bar{Y}^{(k)}$ $(k = 1, \ldots, n)$ are as in the statement of the lemma.

It is trivial to verify that $\sum_{k=1}^{n} \langle J, \bar{Y}^{(k)}\rangle = 1$, and that the matrices $\bar{Y}^{(k)}$ $(k = 1, \ldots, n)$ are doubly nonnegative, by construction.

To show the complete symmetry of $\bar{Y}^{(k)}_{ij}$, consider, for fixed $i, j, k \in \{1, \ldots, n\}$,

$$\begin{aligned} \bar{Y}^{(k)}_{ij} &= \frac{1}{|\mathcal{G}|} \sum_{\pi \in \mathcal{G}} Y^{(\pi(k))}_{\pi(i),\pi(j)} \\ &= \frac{1}{|\mathcal{G}|} \sum_{\pi \in \mathcal{G}} Y^{(\pi(i))}_{\pi(j),\pi(k)} \\ &\equiv \bar{Y}^{(i)}_{jk}, \end{aligned}$$

where the second equality follows from the complete symmetry $Y^{(k)}_{ij} = Y^{(i)}_{jk} = Y^{(j)}_{ik}$.

Finally, since $P_\pi^\mathsf{T} Q P_\pi = Q$ for all $\pi \in \mathcal{G}$, one has

$$\begin{aligned}
\sum_{k=1}^n \langle Q, Y^{(k)} \rangle &= \frac{1}{|\mathcal{G}|} \sum_{\pi\in\mathcal{G}} \sum_{k=1}^n \langle P_\pi^\mathsf{T} Q P_\pi, Y^{(k)} \rangle \\
&= \sum_{k=1}^n \left\langle Q, \frac{1}{|\mathcal{G}|} \sum_{\pi\in\mathcal{G}} P_\pi Y^{(k)} P_\pi^\mathsf{T} \right\rangle \\
&\equiv \sum_{k=1}^n \langle Q, \bar{Y}^{(k)} \rangle.
\end{aligned}$$

This completes the proof. ■

The next useful observation is that an optimal $Y^{(k)}$ may be assumed to belong to the centralizer ring of the stabilizer subgroup $\mathcal{G}[k]$.

Lemma 11. *There exists an optimal solution of ($stQP_{SDP+RLT-2}$) that satisfies*

$$Y^{(k)} \in \mathcal{A}_{\mathcal{G}[k]} \quad (k = 1, \ldots, n).$$

Proof. By the last lemma, we may assume that an optimal solution satisfies

$$Y^{(k)} = \frac{1}{|\mathcal{G}|} \sum_{\pi\in\mathcal{G}} P_\pi^\mathsf{T} Y^{(\pi(k))} P_\pi \quad (k = 1, \ldots, n).$$

Now fix $i, j, k \in \{1, \ldots, n\}$, and $\sigma \in \mathcal{G}[k]$. One now has

$$Y^{(k)}_{\sigma(i),\sigma(j)} = Y^{(\sigma(k))}_{\sigma(i),\sigma(j)} = \frac{1}{|\mathcal{G}|} \sum_{\pi\in\mathcal{G}} Y^{(\pi(\sigma(k)))}_{\pi(\sigma(i)),\pi(\sigma(j))}.$$

Setting $\tau = \pi \circ \sigma$, this yields

$$Y^{(k)}_{\sigma(i),\sigma(j)} = \frac{1}{|\mathcal{G}|} \sum_{\tau\in\mathcal{G}} Y^{(\tau(k))}_{\tau(i),\tau(j)} \equiv Y^{(k)}_{ij}.$$

Thus $Y^{(k)} \in \mathcal{A}_{\mathcal{G}[k]}$, as required. ■

Finally, if $\mathcal{G}$ is transitive, we may assume that the matrices $Y^{(k)}$ $(k = 1, \ldots, n)$ are not independent, but may all be written in terms of $Y^{(1)}$, as the next lemma shows.

Lemma 12. *If $\mathcal{G}$ acts transitively on $\{1, \ldots, n\}$, then there exists an optimal solution of ($stQP_{SDP+RLT-2}$) that satisfies*

$$Y^{(k)} = P_{\pi_k}^\mathsf{T} Y^{(1)} P_{\pi_k},$$

for any $\pi_k \in \mathcal{G}$ such that $\pi_k(k) = 1$ $(k = 1, \ldots, n)$.

Proof. By Lemma 10, we may assume that optimal $Y^{(k)}$ $(k = 1, \ldots, n)$ satisfy

$$Y^{(k)} = \frac{1}{|\mathcal{G}|} \sum_{\pi\in\mathcal{G}} P_\pi^\mathsf{T} Y^{(\pi(k))} P_\pi \quad (k = 1, \ldots, n).$$

Fix $\pi_k \in \mathcal{G}$ such that $\pi_k(k) = 1$ $(k = 1, \ldots, n)$. One now has

$$\begin{aligned} P_{\pi_k}^\top Y^{(1)} P_{\pi_k} &= \frac{1}{|\mathcal{G}|} \sum_{\pi \in \mathcal{G}} P_{\pi_k}^\top P_\pi^\top Y^{\pi(1)} P_\pi P_{\pi_k} \\ &= \frac{1}{|\mathcal{G}|} \sum_{\pi \in \mathcal{G}} (P_\pi P_{\pi_k})^\top Y^{\pi(1)} P_\pi P_{\pi_k}. \end{aligned}$$

Denoting $\sigma_k = \pi \circ \pi_k$ so that $\sigma_k(k) = \pi(1)$, this becomes

$$P_{\pi_k}^\top Y^{(1)} P_{\pi_k} = \frac{1}{|\mathcal{G}|} \sum_{\sigma_k \in \mathcal{G}} P_{\sigma_k}^\top Y^{(\sigma_k(k))} P_{\sigma_k} \equiv Y^{(k)},$$

as required. ■

We may now simplify problem $(stQP_{SDP+RLT-2})$ by using the results of the last three lemmas. To this end, let $A_1, \ldots, A_d$ denote a 0-1 basis of $\mathcal{A}_{\mathcal{G}[1]}$ given by the 2-orbits of $\mathcal{G}[1]$.

By the results of this section, we may assume that an optimal solution takes the form

$$Y^{(1)} = \sum_{i=1}^d y_i A_i, \quad Y^{(k)} = P_{\pi_k}^\top Y^{(1)} P_{\pi_k} = \sum_{i=1}^d y_i P_{\pi_k}^\top A_i P_{\pi_k} \quad (k = 2, \ldots, n),$$

for some nonnegative scalar variables $y_1, \ldots, y_d$, if $\mathcal{G}$ is transitive. Thus,

$$\begin{aligned} \sum_{k=1}^n \langle J, Y^{(k)} \rangle &= \langle J, Y^{(1)} \rangle + \sum_{k=2}^n \langle J, P_{\pi_k}^\top Y^{(1)} P_{\pi_k} \rangle \\ &= n \langle J, Y^{(1)} \rangle, \end{aligned}$$

so that the constraint $\sum_{k=1}^n \langle J, Y^{(k)} \rangle = 1$ becomes $\langle J, Y^{(1)} \rangle = 1/n$.

The complete symmetry conditions $Y_{ij}^{(k)} = Y_{jk}^{(i)} = Y_{ik}^{(j)}$ imply that some of the y_i variables are equal. To make this precise, note that:

$$\begin{aligned} Y_{ij}^{(k)} &= \sum_{u=1}^d y_u (A_u)_{\pi_k(i), \pi_k(j)}, \\ Y_{ik}^{(j)} &= \sum_{v=1}^d y_v (A_v)_{\pi_j(i), \pi_j(k)}, \\ Y_{jk}^{(i)} &= \sum_{t=1}^d y_t (A_t)_{\pi_i(j), \pi_i(k)}. \end{aligned}$$

If we fix $(i, j, k) \in \{1, \ldots, n\}^3$, then there are unique $(u, v, t) \in \{1, \ldots, d\}^3$ such that

$$1 = (A_u)_{\pi_k(i), \pi_k(j)} = (A_v)_{\pi_j(i), \pi_j(k)} = (A_t)_{\pi_i(j), \pi_i(k)},$$

and it must hold that $y_u = y_v = y_t$. Note that one always get the same triple (u, v, t) for a fixed (i, j, k) independently from the choice of permutations π_i, π_j, π_k. Indeed, if π_i and $\tilde{\pi}_i$ are in $\mathcal{G}$ and both map i to 1, then there is a permutation ρ from $\mathcal{G}[1]$ such that $\rho\pi_i = \tilde{\pi}_i$. But A_u is in the algebra $\mathcal{A}_{\mathcal{G}[1]}$, that is, it is invariant under the permutation ρ. Therefore $(A_u)_{\pi_i(j), \pi_i(k)} = (A_u)_{\tilde{\pi}_i(j), \tilde{\pi}_i(k)}$.

Definition 13. *We will write $u \sim v$ if there exists a triple (i,j,k) such that $1 = (A_u)_{\pi_k(i),\pi_k(j)} = (A_v)_{\pi_j(i),\pi_j(k)}$.*

Thus the total symmetry condition becomes $y_u = y_v$ if $u \sim v$.

In summary, we may write problem ($stQP_{SDP+RLT-2}$) in the following form.

Theorem 14. *Consider problem ($stQP_{SDP+RLT-2}$) and assume that $\mathcal{G} = Aut(Q)$ is transitive. Let $A_1, \ldots, A_d$ denote the 0-1 basis of $\mathcal{A}_{\mathcal{G}[1]}$. Then the optimal value is given by:*

$$\min_{y\geq 0} \left\{ n\sum_{i=1}^{d} y_i\langle A_i, Q\rangle \;\middle|\; \sum_{i=1}^{d} y_i\langle A_i, J\rangle = \frac{1}{n},\ y_u = y_v \text{ if } u\sim v,\ \sum_{i=1}^{d} y_i A_i \succeq 0 \right\},$$

where the '$\sim$'-relation is from Definition 13.

It is important to remember that the linear matrix inequality $\sum_{i=1}^d y_i A_i \succeq 0$ may be replaced by $\sum_{i=1}^d y_i \phi(A_i) \succeq 0$ for any algebra $*$-isomorphism ϕ with domain $\mathcal{A}_{\mathcal{G}[1]}$.

6 Symmetry reduction of ($QAP_{SDP+RLT-2}$)

We now consider the symmetry reduction of ($QAP_{SDP+RLT-2}$) for the QAP

$$\min_{P\in\Pi_n} \operatorname{trace}(AP^{\mathsf{T}}BP)$$

in the case when the $n \times n$ symmetric matrices A and B have large automorphism groups.

First of all, we may eliminate the matrix variable Y from ($QAP_{SDP+RLT-2}$), by using $Y = 1/n\sum_{i,j} Z^{[ij]}$, to obtain the formulation:

$$\begin{aligned}
\min\ & \frac{1}{n}\sum_{i,j=1}^{n} \left\langle A\otimes B, Z^{[ij]}\right\rangle \\
\text{s.t.}\ & \sum_{i,j=1}^{n} \left\langle I_n\otimes E_{kk}, Z^{[ij]}\right\rangle = n,\ \sum_{i,j=1}^{n} \left\langle E_{kk}\otimes I_n, Z^{[ij]}\right\rangle = n,\quad k=1,\ldots,n,\\
& \sum_{i,j=1}^{n} \left\langle I_n\otimes (J_n - I_n) + (J_n - I_n)\otimes I_n, Z^{[ij]}\right\rangle = 0,\\
& \sum_{i,j=1}^{n} \left\langle J_n\otimes J_n, Z^{[ij]}\right\rangle = n^3,\\
& \sum_{k=1}^{n} Z^{[kj]} = \sum_{k=1}^{n} Z^{[ik]},\quad i,j=1,\ldots,n,\\
& Z^{[ij]} \in D_{n^2},\quad i,j=1,\ldots,n,\\
& Z^{[ij](lq)}_{(kp)} = Z^{[kl](jq)}_{(ip)} = Z^{[pq](jl)}_{(ik)},\quad i,j,k,l,p,q=1,\ldots,n.
\end{aligned} \qquad (QAP_{SDP+RLT-2})$$

To describe the symmetry, we define $\mathcal{G}_A := \operatorname{Aut}(A)$, $\mathcal{G}_B := \operatorname{Aut}(B)$ and $\mathcal{G}_{AB} := \operatorname{Aut}(A\otimes B)$ as in (11).

The following results are analogous to the results for the symmetry reduction of the standard quadratic program. Where possible, we therefore omit the proofs.

Lemma 15. *Let $Z^{[ij]}$ $(i,j=1,\ldots,n)$ be an optimal solution of $(QAP_{SDP+RLT-2})$, and let $\pi_A \in \mathcal{G}_A$ and $\pi_B \in \mathcal{G}_B$. Then*

$$\widetilde{Z}^{[ij]} = (P_{\pi_A} \otimes P_{\pi_B})^\mathsf{T} Z^{[\pi_A(i),\pi_B(j)]}(P_{\pi_A} \otimes P_{\pi_B}) \quad (i,j=1,\ldots,n)$$

is also optimal.

Proof. One has

$$\langle I_n \otimes E_{kk}, \widetilde{Z}^{[ij]}\rangle = \langle I_n \otimes P_{\pi_B} E_{kk} P_{\pi_B}^\mathsf{T}, Z^{[\pi_A(i),\pi_B(j)]}\rangle = \langle I_n \otimes E_{\pi_B^{-1}(k),\pi_B^{-1}(k)}, Z^{[\pi_A(i),\pi_B(j)]}\rangle,$$

so that

$$\begin{aligned}\sum_{i,j=1}^n \left\langle I_n \otimes E_{kk}, \widetilde{Z}^{[ij]}\right\rangle &= \sum_{i,j=1}^n \left\langle I_n \otimes E_{\pi_B^{-1}(k),\pi_B^{-1}(k)}, Z^{[\pi_A(i),\pi_B(j)]}\right\rangle \\ &= \sum_{i,j=1}^n \left\langle I_n \otimes E_{\pi_B^{-1}(k),\pi_B^{-1}(k)}, Z^{[i,j]}\right\rangle = n.\end{aligned}$$

In the same way, one may show that

$$\sum_{i,j=1}^n \left\langle E_{kk} \otimes I_n, \widetilde{Z}^{[ij]}\right\rangle = n.$$

The matrices $I, J-I$ are invariant under all row and column permutations, so that the constraints

$$\sum_{i,j=1}^n \langle I_n \otimes (J_n - I_n) + (J_n - I_n) \otimes I_n, Z^{[ij]}\rangle = 0,\ \sum_{i,j=1}^n \langle J_n \otimes J_n, Z^{[ij]}\rangle = n^3$$

are satisfied by $Z^{[ij]} = \widetilde{Z}^{[ij]}$.

The matrices $\widetilde{Z}^{[ij]}$ $(i,j=1,\ldots,n)$ are doubly nonnegative, by construction. Moreover, for fixed $j \in \{1,\ldots,n\}$,

$$\begin{aligned}\sum_{i=1}^n \widetilde{Z}^{[ij]} &= \sum_{i=1}^n (P_{\pi_A} \otimes P_{\pi_B})^\mathsf{T} Z^{[\pi_A(i),\pi_B(j)]}(P_{\pi_A} \otimes P_{\pi_B}) \\ &= (P_{\pi_A} \otimes P_{\pi_B})^\mathsf{T} \left(\sum_{k=1}^n Z^{[k,\pi_B(j)]}\right)(P_{\pi_A} \otimes P_{\pi_B}).\end{aligned} \tag{12}$$

Similarly, for fixed $i \in \{1,\ldots,n\}$,

$$\begin{aligned}\sum_{j=1}^n \widetilde{Z}^{[ij]} &= \sum_{j=1}^n (P_{\pi_A} \otimes P_{\pi_B})^\mathsf{T} Z^{[\pi_A(i),\pi_B(j)]}(P_{\pi_A} \otimes P_{\pi_B}) \\ &= (P_{\pi_A} \otimes P_{\pi_B})^\mathsf{T} \left(\sum_{k=1}^n Z^{[\pi_A(i),k]}\right)(P_{\pi_A} \otimes P_{\pi_B}).\end{aligned} \tag{13}$$

Since $\sum_k Z^{[i,k]} = \sum_k Z^{[k,j]}$ for all i,j, the expressions in (12) and (13) are equal. Consequently, the constraint $\sum_{k=1}^n \widetilde{Z}^{[kj]} = \sum_{k=1}^n \widetilde{Z}^{[ik]}$ is satisfied for all i,j.

The tensor $\widetilde{Z}$ is also fully symmetric, since

$$\widetilde{Z}_{kp}^{[ij](lq)} = Z_{\pi_A(k),\pi_A(p)}^{[\pi_A(i),\pi_B(j)](\pi_B(l),\pi_B(q))} = Z_{\pi_A(i),\pi_A(p)}^{[\pi_A(k),\pi_B(l)](\pi_B(j),\pi_B(q))} = \widetilde{Z}_{ip}^{[kl](jq)},$$

etc. Finally, the objective value at $\widetilde{Z}^{[ij]}$ is

$$\frac{1}{n}\sum_{i,j=1}^n \left\langle A\otimes B, \widetilde{Z}^{[ij]}\right\rangle = \frac{1}{n}\sum_{i,j=1}^n \left\langle P_{\pi_A}^{\mathsf{T}} A P_{\pi_A} \otimes P_{\pi_B}^{\mathsf{T}} B P_{\pi_B}, Z^{[\pi_A(i),\pi_B(j)]}\right\rangle = \frac{1}{n}\sum_{i,j=1}^n \left\langle A\otimes B, Z^{[ij]}\right\rangle.$$

This completes the proof. ■

Corollary 16. *If $Z^{[ij]}$ $(i,j=1,\ldots,n)$ denotes an optimal solution of $(QAP_{SDP+RLT-2})$, then*

$$Z_{kp}^{*[ij](lq)} = \frac{1}{|\mathcal{G}_{AB}|}\sum_{\pi_A\in\mathcal{G}_A}\sum_{\pi_B\in\mathcal{G}_B} Z_{\pi_A(k),\pi_A(p)}^{[\pi_A(i),\pi_B(j)](\pi_B(l),\pi_B(q))}$$

is also optimal.

Proof. The result follows immediately from the fact that the optimal set of $(QAP_{SDP+RLT-2})$ is convex. ■

The next result is similar to Lemma 11, and its proof is therefore omitted.

Lemma 17. *Problem $(QAP_{SDP+RLT-2})$ has an optimal solution that satisfies $Z^{[ij]} \in \mathcal{A}_{\mathcal{G}_{AB}[i,j]}$, where $\mathcal{G}_{AB}[i,j] \subset \mathcal{S}_{n^2}$ is the group with permutation matrix representation*

$$\{P_{\pi_A}\otimes P_{\pi_B} \mid \pi_A \in \mathcal{G}_A[i],\ \pi_B\in\mathcal{G}_B[j]\}.$$

The next lemma is similar to Lemma 12, and shows that — under suitable symmetry assumptions — we may write all the $Z^{[ij]}$ in terms of $Z^{[11]}$. Once again, we omit the proof, since it is similar to that of Lemma 12.

Lemma 18. *Assume that $\mathcal{G}_A$ and $\mathcal{G}_B$ act transitively on $\{1,\ldots,n\}$. Let $\pi_k^A\in\mathcal{G}_A$ and $\pi_k^B\in\mathcal{G}_B$ map k to 1 $(k=1,\ldots,n)$. Then there exists an optimal solution of $(QAP_{SDP+RLT-2})$ that satisfies*

$$Z^{[ij]} = (P_{\pi_i^A}\otimes P_{\pi_j^B})^{\mathsf{T}} Z^{[11]} (P_{\pi_i^A}\otimes P_{\pi_j^B}) \quad (i,j=1,\ldots,n).$$

In what follows we let $\{A_1,\ldots,A_{d_A}\}$ and $\{B_1,\ldots,B_{d_B}\}$ denote the 0-1 bases of the centralizer rings of $\mathcal{G}_A$ and $\mathcal{G}_B$ respectively. Moreover, we let $\{A_1',\ldots,A_{d_A'}'\}$ denote the 0-1 basis of the centralizer ring of $\mathcal{G}_A[1]$, and define $\{B_1',\ldots,B_{d_B'}'\}$ similarly. By the last lemma, we may now write the $Z^{[ij]}$ in terms of these bases as follows:

$$Z^{[11]} = \sum_{p=1}^{d_A'}\sum_{q=1}^{d_B'} z_{pq} A_p'\otimes B_q',$$

and, consequently,

$$
\begin{aligned}
Z^{[ij]} &= \sum_{p=1}^{d'_A}\sum_{q=1}^{d'_B} z_{pq}(P_{\pi_i^A}\otimes P_{\pi_j^B})^{\mathsf{T}} A'_p \otimes B'_q (P_{\pi_i^A}\otimes P_{\pi_j^B}) \\
&= \sum_{p=1}^{d'_A}\sum_{q=1}^{d'_B} z_{pq}\left(P_{\pi_i^A}^{\mathsf{T}} A'_p P_{\pi_i^A}\right)\otimes\left(P_{\pi_j^B}^{\mathsf{T}} B'_q P_{\pi_j^B}\right). \qquad (14)
\end{aligned}
$$

Next, we consider the total symmetry conditions for the $Z^{[ij]}$. Recalling that $Z^{[ij](\gamma\delta)}_{(\alpha\beta)} = [x_{ij}x_{\alpha\gamma}x_{\beta\delta}]_L$, the total symmetry conditions are

$$
Z^{[ij](\gamma\delta)}_{\alpha\beta} = Z^{[\alpha\gamma](\delta j)}_{\beta i} = Z^{[\beta\delta](j\gamma)}_{i\alpha} \qquad (15)
$$

together with $Z^{[ij]} = \left(Z^{[ij]}\right)^{\mathsf{T}}$, where all indices range from 1 to n.

Clearly, the total symmetry conditions will translate to certain variables z_{pq} being equal. In particular, for every index set $(i,j,\alpha,\beta,\gamma,\delta)$ there is exactly one pair (p,q) such that $Z^{[ij](\gamma\delta)}_{\alpha\beta} = z_{pq}$. In particular, one has

$$
Z^{[ij](\gamma\delta)}_{\alpha\beta} = z_{pq} \text{ iff } \left(P_{\pi_i^A}^{\mathsf{T}} A'_p P_{\pi_i^A}\right)_{\alpha\beta} = 1 \text{ and } \left(P_{\pi_j^B}^{\mathsf{T}} B'_q P_{\pi_j^B}\right)_{\gamma\delta} = 1.
$$

To proceed, we require some notation analogous to that of Definition 13.

Definition 19. *We define two relations $\sim_{1A}$ and $\sim_{2A}$ that partition $\{1,\ldots,d'_A\}$ as follows*

$$
p \sim_{1A} \tilde{p} \iff \exists(i,\alpha,\beta)\ :\ \left(P_{\pi_i^A}^{\mathsf{T}} A'_p P_{\pi_i^A}\right)_{\alpha\beta} = 1 \text{ and } \left(P_{\pi_\alpha^A}^{\mathsf{T}} A'_{\tilde{p}} P_{\pi_\alpha^A}\right)_{\beta i} = 1,
$$

$$
p \sim_{2A} \tilde{p} \iff \exists(i,\alpha,\beta)\ :\ \left(P_{\pi_i^A}^{\mathsf{T}} A'_p P_{\pi_i^A}\right)_{\alpha\beta} = 1 \text{ and } \left(P_{\pi_\beta^A}^{\mathsf{T}} A'_{\tilde{p}} P_{\pi_\beta^A}\right)_{i\alpha} = 1,
$$

where $1 \le p,\tilde{p} \le d'_A$, and $1 \le i,\alpha,\beta \le n$.

Similarly, we define two relations $\sim_{1B}$ and $\sim_{2B}$ that partition $\{1,\ldots,d'_B\}$ as follows

$$
q \sim_{1B} \tilde{q} \iff \exists(j,\gamma,\delta)\ :\ \left(P_{\pi_j^B}^{\mathsf{T}} B'_q P_{\pi_j^B}\right)_{\gamma\delta} = 1 \text{ and } \left(P_{\pi_\gamma^B}^{\mathsf{T}} B'_{\tilde{q}} P_{\pi_\gamma^B}\right)_{\delta j} = 1,
$$

$$
q \sim_{2B} \tilde{q} \iff \exists(j,\gamma,\delta)\ :\ \left(P_{\pi_j^B}^{\mathsf{T}} B'_q P_{\pi_j^B}\right)_{\gamma\delta} = 1 \text{ and } \left(P_{\pi_\delta^B}^{\mathsf{T}} B'_{\tilde{q}} P_{\pi_\delta^B}\right)_{j\gamma} = 1,
$$

where $1 \le q,\tilde{q} \le d'_A$, and $1 \le j,\delta,\gamma \le n$.

We now state the final form of the total symmetry conditions. The proof is an easy consequence of (14) and (15).

Lemma 20. *Using the notation in Definition 19, the total symmetry conditions (15) become:*

$$
z_{pq} = z_{\tilde{p}\tilde{q}} \iff (p \sim_{1A} \tilde{p} \text{ and } q \sim_{1B} \tilde{q}) \text{ or } (p \sim_{2A} \tilde{p} \text{ and } q \sim_{2B} \tilde{q}). \qquad (16)
$$

The final step in the symmetry reduction of problem $(QAP_{SDP+RLT-2})$ is to rewrite the constraints:

$$\sum_{k=1}^{n} Z^{[kj]} = \sum_{k=1}^{n} Z^{[ik]} \ \ (i,j=1,\ldots,n). \tag{17}$$

Using (14), the left-hand-side may be written as

$$\sum_{k=1}^{n} Z^{[kj]} = \sum_{p=1}^{d'_A}\sum_{q=1}^{d'_B} z_{pq}\left(\sum_{k=1}^{n} P^{\mathsf{T}}_{\pi_k^A} A'_p P_{\pi_k^A}\right) \otimes \left(P^{\mathsf{T}}_{\pi_j^B} B'_q P_{\pi_j^B}\right). \tag{18}$$

By Lemma 9,

$$\sum_{k=1}^{n} P^{\mathsf{T}}_{\pi_k^A} A'_p P_{\pi_k^A} = \frac{n\langle A'_p, J\rangle}{\langle A_{f_A(p)}, J\rangle} A_{f_A(p)}$$

where $f_A(p) \in \{1,\ldots,d_A\}$ is the unique value such that support$(A'_p) \subseteq$ support$(A_{f_A(p)})$. Moreover, we have $B_s = \sum_{q\in I_B(s)} B'_q$ for some index set $I_B(s) \subset \{1,\ldots,d'_B\}$. In particular, if we define f_B analogously to f_A, then $I_B(s) = \{q \mid f_B(q) = s\}$.

Using these relations, equation (18) becomes

$$\sum_{k=1}^{n} Z^{[kj]} = \sum_{p=1}^{d'_A}\sum_{q=1}^{d'_B} z_{pq}\left(\frac{n\langle A'_p, J\rangle}{\langle A_{f_A(p)}, J\rangle} A_{f_A(p)}\right) \otimes \left(P^{\mathsf{T}}_{\pi_j^B} B'_q P_{\pi_j^B}\right).$$

In a similar way, one may show that

$$\sum_{k=1}^{n} Z^{[ik]} = \sum_{p=1}^{d'_A}\sum_{q=1}^{d'_B} z_{pq}\left(P^{\mathsf{T}}_{\pi_i^A} A'_p P_{\pi_i^A}\right) \otimes \left(\frac{n\langle B'_q, J\rangle}{\langle B_{f_B(q)}, J\rangle} B_{f_B(q)}\right).$$

Equating coefficients of $A_r \otimes B_s$ $(1 \le r \le d_A,\ 1 \le s \le d_B)$ in the last two expressions, we find that (17) will hold if and only if

$$\sum_{\bar p : f_A(\bar p) = r} \frac{\langle A'_{\bar p}, J\rangle}{\langle A_r, J\rangle} z_{\bar p q} = \sum_{\bar q : f_B(\bar q) = s} \frac{\langle B'_{\bar q}, J\rangle}{\langle B_s, J\rangle} z_{p\bar q} \ \ \forall\, p \in I_A(r),\ q \in I_B(s)\ (1 \le r \le d_A,\ 1 \le s \le d_B).$$

We end this section by stating the final reformulation of the relaxation $(QAP_{SDP+RLT-2})$ as a theorem.

Theorem 21. *Consider the QAP problem* $\min_{P\in\Pi_n} \operatorname{trace} AP^{\mathsf{T}}BP$ *and assume that* $Aut(A)$ *and* $Aut(B)$ *act transitively on* $\{1,\ldots,n\}$. *Let* $\{A_1,\ldots,A_{d_A}\}$ *and* $\{B_1,\ldots,B_{d_B}\}$ *denote the 0-1 bases of the centralizer rings of* $\mathcal{G}_A := Aut(A)$ *and* $\mathcal{G}_B := Aut(B)$ *respectively. Moreover, let* $\{A'_1,\ldots,A'_{d'_A}\}$ *denote the 0-1 basis of the centralizer ring of* $\mathcal{G}_A[1]$, *and define* $\{B'_1,\ldots,B'_{d'_B}\}$ *similarly.*

Assume that $\pi_k^A \in \mathcal{G}_A$ *are given such that* $\pi_k^A(k) = 1$ $(k=1,\ldots,n)$, *and define* $\pi_k^B \in \mathcal{G}_B$ *in the same way.*

Then the optimal value of problem $(QAP_{SDP+RLT-2})$ *is given by*

$$\min n \sum_{r=1}^{d'_A}\sum_{s=1}^{d'_B} z_{rs}\langle A, A'_r\rangle\langle B, B'_s\rangle$$

subject to

$$\sum_{r=1}^{d'_A}\sum_{s=1}^{d'_B} z_{rs}\,\mathrm{trace}(A'_r)(B'_s)_{ii} = \frac{1}{n} \quad (i=1,\ldots,n),$$
$$\sum_{r=1}^{d'_A}\sum_{s=1}^{d'_B} z_{rs}\,\mathrm{trace}(B'_s)(A'_r)_{ii} = \frac{1}{n} \quad (i=1,\ldots,n),$$
$$\sum_{r=1}^{d'_A}\sum_{s=1}^{d'_B} z_{rs}\left(\mathrm{trace}(A'_r)\langle J-I, B'_s\rangle + \mathrm{trace}(B'_s)\langle J-I, A'_r\rangle\right) = 0,$$
$$\sum_{r=1}^{d'_A}\sum_{s=1}^{d'_B} z_{rs}\langle J, A'_r\rangle\langle J, B'_s\rangle = n,$$
$$\sum_{\bar{p}:f_A(\bar{p})=r}\frac{\langle A'_{\bar{p}}, J\rangle}{\langle A_r, J\rangle} z_{\bar{p}q} = \sum_{\bar{q}:f_B(\bar{q})=s}\frac{\langle B'_{\bar{q}}, J\rangle}{\langle B_s, J\rangle} z_{p\bar{q}} \;\; \forall\, p\in I_A(r),\; q\in I_B(s)\; (1\le r\le d_A,\; 1\le s\le d_B),$$
$$\sum_{p=1}^{d'_A}\sum_{q=1}^{d'_B} z_{pq}A'_p\otimes B'_q \succeq 0,$$
$$z_{pq} = z_{\tilde{p}\tilde{q}} \text{ if } (p\sim_{1A}\tilde{p} \text{ and } q\sim_{1B}\tilde{q}) \text{ or } (p\sim_{2A}\tilde{p} \text{ and } q\sim_{2B}\tilde{q}),$$
$$z\ge 0,$$

where

- *the relations '$\sim_{1A}$' etc. are defined in Definition 19,*
- *f_A and f_B correspond to f in Lemma 9 for the groups $Aut(A)$ and $Aut(B)$ respectively,*
- *for $r\in\{1\ldots,d_A\}$ and $s\in\{1,\ldots,d_B\}$, $I_A(r)=\{p\mid f_A(p)=r\}$, and $I_B(s)=\{q\mid f_B(q)=s\}$.*

If we have algebra $*$-isomorphisms ϕ_A and ϕ_B defined on $\mathcal{A}_{\mathcal{G}_A[1]}$ and $\mathcal{A}_{\mathcal{G}_B[1]}$ respectively, then we may replace the linear matrix inequality $\sum_{p=1}^{d'_A}\sum_{q=1}^{d'_B} z_{pq}A'_p\otimes B'_q\succeq 0$ in the above formulation by $\sum_{p=1}^{d'_A}\sum_{q=1}^{d'_B} z_{pq}\phi_A(A'_p)\otimes\phi_B(B'_q)\succeq 0$. As before, this may lead to smaller, block diagonal matrices in practice.

7 Numerical examples

In this section we will show how the symmetry reduction works for some specific (stQP) and (QAP) problems.

We will first consider maximum stable set problems on symmetric graphs formulated as (stQP) problems, followed by QAP formulations of certain graph partition problems on symmetric graphs.

7.1 Results for (stQP)

An important application of (stQP) is the *maximum stable set problem* in combinatorial optimization. Recall that a stable set of a graph $G = (V, E)$ is a subset of $V' \subset V$ such that no two vertices in V' are adjacent. The stability number $\alpha(G)$ of G is the cardinality of a maximum stable set in G. By the Motzkin-Straus theorem [32], one has

$$\frac{1}{\alpha(G)} = \min_{x \in \Delta} x^{\mathsf{T}}(A + I)x \tag{19}$$

where A is the adjacency matrix of G.

The so-called $\vartheta'(G)$ upper bound on $\alpha(G)$ is defined as

$$\alpha(G) \leq \vartheta'(G) := \max\{\langle J, X\rangle \mid \langle A + I, X\rangle = 1,\ X \in D_{|V|}\},$$

where $D_{|V|}$ is the doubly nonnegative cone in $\mathbb{R}^{|V|\times|V|}$ as before. The $\vartheta'(G)$ bound corresponds to our $(stQP_{SDP+RLT-1})$ bound when applied to problem (19) in the following sense.

Theorem 22 (see Lemma 5.2 in [23])**.** *Let $G = (V, E)$ be a graph with adjacency matrix A, and let $val(G)$ denote the optimal value of $(stQP_{SDP+RLT-1})$ with $Q = A + I$. Then one has $\frac{1}{val(G)} = \vartheta'(G)$.*

A similar results holds for the $(stQP_{SDP+RLT-2})$ bound, since it coincides with the bound $p^{(1)}$, defined in (6), if $Q = A + I$. The reciprocal of this bound was first studied by De Klerk and Pasechnik [23], and was called $\vartheta^{(1)}$ there. To be precise:

$$\alpha(G) \leq \vartheta^{(1)}(G) := \max\{\langle J, X\rangle \mid \langle A + I, X\rangle = 1,\ X \in \mathcal{K}^{*(1)}_{|V|}\}, \tag{20}$$

where the cone $\mathcal{K}^{*(1)}_{|V|}$ is defined in Section 2.1.

Theorem 23. *Let $G = (V, E)$ be a graph with adjacency matrix A, and let $val(G)$ denote the optimal value of $(stQP_{SDP+RLT-2})$ with $Q = A+I$. Then one has $\frac{1}{val(G)} = \vartheta^{(1)}(G)$, where $\vartheta^{(1)}$ is defined in* (20)*.*

Proof. The proof is an immediate consequence of Theorem 2. ∎

The Hamming graph

Consider now the special case where G is the Hamming graph $H_{n,d}$ defined as follows: the vertex set is $\{0, 1\}^n$ (viewed as binary words of length n), and two vertices are adjacent if their Hamming distance is less than d. The stability number of $H_{n,d}$ is mostly denoted by $A(n, d)$, and is of fundamental importance in coding theory. Possibly the most famous upper bound on $A(n, d)$ is the linear programming bound of Delsarte [12], which coincides with $\vartheta'(H_{n,d})$, as was shown by Schrijver [38]. By Theorem 22, the reciprocal of the $(stQP_{SDP+RLT-1})$ bound therefore also coincides with the Delsarte bound. Consequently, the reciprocal of the $(stQP_{SDP+RLT-2})$ bound (i.e. the $\vartheta^{(1)}(H_{n,d})$ bound) is at least as strong as the Delsarte bound (and sometimes stronger; cf Table 1).

Stronger semidefinite programming bounds were introduced by Schrijver [39], and this has led to further improvements in [29] and [16].

The algebraic symmetry of the Hamming graph $H_{n,d}$ is well-understood. For our purposes it is important to note that $\mathcal{A}_{Aut(H_{n,d})}$ is the Bose-Mesner algebra of the Hamming scheme, and $\mathcal{A}_{Aut(H_{n,d})[1]}$ is the Terwilliger algebra of the Hamming scheme. Thus one has $\dim(\mathcal{A}_{Aut(H_{n,d})}) = n+1$, and $\dim(\mathcal{A}_{Aut(H_{n,d})[1]}) = \binom{n+3}{3}$, and bases for these algebras are known in closed form; see e.g., Chapter 3 in [15]. Moreover, the Wedderburn decompositions of both algebras are also known in closed form; see [39] and [15] for details.

We were therefore able to compute the bound $(stQP_{SDP+RLT-2})$ for problem (19) for the graph $H_{n,d}$, and the reciprocal of the bound ($= \vartheta^{(1)}(H_{n,d})$) is shown in Table 1 for some values of (n,d). Our purpose was to show the difference between the bounds obtained by level 1 RLT cuts (the Delsarte bound) and level 2 RLT cuts (the $\vartheta^{(1)}(H_{n,d})$ bound). Note that a few values of $\vartheta^{(1)}(H_{n,d})$ were already reported in the paper [17], namely $(n,d) \in \{(17,4),(17,6),(17,8)\}$, but no details were given there on the symmetry reduction. Our goal here is therefore to compare the bounds for more (and larger) values of (n,d), and also to give details on the symmetry reduction via Theorem 14.

Computation was done on a Dell Precision T7500 workstation with 32GB of RAM memory, using the semidefinite programming solver SDPA-GMP [33].

The column $A(n,d)$ in Table 1 contains the best known upper and lower bounds on $A(n,d)$ as taken from the table maintained by Andries Brouwer at `http://www.win.tue.nl/~aeb/codes/binary-1.html` for $n \le 28$. This table is an update of the table published in [8]; see also [6]. For $n > 28$ the bounds were taken from [31, Appendix A].

n	d	$A(n,d)$	$1/(stQP_{SDP-RLT2})$ $= \vartheta^{(1)}(H_{n,d})$	CPU time (sec)	$1/(stQP_{SDP-RLT1})$ = Delsarte bound
9	4	20	21	1.05	25
13	4	256	278	6.9	292
13	6	32	33	7.37	40
17	8	36	42	39.93	50
22	6	4096–6941	7672	243.69	7,723
22	10	64–84	92	314.65	95
23	10	80–150	151	375.96	151
25	10	192–466	525	865.65	551
26	10	384–836	983	1214.5	1040
25	12	52–55	63	1004.66	75
26	12	64–96	105	1259.57	113
27	12	128–169	170	1251.75	170
28	12	178–288	288	1622.36	288
30	8	2^{16} – 114,398	114,398	3027.44	114,816
30	12	512 – 1,076	1,076	3706.00	1,131
30	14	64 – 117	117	3892.09	129

Table 1: Upper bounds on $A(n,d)$ via RLT level 1 and level 2 cuts. All upper bounds have been rounded down to the nearest integer.

Note that the $\vartheta^{(1)}(H_{n,d})$ bound is stronger than the Delsarte bound [12] for all instances in the table where the Delsarte bound is not tight, but not as strong as the best known bound for $n \le 27$. For the values $(n,d) \in \{(28,12),(30,8),(30,12),(30,14)\}$, $\vartheta^{(1)}(H_{n,d})$ coincides with the strongest known bound. (The sources of the strongest bounds for these cases are given in [6].) Unfortunately, we were not able to find values of (n, d) where $\vartheta^{(1)}(H_{n,d})$ improves on the best known upper bound on $A(n, d)$.

Finally, we wish to emphasize that computing $\vartheta^{(1)}(H_{n,d})$ is intractable without the use of symmetry reduction for all but the smallest values of n and d. This is because the number of vertices in the Hamming graph $H(n, d)$ equals 2^n, and the size of the SDP matrix variables in the original formulation of $\vartheta^{(1)}(H_{n,d})$ would therefore be of the order 2^{2n}.

7.2 Results for QAP

In this section we will present results for maximum and minimum k-section problems on graphs, formulated as QAPs.

Recall that the maximum (resp. minimum) k-section problem, for a graph $G = (V, E)$ on $n = |V|$ vertices and with adjacency matrix A, is to partition the vertices V into k sets of equal cardinality $m := n/k$, such that the number of edges between partitions is a maximum (resp. minimum).

The QAP reformulation of these problems works as follows: consider the adjacency matrix, say B, of $K_{m,\dots,m}$ (with any fixed labeling of the vertices), e.g.

$$B := (J_k - I_k) \otimes J_m. \tag{21}$$

If P is a permutation matrix that defines a re-labeling of the vertices, then the adjacency matrix after re-labeling is $P^T BP$.

The QAP reformulation of max k-section is therefore given by:

$$\frac{1}{2} \max_{P \in \Pi_{|V|}} \operatorname{trace}(AP^{\mathsf{T}} BP), \tag{22}$$

and min k-section is obtained by replacing 'max' by 'min'.

An SDP bound for min/max k-section by Karisch and Rendl [22] is known to coincide with the $(QAP_{SDP+RLT-1})$ bound considered here, as was shown in [13]; see also [45, Theorem 13]. Our goal here is to improve on this bound by computing the stronger $(QAP_{SDP+RLT-2})$ bound.

We will consider min/max k-section problem on strongly regular graphs. Recall that the adjacency matrix A of a strongly regular graph has exactly two distinct eigenvalues associated with eigenvectors orthogonal to the all-ones vector. These eigenvalues are called the *restricted eigenvalues*, and are usually denoted by $r > 0$ and $s < 0$. A strongly regular graph is completely characterized by the values $(n = |V|, \kappa, r, s)$, where κ is the valency of the graph.

For strongly regular graphs, the Karisch and Rendl [22] bound has a closed form expression, as shown in [25]. Since the closed form expression was only derived for the maximum k-section bound in [25], we state the expression here for the minimum k-section bound as well. The proof is similar to that of [25, Theorem 7], and is therefore omitted.

Theorem 24 (cf. Theorem 7 in [25])**.** *Let $G = (V, E)$ be a strongly regular graph with parameters $(n = |V|, \kappa, r, s)$ where r and s are the restricted eigenvalues, and κ is the valency. Let an integer $k > 0$ be given such that $m = n/k$ is integer. The Karisch-Rendl bound on the minimum k-section of G is now given by*

$$|E| \left(1 - \min \left\{ \frac{n - \kappa - 1 - (s + 1)(m - 1)}{-s(n - \kappa - 1) - (s + 1)\kappa}, (m - 1)/\kappa \right\} \right). \tag{23}$$

Similarly, the Karisch-Rendl bound on the maximum k-section of G is given by

$$\frac{1}{2}\min\{(n-m)(\kappa-s),\kappa n\}. \tag{24}$$

Maximum k-section problems in strongly regular graphs are of interest, since they are related to so-called *Hoffman colorings* and *spreads* of these graphs; see [18] for details and definitions.

We first present results for the Higman-Sims graph [20], where

$$(n=|V|,\kappa,r,s)=(100,22,2,-8).$$

The max k-section problem on this graph was studied in [25], and the best known upper bound of max 4-section was obtained there. In particular, it is known that the Higman-Sims graph has a 4-section into four components of five 5-cycles each. Thus there is a 4-section of weight 1000, but this is not known to be a maximum; for more information on this graph, see the discussion on the web page maintained by Andries Brouwer: `http://www.win.tue.nl/~aeb/graphs/Higman-Sims.html`

In Tables 2 and 3 we compare different bounds on various max k-section and min k-section problems on the Higman-Sims graph respectively.

We computed the bound ($QAP_{SDP+RLT-2}$) for the max/min k-section of the Higman-Sims graph for several values of k. In order to do so, we used the symmetry of the Higman-Sims graph described in [25]. Moreover, we used the symmetry of B as described in Example 8.

Computation was done on a PC with 8GB RAM memory and an Intel(R) Core(TM)2 Quad CPU Q9550 processor, using the semidefinite programming solver SeDuMi [46] under Matlab 7 together with the Matlab package YALMIP [30].

k	($QAP_{SDP+RLT-2}$)	CPU time (s)	Karisch-Rendl bound (24)	Bound from [25]	Lower bound
2	750	0.1758	750	750	750
4	1048	0.2253	1100	1098	1006
5	1100	0.2161	1100	1100	1068

Table 2: Different bounds on the max k-section of the Higman-Sims graph.

The lower bounds in Table 2, and the upper bounds in Table 3 were obtained by using a iterative local search QAP heuristic.

k	($QAP_{SDP+RLT-2}$)	CPU time (s)	Karisch-Rendl bound (23)	Upper bound
2	500	0.1623	500	500
4	750	0.2016	750	756
5	800	0.9491	800	800
10	900	0.1951	900	900
20	975	0.2746	950	980
25	1000	0.281	960	1000

Table 3: Different bounds on the min k-section of the Higman-Sims graph.

The ($QAP_{SDP+RLT-2}$) bound gave improvements for max 4-section, min 20-section, and min 25-section. Note that the upper and lower bounds for min 25-section coincide, proving optimality.

Moreover, it is worth noting that the computational time required was less than a second for each instance. (The computational time for the Karisch-Rendl bound is negligible, due to its closed form expression in (23).) This shows that it is indeed possible to compute the ($QAP_{SDP+RLT-2}$) bound when the QAP problem has suitable symmetry.

Similar results are shown in Table 4, for min/max 11-section on another strongly regular graph, namely the Cameron graph [10] with parameters $(n = |V|, \kappa, r, s) = (231, 30, 9, -3)$; see also `http://www.win.tue.nl/~aeb/graphs/Cameron.html` for more details on this graph. The column 'Heuristic' gives the best heuristic solutions that were obtained with the iterative local search heuristic (i.e. the heuristic solution provides a lower bound for the maximization problem and an upper bound for minimization). For the min-11-section problem, the ($QAP_{SDP+RLT-2}$)

min/max	k	($QAP_{SDP+RLT-2}$)	CPU time (s)	Karisch-Rendl bound (23)	Heuristic
min	11	2349	1.7018	2205	2458
max	11	3465	0.8365	3465	3440

Table 4: Different bounds on the min/max 11-section of the Cameron graph.

bound is strictly better than the Karisch-Rendl bound (23). Once again, the computational time required to compute the ($QAP_{SDP+RLT-2}$) bound is of the order of a second after symmetry reduction.

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