

SEMIDEFINITE PROGRAMMING RELAXATIONS FOR THE QUADRATIC ASSIGNMENT PROBLEM*

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Abstract

Semidefinite programming (SDP) relaxations for the quadratic assignment problem (QAP) are derived using the dual of the (homogenized) Lagrangian dual of appropriate equivalent representations of QAP. These relaxations result in the interesting, special, case where only the dual problem of the SDP relaxation has strict interior, i.e. the Slater constraint qualification always fails for the primal problem. Although there is no duality gap in theory, this indicates that the relaxation cannot be solved in a numerically stable way. By exploring the geometrical structure of the relaxation, we are able to find projected SDP relaxations. These new relaxations, and their duals, satisfy the Slater constraint qualification, and so can be solved numerically using primal-dual interior-point methods.

For one of our models, a preconditioned conjugate gradient method is used for solving the large linear systems which arise when finding the Newton direction. The preconditioner is found by exploiting the special structure of the relaxation. See e.g. [41] for a similar approach for solving SDP problems arising from the control applications.

Numerical results are presented which indicate that the described methods yield at least competitive lower bounds.

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1 INTRODUCTION

Semidefinite programming (SDP) has proven to be very successful in providing tight relaxations for hard combinatorial problems, such as the max-cut problem. The quadratic assignment problem (QAP) is a well known *NP*-hard combinatorial problem where problems of dimension $n = 16$ can be considered large. We study SDP relaxations for QAP. In the process we handle several interesting complications that arise, e.g. no constraint qualification for the SDP relaxation and loss of sparsity when solving for the search direction.

1.1 The Quadratic Assignment Problem

The QAP in the trace formulation is

$$(QAP) \quad \mu^* := \min_{X \in \Pi} \text{trace } AXBX^T - 2CX^T,$$

where A, B are real symmetric $n \times n$ matrices, C is a real $n \times n$ matrix, and Π denotes the set of permutation matrices. (We assume $n \geq 4$ to avoid trivialities.) QAP is used to model the

problem of allocating a set of n facilities to a set of n locations while minimizing the quadratic objective arising from the distance between the locations in combination with the flow between the facilities. The QAP is well known to be *NP*-hard [39] and, in practice, problems of moderate sizes, such as $n = 16$, are still considered very hard. For recent surveys on QAP, see the articles Burkard [6], and Rendl, Pardalos, Wolkowicz [30]. An annotated bibliography is given by Burkard and Çela [7].

The QAP is a classic problem that still defies all approaches for its solution and where problems of dimension $n \geq 16$ can be considered large scale. A “Nugent type” test problem of dimension $n = 22$ (based on the problems introduced in [29] and obtainable from QAPLIB [8]) has only recently been solved to optimality by Brügger et al. [1] using high power computing facilities and the classical Gilmore-Lalwer bound (GLB) [13, 26]. The failure to solve larger problems using branch and bound techniques is due mainly to the lack of bounds which are tight and at the same time cheap to compute. Even though GLB is cheap to compute, it is in general not very tight. For solving the Nugent type problem of dimension $n = 22$, more than 48 billion (!) subproblems had to be solved (see [1]).

Stronger bounds based on linear programming relaxations are used by Adams and Johnson [2], and by Resende, Ramakrishnan and Drezner [37]. These are quite expensive to compute and can only be applied to problems of dimension $n \leq 30$. The latter bounds have been applied in branch and bound for instances of dimension $n \leq 15$, see Ramakrishnan, Resende and Pardalos [34]. More recently, Rijal [38], and Jünger and Kaibel [21] studied the QAP polytope and found tighter linear relaxations of QAP.

Another class of lower bounds is the class of eigenvalue bounds which are based on orthogonal relaxations, see e.g. [12, 16, 36, 23]. Even though they are stronger for many (symmetric) problems of dimension $n \geq 20$ and are of reasonable computational cost for all instances in QAPLIB, they are not very well suited for application in branch and bound methods, since their quality deteriorates in lower levels of the branching tree, see Clausen et al. [10].

1.2 Semidefinite Programming

Semidefinite programming is an extension of linear programming where the nonnegativity constraints are replaced by positive semidefiniteness constraints on matrix variables. SDP has been shown to be a very powerful tool in several different areas, e.g. positive definite completion problems, maximum entropy estimation, and bounds for hard combinatorial problems, see e.g. the survey of Vandenberghe and Boyd [42].

Though SDP has been studied in the past, as part of the more general cone programming problem, see e.g. [11, 43], there has been a renewed interest due to the successful applications to discrete optimization [27, 14] and to systems theory [5]. In addition, the relaxations are equivalent to the reformulation and linearization technique, see e.g. the survey discussion in [40], which provides further evidence of successful applications.

1.3 Goals

In this paper we test the efficacy of using semidefinite programming to provide strong relaxations for QAP. We try to address the following questions:

1. How to overcome many interesting numerical and theoretical difficulties, e.g. loss of constraint qualification and loss of sparsity in the optimality conditions?
2. Can the new bound compete with other bounding techniques in speed and quality?
3. Can we improve the bounds or solve existing tough instances of QAP, e.g. the Nugent test problems?
4. Can we improve the bound further by adding new facet inequalities?

1.4 Main Results

Motivated by the numerical and theoretical success of SDP for e.g. the max-cut problem [17, 19, 14, 15], we study SDP relaxations for QAP. These relaxations also prove to be numerically successful. In addition, the relaxation of the linear equality constraints, corresponding to the doubly stochastic property of permutation matrices, implies that the SDP relaxation does not satisfy the Slater constraint qualification. Although there is no duality gap in theory, since the dual does satisfy Slater's constraint qualification, this leads to an unbounded dual optimal solution set. Numerical difficulties can arise when trying to implement interior-point methods, see Example 3.1 below. However, the *minimal face* of the semidefinite cone can be found using the structure of the barycenter of the convex hull of the permutation matrices. In fact, the minimal face is completely defined by the row and column sum property of permutation matrices. Surprisingly, the 0,1 property does not change the minimal face. Then, the primal problem can be projected onto the minimal face. This yields a regularized SDP of smaller dimension.

The special structure of the minimal face can be exploited to find an inexpensive preconditioner. This enables us to solve the large linear system arising from the Newton equation in interior-point methods.

We also present numerical results which indicate that this new approach yields at least competitive bounds.

1.5 Outline

We complete this section with basic notation and some preliminary results. (We include an appendix with a list of notation at the end of the paper.) In Section 2 we derive the SDP relaxations. We initially use the dual of the homogenized Lagrangian dual to get a preliminary relaxation. In Section 3 we study the geometry of the semidefinite relaxation and show how to project onto the minimal face of the relaxation. This guarantees that Slater's constraint qualification holds. This yields a basic semidefinite relaxation which is then tightened by adding additional constraints (in Section 4). We describe practical aspects of applying a primal-dual interior-point method in Section 5. We conclude with our numerical results in Section 6.

1.6 Preliminaries

We work with the space of $t \times t$ *real matrices* denoted \mathcal{M}_t , and the space of $t \times t$ *symmetric matrices* denoted \mathcal{S}_t . $\text{Diag}(v)$ denotes the diagonal matrix formed from the vector v and conversely, (the adjoint of $\text{Diag}(v)$) $\text{diag}(M)$ is the vector of the diagonal elements of the matrix

M ; $\mathcal{R}(M)$, $\mathcal{N}(M)$ denote the *range space* and *null space*, respectively; e is the vector of ones and e_i is the i -th unit vector; E denotes the matrix of ones and $E_{ij} := e_i e_j^T$; $M_{:,t:j}$ refers to the columns t to j of M and $M_{i:s,:}$ refers to the rows i to s of M . The set of matrices with row and column sums one, is denoted by $\mathcal{E} := \{X : Xe = X^T e = e\}$ and is called the set of *assignment constraints*; the set of $(0,1)$ -matrices is denoted by $\mathcal{Z} := \{X : X_{ij} \in \{0,1\}\}$; the set of *nonnegative matrices* is denoted by $\mathcal{N} := \{X : X_{ij} \geq 0\}$; while the set of orthogonal matrices is denoted by $\mathcal{O} := \{X : XX^T = X^T X = I\}$, where I is the identity matrix.

For symmetric matrices $M_1 \preceq M_2$ ($M_1 \prec M_2$) refers to the Löwner partial order, i.e. that $M_1 - M_2$ is negative semidefinite (negative definite, respectively); similar definitions hold for positive semidefinite and positive definite; $V \leq W$, ($V < W$) refers to elementwise ordering of the matrices. The space of symmetric matrices is considered with the trace inner product $\langle M, N \rangle = \text{trace } MN$.

We use the *Kronecker product*, or tensor product, of two matrices, $A \otimes B$, when discussing the quadratic assignment problem QAP; $\text{vec}(X)$ denotes the vector formed from the columns of the matrix X , while $\text{Mat}(x)$ denotes the matrix formed from the vector x . Note that, see e.g. [20],

1. $(A \otimes B)(U \otimes V) = AU \otimes BV$.
2. $\text{vec}(AYB) = (B^T \otimes A)\text{vec}(Y)$.
3. $(A \otimes B)^T = A^T \otimes B^T$.

The *Hadamard product* or elementwise product of two matrices A and B is denoted $A \circ B$.

We partition a symmetric matrix $Y \in \mathcal{S}_{n^2+1}$ into blocks as follows.

$$Y = \left[\begin{array}{c|c} y_{00} & Y_0^T \\ \hline Y_0 & Z \end{array} \right] = \left[\begin{array}{c|ccc} y_{00} & Y^{01} & \dots & Y^{0n} \\ \hline Y^{10} & Y^{11} & \dots & Y^{1n} \\ \vdots & \vdots & \ddots & \vdots \\ Y^{n0} & Y^{n1} & \dots & Y^{nn} \end{array} \right], \quad (1.1)$$

where we use the index 0 for the first row and column. Hence $Y_0 \in \mathbb{R}^{n^2}$, $Z \in \mathcal{S}_{n^2}$, $Y^{pq} \in \mathbb{R}^n$, and $Y^{pq} \in \mathcal{M}_n$. When referring to entry $r, s \in \{1, 2, \dots, n^2\}$ of Z , we also use the pairs $(i, j), (k, l)$ with $i, j, k, l \in \{1, 2, \dots, n\}$. This identifies the element in row $r = (i-1)n + j$ and column $s = (k-1)n + l$ by $Y_{(i,j),(k,l)}$. This notation is going to simplify both the modeling and the presentation of properties of the relaxations. If we consider Z as a matrix consisting of $n \times n$ blocks Y^{ik} , then $Y_{(i,j),(k,l)}$ is just element (j, l) of block (i, k) .

2 SDP and LAGRANGIAN RELAXATION

In this section we present a “first” SDP relaxation for QAP. This comes from “lifting” the problem into a higher dimensional space of symmetric matrices. The QAP is a quadratic $(0,1)$ -problem with additional constraints prescribed by the permutation matrices $X \in \Pi$, which can also be represented by binary vectors $\text{vec}(X)$. The embedding in \mathcal{S}_{n^2+1} is obtained by

$$\begin{pmatrix} 1 \\ \text{vec}(X) \end{pmatrix} (1, \text{vec}(X)^T),$$

which is due to its construction as diadic product a symmetric and positive semidefinite matrix.

However, it is interesting and useful to know that the relaxation comes from the dual of the (homogenized) Lagrangian dual. Thus SDP relaxation is equivalent to Lagrangian relaxation for an appropriately constrained problem. (See also [32].) In the process we see several of the interesting operators that arise in the relaxation. The structure of this SDP relaxation is then used to find the projected relaxation which is the actual one we use for our bounds. As in [32], we see that adding, possibly redundant, quadratic constraints often tightens the SDP relaxation obtained through the Lagrangian dual.

It is well known that the set of permutation matrices Π can be characterized as the intersection of $(0,1)$ -matrices with \mathcal{E} and \mathcal{O} , i.e.

$$\Pi = \mathcal{E} \cap \mathcal{Z} = \mathcal{O} \cap \mathcal{Z}, \quad (2.1)$$

see e.g. [16]. Therefore, we can rewrite QAP as

$$(QAP_{\mathcal{E}}) \quad \begin{aligned} \mu^* := \min \quad & \text{trace } AXBX^T - 2CX^T \\ \text{s.t.} \quad & XX^T = X^T X = I \\ & Xe = X^T e = e \\ & X_{ij}^2 - X_{ij} = 0, \quad \forall i, j. \end{aligned}$$

We can see that there are a lot of redundant constraints in $(QAP_{\mathcal{E}})$. However, as we show below, they are not necessarily redundant in the SDP relaxations.

Additional redundant (but useful in the relaxation) constraints will be added below, e.g. we can use the fact that the rank-one matrices formed from the columns of X , i.e. $X_{:i}X_{:j}^T$, are diagonal matrices if $i = j$; while their diagonals are 0 if $i \neq j$.

2.1 The Direct Approach to SDP Relaxation

We first show how the SDP relaxation can be obtained directly from QAP. This involves *lifting* the vector $x = \text{vec}(X)$ into the matrix space S_{n^2+1} .

We now outline this for the quadratic constraints that arise from the fact that X is a $(0,1)$, orthogonal matrix. Let $X \in \Pi_n$ be a permutation matrix and, again, let $x = \text{vec}(X)$ and $c = \text{vec}(C)$. Then the objective function for QAP is

$$\begin{aligned} q(X) &= \text{trace } AXBX^T - 2CX^T \\ &= x^T(B \otimes A)x - 2c^T x \\ &= \text{trace } xx^T(B \otimes A) - 2c^T x \\ &= \text{trace } L_Q Y_X, \end{aligned}$$

where we define the $(n^2 + 1) \times (n^2 + 1)$ matrices

$$L_Q := \begin{bmatrix} 0 & -\text{vec}(C)^T \\ -\text{vec}(C) & B \otimes A \end{bmatrix}, \quad (2.2)$$

and

$$Y_X := \begin{bmatrix} x_0 & x^T \\ x & xx^T \end{bmatrix}. \quad (2.3)$$

This shows how the objective function of QAP is transformed into a linear function in the SDP relaxation; where we have added the constraint $(Y_X)_{00} = 1$. Note that if we denote $Y = Y_X$, then the element $Y_{(i,j),(k,l)}$ corresponds to $x_{ij}x_{kl}$.

We already have three constraints on the matrix Y , i.e. it is positive semidefinite, the top-left component $y_{00} = 1$, and it is rank-one. The first two constraints are tractable constraints; while the rank-one constraint is too hard to satisfy and is discarded in the SDP relaxation.

In order to guarantee that the matrix Y , in the case that it is rank one, arises from a permutation matrix X , we need to add additional constraints. For example, the (0,1)-constraints $X_{ij}^2 - x_0 X_{ij} = 0$ are equivalent to the restriction that the diagonal of Y is equal to its first row (or column). This results in the arrow constraint, see (2.15) below. Similarly, the orthogonality constraint, $XX^T = I$ can be written as

$$XX^T = \sum_{k=1}^n X_{:k} X_{:k}^T = I.$$

Each rank-one matrix in the sum is a diagonal $n \times n$ block of Y , i.e. we get the block diagonal constraint, see (2.16). Similarly, the orthogonality constraint written as $X^T X = I$ results in the block off diagonal constraints, see (2.17). The SDP relaxation with these constraints, as well as the ones arising from the row and column sums equal 1, is given below in (2.14). Also, we will see below that the SDP relaxation is exact if we do not relax the rank-one constraint on Y . (See Theorem 2.1.)

2.2 Lagrangian Relaxation

In this section we will investigate the relaxation of the constraints in $(QAP_{\mathcal{E}})$ via Lagrangian duality. We show that the dual of the Lagrangian dual results in an SDP relaxation. Also, there is no duality gap between the Lagrangian relaxation and its dual, so solving the SDP relaxation is equivalent to solving the Lagrangian relaxation. Though SDP relaxations can be obtained more simply in a direct fashion, once the form of the relaxation is known, it is important to know where the relaxation comes from in order to recover good approximate feasible solutions. More precisely, we can use the optimal solution of the dual of the SDP in the Lagrangian relaxation of $(QAP_{\mathcal{E}})$ and then find the optimal matrix X where this Lagrangian attains its minimum. This X is then a good approximation for the original QAP, see [25].

After changing the row and column sum constraints into $\|Xe - e\|^2 + \|X^T e - e\|^2 = 0$ we consider the following equivalent problem to QAP.

$$(QAP_{\mathcal{O}}) \quad \begin{aligned} \mu_{\mathcal{O}} := \min \quad & \text{trace } AXBX^T - 2CX^T \\ \text{s.t.} \quad & XX^T = I \\ & X^T X = I \\ & \|Xe - e\|^2 + \|X^T e - e\|^2 = 0 \\ & X_{ij}^2 - X_{ij} = 0, \quad \forall i, j. \end{aligned}$$

We first add the (0,1) and row-column sum constraints to the objective function using Lagrange multipliers W_{ij} and u_0 respectively.

$$\mu_{\mathcal{O}} = \min_{XX^T = X^T X = I} \max_{W, u_0} \{ \text{trace } AXBX^T - 2CX^T + \sum_{ij} W_{ij} (X_{ij}^2 - X_{ij}) + u_0 (\|Xe - e\|^2 + \|X^T e - e\|^2) \}. \quad (2.4)$$

Interchanging min and max yields

$$\mu_{\mathcal{O}} \geq \mu_{\mathcal{L}} := \max_{W, u_0} \min_{XX^T = X^T X = I} \{ \text{trace } AXBX^T - 2CX^T + \sum_{ij} W_{ij}(X_{ij}^2 - X_{ij}) + u_0(\|Xe - e\|^2 + \|X^T e - e\|^2) \}. \quad (2.5)$$

We now continue with the relaxation and homogenize the objective function by multiplying by a constrained scalar x_0 and increasing the dimension of the problem by 1. We homogenize the problem since that simplifies the transition to a semidefinite programming problem.

$$\mu_{\mathcal{O}} \geq \mu_{\mathcal{L}} = \max_W \min_{XX^T = X^T X = I, x_0^2 = 1} \{ \text{trace } [AXBX^T + W(X \circ X)^T + u_0(\|Xe\|^2 + \|X^T e\|^2) - x_0(2C + W)X^T] - 2x_0 u_0 e^T (X + X^T)e + 2nu_0 \}. \quad (2.6)$$

Introducing a Lagrange multiplier w_0 for the constraint on x_0 and Lagrange multipliers S_b for $XX^T = I$ and S_o for $X^T X = I$ we get the lower bound μ_R

$$\mu_{\mathcal{O}} \geq \mu_{\mathcal{L}} \geq \mu_R := \max_{W, S_b, S_o, u_0, w_0} \min_{X, x_0} \{ \text{trace } [AXBX^T + u_0(\|Xe\|^2 + \|X^T e\|^2) + W(X \circ X)^T + w_0 x_0^2 + S_b XX^T + S_o X^T X] - \text{trace } x_0(2C + W)X^T - 2x_0 u_0 e^T (X + X^T)e - w_0 - \text{trace } S_b - \text{trace } S_o + 2nu_0 \}. \quad (2.7)$$

Both inequalities can be strict, i.e. there can be duality gaps in each of the Lagrangian relaxations. Following is an example of a duality gap that arises from the Lagrangian relaxation of the orthogonality constraint.

Example 2.1 Consider the the pure quadratic, orthogonally constrained problem

$$\mu^* := \min_{s.t.} \text{trace } AXBX^T \quad XX^T = I, \quad (2.8)$$

with 2×2 matrices

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad B = \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix}.$$

The dual problem is

$$\mu^D := \max_{s.t.} -\text{trace } S \quad (B \otimes A + I \otimes S) \succeq 0 \quad S = S^T. \quad (2.9)$$

Then $\mu^* = 10$. But is the dual optimal value μ^D also 10? We have

$$B \otimes A = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 8 \end{pmatrix}.$$

Then in order to satisfy dual feasibility, we must have $S_{11} \geq -3$ and $S_{22} \geq -6$. In order to maximize the dual, equality must hold. Therefore $-\text{trace } S = 9$ in the optimum. Thus we have duality gap for this simple example.

In (2.7), we grouped the quadratic, linear, and constant terms together. We now define $x := \text{vec}(X)$, $y^T := (x_0, x^T)$ and $w^T := (w_0, \text{vec}(W)^T)$ and get

$$\mu_R = \max_{w, S_b, S_o, u_0} \min_y \{y^T [L_Q + \text{Arrow}(w) + \text{B}^0\text{Diag}(S_b) + \text{O}^0\text{Diag}(S_o) + u_0 D] y - w_0 - \text{trace } S_b - \text{trace } S_o\}, \quad (2.10)$$

where L_Q is as above and the linear operators

$$\text{Arrow}(w) := \begin{bmatrix} w_0 & -\frac{1}{2}w_{1:n^2}^T \\ -\frac{1}{2}w_{1:n^2} & \text{Diag}(w_{1:n^2}) \end{bmatrix}, \quad (2.11)$$

$$\text{B}^0\text{Diag}(S) := \begin{bmatrix} 0 & 0 \\ 0 & I \otimes S_b \end{bmatrix}, \quad (2.12)$$

$$\text{O}^0\text{Diag}(S) := \begin{bmatrix} 0 & 0 \\ 0 & S_o \otimes I \end{bmatrix}, \quad (2.13)$$

and

$$D := \begin{bmatrix} n & -e^T \otimes e^T \\ -e \otimes e & I \otimes E \end{bmatrix} + \begin{bmatrix} n & -e^T \otimes e^T \\ -e \otimes e & E \otimes I \end{bmatrix}.$$

There is a hidden semidefinite constraint in (2.10), i.e. the inner minimization problem is bounded below only if the Hessian of the quadratic form is positive semidefinite. In this case the quadratic form has minimum value 0. This yields the following SDP.

$$(D_{\mathcal{O}}) \quad \begin{array}{ll} \max & -w_0 - \text{trace } S_b - \text{trace } S_o \\ \text{s.t.} & L_Q + \text{Arrow}(w) + \text{B}^0\text{Diag}(S_b) + \text{O}^0\text{Diag}(S_o) + u_0 D \succeq 0. \end{array}$$

We now obtain our desired SDP relaxation of $(QAP_{\mathcal{O}})$ as the Lagrangian dual of $(D_{\mathcal{O}})$. We introduce the $(n^2 + 1) \times (n^2 + 1)$ dual matrix variable $Y \succeq 0$ and derive the dual program to the SDP $(D_{\mathcal{O}})$.

$$(SDP_{\mathcal{O}}) \quad \begin{array}{ll} \min & \text{trace } L_Q Y \\ \text{s.t.} & \text{b}^0\text{diag}(Y) = I, \quad \text{o}^0\text{diag}(Y) = I \\ & \text{arrow}(Y) = e_0, \quad \text{trace } DY = 0 \\ & Y \succeq 0, \end{array} \quad (2.14)$$

where the *arrow operator*, acting on the $(n^2 + 1) \times (n^2 + 1)$ matrix Y , is the adjoint operator to $\text{Arrow}(\cdot)$ and is defined by

$$\text{arrow}(Y) := \text{diag}(Y) - (0, (Y_{0,1:n^2})^T), \quad (2.15)$$

i.e. the arrow constraint guarantees that the diagonal and 0-th row (or column) are identical.

The *block-0-diagonal operator* and *off-0-diagonal operator* acting on Y are defined by

$$\text{b}^0\text{diag}(Y) := \sum_{k=1}^n Y_{(k,\cdot),(k,\cdot)} \quad (2.16)$$

and

$$\text{o}^0 \text{diag}(Y) := \sum_{k=1}^n Y_{(\cdot,k),(\cdot,k)}. \quad (2.17)$$

These are the adjoint operators of $\text{B}^0 \text{Diag}(\cdot)$ and $\text{O}^0 \text{Diag}(\cdot)$, respectively. The block-0-diagonal operator guarantees that the sum of the diagonal blocks equals the identity. The off-0-diagonal operator guarantees that the trace of each diagonal block is 1, while the trace of the off-diagonal blocks is 0. These constraints come from the orthogonality constraints, $XX^T = I$ and $X^T X = I$, respectively.

We have expressed the orthogonality constraints with both $XX^T = I$ and $X^T X = I$. It is interesting to note that this redundancy adds extra constraints into the relaxation which are not redundant. These constraints reduce the size of the feasible set and so tighten the bounds.

Proposition 2.1 *Suppose that Y is feasible for the SDP relaxation (2.14). Then Y is singular.*

Proof. Note that $D \neq 0$ is positive semidefinite. Therefore Y has to be singular in order to satisfy the constraint $\text{trace } DY = 0$.

□

This means that the feasible set of the primal problem ($\text{SDP}_{\mathcal{O}}$) has no interior. It is not difficult to find an interior-point for the dual ($D_{\mathcal{O}}$), which means that Slater's constraint qualification (strict feasibility) holds for ($D_{\mathcal{O}}$). Therefore ($\text{SDP}_{\mathcal{O}}$) is attained and there is no duality gap in theory, for the usual primal-dual pair. However, if Slater's constraint qualification fails, then this is not the proper dual, since perturbations in the right-hand-side will not result in the dual value. This is because we cannot stay exactly feasible in the dual, $\succeq 0$, since the interior is empty, see [35]. In fact we may never attain the supremum of ($D_{\mathcal{O}}$), which may cause instability when implementing any kind of interior-point method. Since Slater's constraint qualification fails for the primal, the set of optimal solutions of the dual is an unbounded set, and an interior-point method may never converge. Therefore we have to express the feasible set of ($\text{SDP}_{\mathcal{O}}$) in some lower dimensional space. We study this below when we project the problem onto a face of the semidefinite cone.

However, if we add the rank-one condition, then the relaxation is exact.

Theorem 2.1 *Suppose that Y is restricted to be rank-one in ($\text{SDP}_{\mathcal{O}}$), i.e. $Y = \begin{pmatrix} 1 \\ x \end{pmatrix} (1 \ x^T)$,*

for some $x \in \mathbb{R}^{n^2}$. Then the optimal solution of ($\text{SDP}_{\mathcal{O}}$) provides the permutation matrix $X = \text{Mat}(x)$ that solves the QAP.

Proof. The arrow-constraint in ($\text{SDP}_{\mathcal{O}}$) guarantees that the diagonal of Y is 0 or 1. The 0-diagonal and assignment constraint now guarantee that $\text{Mat}(x)$ is a permutation matrix. Therefore the optimization is over the permutation matrices and so the optimum of QAP is obtained.

□

3 GEOMETRY of the RELAXATION

We define $F_{\mathcal{O}}$ to be the feasible set of the semidefinite relaxation ($\text{SDP}_{\mathcal{O}}$). There are two difficulties regarding our feasible set $F_{\mathcal{O}}$. It is easy to see that there are redundant constraints

in $(SDP_{\mathcal{O}})$. The other difficulty is that $F_{\mathcal{O}}$ has no positive definite feasible point. Hence, the optimal set of the dual is unbounded and we cannot apply an (feasible or infeasible) interior-point method directly. In fact, the dual can be unattained.

Example 3.1 Consider the SDP pair

$$(P) \quad \begin{array}{ll} \min & 2X_{12} \\ \text{s.t.} & \text{diag}(X) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ & X \succeq 0 \end{array} \quad (D) \quad \begin{array}{ll} \max & y_2 \\ \text{s.t.} & \begin{bmatrix} y_1 & 0 \\ 0 & y_2 \end{bmatrix} \preceq \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \end{array}$$

Slater's condition holds for the dual but not for the primal. The optimal value for both is 0. The primal is attained, but the dual is not.

3.1 The Minimal Face

In order to overcome the above difficulties, we need to explore the geometrical structure of $F_{\mathcal{O}}$. It is easy to see that

$$Y_X := \begin{pmatrix} 1 \\ \text{vec}(X) \end{pmatrix} (1 \ \text{vec}(X)^T), \quad X \in \Pi$$

are feasible points of $F_{\mathcal{O}}$. Moreover, these points are rank-one matrices and are, therefore, contained in the set of extreme points of $F_{\mathcal{O}}$, see e.g. Pataki [31]. We need only consider faces of $F_{\mathcal{O}}$ which contain all of these extreme points. Therefore we are only interested in the *minimal face*, which is the intersection of all these faces.

We need to take a closer look at the assignment (row and column sums) constraints defined by \mathcal{E} .

Surprisingly, it is only these constraints that are needed to define the minimal face. (This is not true in general, see Example 3.2 below.) Alternatively, we can describe these constraints as follows. With $x = \text{vec}(X)$, the constraints are

$$X^T e = e \iff \begin{bmatrix} e^T & 0 & \dots & \dots & 0 \\ 0 & e^T & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & 0 & e^T \end{bmatrix} x = e$$

and

$$X e = e \iff \begin{bmatrix} I & I & \dots & \dots & I \end{bmatrix} x = e.$$

Thus, the assignment constraints are equivalent to

$$T x = e,$$

where

$$T := \begin{bmatrix} I \otimes e^T \\ e^T \otimes I \end{bmatrix}. \quad (3.1)$$

We now multiply with x^T from the right and use the fact that x is a binary vector. We get

$$Txx^T = e(\text{diag}(xx^T))^T,$$

and also

$$T\text{diag}(xx^T) = e.$$

These two conditions are equivalent to

$$\hat{T}Y_X = 0, \tag{3.2}$$

where $\hat{T} := [-e|T]$; and (3.2) now corresponds to the embedding of the assignment constraints into \mathcal{S}_{n^2+1} .

Before we characterize the minimal face of $F_{\mathcal{O}}$ we define the following $(n^2+1) \times ((n-1)^2+1)$ matrix.

$$\hat{V} := \left[\begin{array}{c|c} 1 & 0 \\ \hline \frac{1}{n}(e \otimes e) & V \otimes V \end{array} \right], \tag{3.3}$$

where V is an $n \times (n-1)$ matrix containing a basis of the orthogonal complement of e , i.e. $V^T e = 0$. Our choice for V is

$$V := \left[\begin{array}{c} I_{n-1} \\ -e_{n-1}^T \end{array} \right].$$

In fact, \hat{V} is a basis of the null space of \hat{T} , i.e. $\hat{T}\hat{V} = 0$.

The following theorem characterizes the minimal face by finding the barycenter of the convex hull of the permutation matrices. The barycenter has a very simple and elegant structure.

Theorem 3.1 *Define the barycenter*

$$\hat{Y} := \frac{1}{n!} \sum_{X \in \Pi_n} Y_X. \tag{3.4}$$

Then:

1. \hat{Y} has a 1 in the $(0,0)$ position and n diagonal $n \times n$ blocks with diagonal elements $1/n$. The first row and column equal the diagonal. The rest of the matrix is made up of $n \times n$ blocks with all elements equal to $1/(n(n-1))$ except for the diagonal elements which are 0.

$$\hat{Y} = \left[\begin{array}{c|c} 1 & \frac{1}{n}e^T \\ \hline \frac{1}{n}e & \left[\frac{1}{n^2}E \otimes E \right] + \left[\frac{1}{n^2(n-1)}(nI - E) \otimes (nI - E) \right] \end{array} \right].$$

2. The rank of \hat{Y} is given by

$$\text{rank}(\hat{Y}) = (n-1)^2 + 1.$$

3. The n^2+1 eigenvalues of \hat{Y} are given in the vector

$$\left(2, \frac{1}{n-1}e_{(n-1)^2}^T, 0e_{2n-1}^T \right)^T.$$

4. The null space and range space are

$$\mathcal{N}(\hat{Y}) = \mathcal{R}(\hat{T}^T) \text{ and } \mathcal{R}(\hat{Y}) = \mathcal{R}(\hat{V}) \text{ (so that } \mathcal{N}(\hat{T}) = \mathcal{R}(\hat{V}) \text{)}.$$

Proof. Fix $X \in \Pi$ and let

$$Y = Y_X = \begin{pmatrix} 1 \\ \text{vec}(X) \end{pmatrix} (1 \text{ vec}(X)^T).$$

We now proceed to find the structure of \hat{Y} . Consider the entries of the 0th row of Y . Since $Y_{0,(i-1)n+j} = 1$ means i is assigned to j , there are $(n-1)!$ such permutations. We conclude that the components of the 0 row (and column) of \hat{Y} are given by

$$\hat{Y}_{0,(i-1)n+j} = \frac{1}{n!}(n-1)! = \frac{1}{n}.$$

Now consider the entries of Y in the other rows, denoted $Y_{(p,q),(i,j)}$.

- i) If $p = i$ and $q = j$, then $Y_{(p,q),(i,j)} = 1$ means that i is assigned to j and there are $(n-1)!$ such permutations. Therefore the diagonal elements are

$$\hat{Y}_{(i,j),(i,j)} = \frac{1}{n!}(n-1)! = \frac{1}{n}.$$

- ii) Now suppose that $p \neq i$ and $q \neq j$, i.e. the element is an off-diagonal element in an off-diagonal block. Then $Y_{(p,q),(i,j)} = 1$ means that i is assigned to j and p is assigned to q . Since there are $(n-2)!$ such permutations, we get that

$$\hat{Y}_{(p,q),(i,j)} = \frac{1}{n!}(n-2)! = \frac{1}{n(n-1)}.$$

- iii) Otherwise, suppose that $p = i$ or $q = j$, but not both, i.e. we consider the off-diagonal elements of the diagonal blocks and the diagonal elements of the off-diagonal blocks. By the property of permutation matrices, these elements must all be 0, i.e. they correspond to the off-diagonal elements of $X_{:j} \circ X_{:j}^T$ and the diagonal elements of elements of $X_{:q} \circ X_{:j}^T$, $q \neq j$.

This proves the representation of \hat{Y} in 1.

Let us find the rank and eigenvalues of \hat{Y} . We partition

$$\hat{Y} = \begin{bmatrix} 1 & \frac{1}{n}e^T \\ \frac{1}{n}e & Z \end{bmatrix},$$

thus defining the block Z . We have

$$\begin{bmatrix} 1 & 0 \\ \frac{1}{n}e & I \end{bmatrix} \hat{Y} \begin{bmatrix} 1 & \frac{1}{n}e^T \\ 0 & I \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & S \end{bmatrix}, \quad (3.5)$$

where $S = Z - \frac{1}{n^2}E$. As a result, we have

$$\text{rank}(\hat{Y}) = 1 + \text{rank}(S).$$

From the structure of \hat{Y} , we see that

$$S = \frac{1}{n^2(n-1)}(nI_{n-1} - E) \otimes (nI_{n-1} - E).$$

The eigenvalues of $nI_{n-1} - E$ are n (with multiplicity $n-1$) and 0 . By the fact that the eigenvalues of a Kronecker product are found from the Kronecker product of eigenvalues, we have that the eigenvalues of S are $1/(n-1)$ (with multiplicity $(n-1)^2$) and 0 (with multiplicity $2n-1$). Therefore, we have

$$\text{rank}(\hat{Y}) = 1 + \text{rank}(S) = (n-1)^2 + 1.$$

This proves 2.

By (3.5) and the rank, we see that the eigenvalues of \hat{Y} are $1/(n-1)$ (with multiplicity $(n-1)^2$) and 2 and 0 (with multiplicity $2n-1$). This proves 3.

Note that

$$u \in \mathcal{N}(S) \Leftrightarrow \begin{pmatrix} -\frac{1}{n}e^T u \\ u \end{pmatrix} \in \mathcal{N}(\hat{Y}). \quad (3.6)$$

It is well known that $\text{rank}(T) = 2n-1$ and we can verify that $ST^T = 0$. So we have

$$\mathcal{N}(\hat{Y}) = \left\{ \begin{pmatrix} -\frac{1}{n}e^T u \\ u \end{pmatrix} : u \in \mathcal{R}(T^T) \right\}.$$

In addition, we can now verify that

$$\hat{V}^T \begin{pmatrix} -\frac{1}{n}e^T u \\ u \end{pmatrix} = 0 \text{ for } u \in \mathcal{R}(T^T).$$

This proves 4. □

With the above characterization of the barycenter, we can find the minimal face of \mathcal{P} that contains the feasible set of the relaxation SDP. We let $t(n) := \frac{n(n+1)}{2}$.

Corollary 3.1 *The dimension of the minimal face is $t((n-1)^2 + 1)$. Moreover, the minimal face can be expressed as $\hat{V} \mathcal{S}_{(n-1)^2+1} \hat{V}^T$.*

The above characterization of the barycenter yields a characterization of the minimal face. At first glance it appears that there would be a simpler proof for this characterization, the proof would use only the row and column sums constraints. Finding the barycenter is the key in exploiting the geometrical structure of a given problem with an assignment structure. However, it is not always true that the other constraints in the relaxation are redundant, as the following shows.

Example 3.2 Consider the constraints

$$\begin{array}{rcccc} x_1 & & & & = 1 \\ x_1 & +x_2 & +x_3 & +x_4 & = 1 \\ x_1, & x_2, & x_3, & x_4 & \geq 0 \end{array}$$

The only solution is $(1, 0, 0, 0)$. Hence the barycenter of the relaxation is the set with only a rank one matrix in it. However, the null space of the above system has dimension 3. Thus the projection using the null space yields a minimal face with matrices of dimension greater than 1.

3.2 The Projected SDP Relaxation

In Theorem 3.1, we presented explicit expressions for the range and null space of the barycenter, denoted \hat{Y} . It is well known, see e.g. [4], that the faces of the positive semidefinite cone are characterized by the nullspace of points in their relative interior, i.e. \mathcal{K} is a face if

$$\mathcal{K} = \{X \succeq 0 : \mathcal{N}(X) \supset S\} = \{X \succeq 0 : \mathcal{R}(X) \subset S^\perp\},$$

and

$$\text{relint } \mathcal{K} = \{X \succeq 0 : \mathcal{N}(X) = S\} = \{X \succeq 0 : \mathcal{R}(X) = S^\perp\},$$

where S is a given subspace. In particular, if $\hat{X} \in \text{relint } \mathcal{K}$, the matrix V is $n \times k$, and $\mathcal{R}(V) = \mathcal{R}(\hat{X})$, then

$$\mathcal{K} = V\mathcal{P}_k V^T.$$

Therefore, using \hat{V} in Theorem 3.1, we can project the SDP relaxation $(SDP_{\mathcal{O}})$ onto the minimal face. The projected problem is

$$(QAP_{R1}) \quad \begin{array}{ll} \mu_{R1} := \min & \text{trace}(\hat{V}^T L_Q \hat{V})R \\ \text{s.t.} & \text{b}^0 \text{diag}(\hat{V}R\hat{V}^T) = I, \quad \text{o}^0 \text{diag}(\hat{V}R\hat{V}^T) = I \\ & \text{arrow}(\hat{V}R\hat{V}^T) = e_0, \quad R \succeq 0 \end{array} \quad (3.7)$$

Note that the constraint $\text{trace}(\hat{V}^T D\hat{V})R = 0$ can be dropped since it is always satisfied, i.e. $D\hat{V} = 0$. We are going to refer to (QAP_{R1}) as the *basic relaxation* of QAP.

By construction, this program satisfies the generalized Slater constraint qualification for both primal and dual. Therefore there will be no duality gap, the optimal solutions are attained for both primal and dual, and both the primal and dual optimal solution sets are bounded.

Using the fact that $\hat{T}\hat{V} = 0$, we get the following lemma which gives some interesting properties of matrices of the form $\hat{V}R\hat{V}^T$, i.e. of matrices in the span of the minimal face. These properties are closely related to the row and column sums equal 1 constraints. We will see below that these properties cause some of the other constraints to be redundant in the SDP relaxation.

Lemma 3.1 Let $R \in \mathcal{S}_{(n-1)^2+1}$ be arbitrary and let

$$Y = \hat{V}R\hat{V}^T,$$

where \hat{V} is given in (3.3). Then, using the block notation of (1.1), we have

- a) $y_{00} = r_{00}$, $Y^{0j}e = r_{00}$, and $\sum_{j=1}^n Y^{0j} = r_{00}e^T$.
- b) $Y^{0j} = e^T Y^{ij}$, for $i, j = 1, \dots, n$.
- c) $\sum_{i=1}^n Y^{ij} = eY^{0j}$ and $\sum_{i=1}^n \text{diag}(Y^{ij}) = Y^{j0}$, for $j = 1, \dots, n$.

Proof. We can verify that $y_{00} = r_{00}$ from the definitions. Using the fact that $\hat{T}\hat{V} = \begin{bmatrix} -e & | & T \end{bmatrix} \hat{V} = 0$, we have

$$\hat{T}Y = \hat{T}\hat{V}R\hat{V}^T = 0.$$

The rest of the proof follows from expanding $\hat{T}Y = 0$. □

The projection eliminates the constraints $\hat{T}Y = 0$. After the projection, one problem remains. There are still redundant constraints in the relaxation. This creates unnecessary complications when applying interior-point methods, i.e. the linear systems do not necessarily have unique solutions. But, using Lemma 3.1, we can observe that in the basic relaxation (QAP_{R1}) parts of the block-0-diag and off-0-diag operators are redundant. This is because the implicit presence of the assignment constraints in combination with the arrow operator forces $y_{00} = 1$. The main diagonal elements of the images of both operators are equal to one automatically. Part b) of Lemma 3.1 relates the row sums of the diagonal blocks to the corresponding parts of the 0 column of Y . Therefore the sum of the diagonal blocks has row sums equal to one, which makes one additional element per row dependent. The same can be observed for the off-0-diag operator. The dimension of the image space of both operators now reduces to $(n^2 - 3n)/2$. We assume from now on that the operators are defined such that they cover only a set of $(n^2 - 3n)/2$ linearly independent equalities.

4 TIGHTENING THE RELAXATION

4.1 The Gangster Operator

The feasible set of the SDP relaxation is convex but not polyhedral. It contains the set of matrices of the form Y_X corresponding to the permutation matrices $X \in \Pi$. But the SDP relaxations, discussed above, can contain many points that are not in the affine hull of these Y_X . In particular, it can contain matrices with nonzeros in positions that are zero in the affine hull of the Y_X . We can therefore strengthen the relaxation by adding constraints corresponding to these zeros.

Note that the barycenter \hat{Y} is in the relative interior of the feasible set. Therefore the null space of \hat{Y} determines the dimension of the minimal face which contains the feasible set. However, the dimension of the feasible set can be (and is) smaller. We now take a closer look at the structure of \hat{Y} to determine the 0 entries. The relaxation is obtained from

$$Y_X = \begin{pmatrix} 1 \\ \text{vec}(X) \end{pmatrix} (1 \text{ vec}(X)^T)$$

$$= \begin{pmatrix} 1 \\ X_{:1} \\ X_{:2} \\ \vdots \\ X_{:n} \end{pmatrix} (1 \ X_{:1}^T \ X_{:2}^T \ \vdots \ X_{:n}^T)$$

which contains the n^2 blocks

$$(X_{:i} X_{:j}^T).$$

We then have

$$\text{diag}(X_{:i} X_{:j}^T) = X_{:i} \circ X_{:j} = 0, \text{ if } i \neq j,$$

and

$$X_{:i} \circ X_{:j} = 0, \text{ if } i \neq j,$$

i.e. the diagonal of the off-diagonal blocks are identically zero and the off-diagonal of the diagonal blocks are identically zero. These are exactly the zeros of the barycenter \hat{Y} .

The above description defines the so-called gangster operator. Let $J \subset \{(i, j) : 1 \leq i, j \leq n^2 + 1\}$. The operator $\mathcal{G}_J : \mathcal{S}_{n^2+1} \rightarrow \mathcal{S}_{n^2+1}$ is called the *Gangster* operator. For matrix Y , and $i, j = 1, \dots, n^2 + 1$, the ij component of the image of the gangster operator is defined as

$$(\mathcal{G}_J(Y))_{ij} := \begin{cases} Y_{ij} & \text{if } (i, j) \in J \\ 0 & \text{otherwise.} \end{cases} \quad (4.1)$$

The subspace of $(n^2 + 1) \times (n^2 + 1)$ symmetric matrices with nonzero index set J is denoted \mathcal{S}_J , i.e.,

$$\mathcal{S}_J := \{X \in \mathcal{S}_{n^2+1} : X_{ij} = 0 \text{ if } (i, j) \notin J\}.$$

From the definition of the gangster operator, we can easily see the following.

$$\mathcal{R}(\mathcal{S}_J) = \mathcal{S}_J$$

and

$$\mathcal{N}(\mathcal{S}_{-J}) = \mathcal{S}_{-J},$$

where $-J$ is denoted as the complementary set of J . Therefore, let $J = \{(i, j) : \hat{Y}_{ij} = 0\}$, be the zeros found above using the Hadamard product, we have

$$\mathcal{G}_J(\hat{Y}) = 0. \quad (4.2)$$

Thus the gangster operator, acting on a matrix Y , shoots holes (zeros) through the matrix Y in the positions where \hat{Y} is not zero. For any permutation matrix $X \in \Pi$, the matrix Y_X has all its entries either 0 or 1; and \hat{Y} is just a convex combination of all these matrices Y_X for $X \in \Pi$. Hence, from (4.2), we have

$$\mathcal{G}_J(Y_X) = 0, \text{ for all } X \in \Pi.$$

Therefore, we can further tighten our relaxation by adding the constraint

$$\mathcal{G}_J(Y) = 0. \quad (4.3)$$

Note that the adjoint equation

$$\text{trace}(\mathcal{G}_J^*(Z)Y) = \text{trace}(Z\mathcal{G}_J(Y)),$$

implies that the gangster operator is self-adjoint, i.e.

$$\mathcal{G}_J^* = \mathcal{G}_J.$$

4.2 The Gangster Operator and Redundant Constraints

The addition of the gangster operator provides a tighter SDP relaxation. Moreover, it makes many of the existing constraints redundant. We now add the gangster operator and remove all redundant constraints. We maintain the notation from Theorem 3.1.

Suppose that we have added the gangster operator constraint to the projected problem (QAP_{R1}) , i.e. $\mathcal{G}(\hat{V}R\hat{V}^T) = 0$. From Lemma 3.1, if $Y = \hat{V}R\hat{V}^T$, then we have

$$Y^{0j} = e^T Y^{jj} \text{ for } j = 1, \dots, n.$$

Note that the off-diagonal entries for each Y^{jj} are zero. Therefore it follows that the arrow operator is redundant. Furthermore, by part *a*) of Lemma 3.1, we can see that the block-diag operator is redundant. Similarly, the off-block-diag operator is redundant.

We now define a subset \hat{J} of J , of indices of Y , (a union of two sets)

$$\begin{aligned} \hat{J} := & \{(i, j) : i = (p-1)n + q, j = (p-1)n + r, q \neq r\} \cup \\ & \{(i, j) : i = (p-1)n + q, j = (r-1)n + q, p \neq r, (p, r \neq n), \\ & \quad ((r, p), (p, r) \neq (n-2, n-1), (n-1, n-2))\}. \end{aligned}$$

These are the indices for the 0 elements of the barycenter, i.e. (up to symmetry) the off-diagonal elements of the diagonal blocks and the diagonal elements of the off-diagonal blocks. We do not include (up to symmetry) the off-diagonal block $(n-2, n-1)$ or the last column of off-diagonal blocks.

With this new index set \hat{J} we are able to remove all redundant constraints while maintaining the SDP relaxation. First we have the following lemma.

Lemma 4.1 *Let $Y \in \mathcal{S}_{n^2+1}$. Then*

$$\hat{V}^T \mathcal{G}_{\hat{J}}^*(Y) \hat{V} = 0 \implies \mathcal{G}_{\hat{J}}^*(Y) = 0.$$

Proof. First, recall that the gangster operator is self-adjoint. Let $Z = \mathcal{G}_{\hat{J}}^*(Y)$. The matrix Z can be written as the block matrix

$$Z = \left[\begin{array}{c|ccc} 0 & 0 & \dots & 0 \\ 0 & Z^{11} & \dots & Z^{1n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & Z^{n1} & \dots & Z^{nn} \end{array} \right].$$

We let

$$\hat{Z} = (V \otimes V)^t \begin{bmatrix} Z^{11} & \dots & Z^{1n} \\ \vdots & \ddots & \vdots \\ Z^{n1} & \dots & Z^{nn} \end{bmatrix} (V \otimes V).$$

Then, for $i, j \in \{1, \dots, n-1\}$, the $(n-1)^2$ blocks of $\hat{Z} := \hat{V}^T Z \hat{V}$ are

$$\hat{Z}^{ij} = V^T (Z^{ij} - Z^{i,n} - Z^{n,j} + Z^{n,n}) V = 0. \quad (4.4)$$

Note that the definition of \hat{J} implies $Z^{ni} = Z^{in} = 0$, for $i = 1, \dots, n-1$, and $Z^{(n-2), (n-1)} = Z^{(n-1), (n-2)} = 0$. Therefore, with $i = n-1, j = n-2$, (4.4) implies that

$$\hat{Z}^{(n-1), (n-2)} = V^T (Z^{n,n}) V = 0.$$

As a result, we have

$$\hat{Z}^{ij} = V^T Z^{ij} V,$$

for $i, j \in \{1, \dots, n-1\}$.

Since Z^{ij} can be either a diagonal matrix or a matrix with diagonal equal to zeros, we have the following two cases.

Case 1: Z^{ij} is a diagonal matrix.

Let

$$Z^{ij} = \begin{bmatrix} a_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & a_n \end{bmatrix}.$$

Then

$$\hat{Z}^{ij} = \begin{bmatrix} a_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & a_{n-1} \end{bmatrix} + a_n E = 0,$$

which implies that $Z^{ij} = 0$.

Case 2: Z^{ij} is a matrix with diagonal equal to zeros.

Let

$$Z^{ij} = \begin{bmatrix} A & b \\ b^t & 0 \end{bmatrix},$$

where A is a $n-1$ by $n-1$ matrix with diagonal equal to zeros. Thus, we have

$$\hat{Z}^{ij} = A - eb^t - be^t = 0,$$

which implies that $b = 0$ and $A = 0$, i.e., $Z^{ij} = 0$. Therefore, We have $Z = 0$. \square

Note the adjoint relationship

$$\hat{V}^T \mathcal{G}_j^*(\cdot) \hat{V} = (\mathcal{G}_j(\hat{V} \cdot \hat{V}^T))^*.$$

The above Lemma 4.1 states that

$$\mathcal{N}(\hat{V}^T \mathcal{G}_j^*(\cdot) \hat{V}) = \mathcal{N}(\mathcal{G}_j^*(\cdot)).$$

Therefore, the adjoint operator satisfies the following.

Corollary 4.1

$$\mathcal{R}(\mathcal{G}_{\hat{J}}(\hat{V} \cdot \hat{V}^T)) = \mathcal{R}(\mathcal{G}_{\hat{J}}(\cdot)) = \mathcal{S}_{\hat{J}}. \quad (4.5)$$

We can now get rid of all of the redundant constraints that arise from adding the gangster operator \mathcal{G}_J , i.e. we can have an SDP relaxation where the constraint operator is onto. This requires the following.

Theorem 4.1 *Let $Y = \hat{V}R\hat{V}^T$ be written in block matrix form (1.1). Then*

1. $\mathcal{G}_{\hat{J}}(Y) = 0$ implies that $\text{diag}(Y^{1n}) = 0, \dots, \text{diag}(Y^{1,(n-1)}) = 0$, and $\text{diag}(Y^{(n-2),(n-1)}) = 0$.
2. Let $\bar{J} = \hat{J} \cup (0,0)$. Then $\mathcal{G}_{\bar{J}}(\hat{V} \cdot \hat{V}^T)$ has range space equal to $\mathcal{S}_{\bar{J}}$.

Proof. Suppose that $\mathcal{G}_{\hat{J}}(Y) = 0$, i.e. Y has zeros in positions corresponding to the set \hat{J} . From Lemma 3.1, we have, for each $i = 1, \dots, n$,

$$\sum_{j=1}^n \text{diag}(Y^{ij}) = Y^{i0}$$

and

$$\text{diag}(Y^{ii}) = Y^{i0}.$$

Using the zeros of the diagonals of the off-diagonal block, we get that $\text{diag}(Y^{in}) = 0$, for $i = 1, \dots, n-3$. Therefore

$$\begin{cases} \text{diag}(Y^{(n-2),(n-1)}) + \text{diag}(Y^{(n-2),n}) = 0 \\ \text{diag}(Y^{(n-2),(n-1)}) + \text{diag}(Y^{(n-1),n}) = 0 \\ \text{diag}(Y^{(n-2),n}) + \text{diag}(Y^{(n-1),n}) = 0. \end{cases}$$

Therefore

$$\begin{cases} \text{diag}(Y^{(n-2),(n-1)}) = 0 \\ \text{diag}(Y^{(n-2),n}) = 0 \\ \text{diag}(Y^{(n-1),n}) = 0. \end{cases}$$

This completes the proof for 1.

Since $\hat{Y}_{00} = 1$ is definitely a feasible constraint, and the $(0,0)$ index is not involved in the set \hat{J} , part 2 follows from Lemma 4.1 and the observation (4.5). \square

Theorem 4.1 shows that we have eliminated the redundant constraints and obtained a full rank constraint. We can now get a very simple projected relaxation.

$$\begin{aligned} \mu_{R2} := \min & \text{ trace}(\hat{V}^T L_Q \hat{V}) R \\ (QAP_{R2}) \quad \text{s.t.} & \mathcal{G}_{\bar{J}}(\hat{V} R \hat{V}^T) = E_{00} \\ & R \succeq 0. \end{aligned} \quad (4.6)$$

The dimension of the range space is determined by the cardinality of the set \bar{J} , i.e. there are $n^3 - 2n^2 + 1$ constraints.

The dual problem is

$$\begin{aligned} \mu_{R2} := \max \quad & -Y_{00} \\ \text{s.t.} \quad & \hat{V}^T(L_Q + \mathcal{G}_{\bar{J}}^*(Y))\hat{V} \succeq 0. \end{aligned}$$

Note $\mathcal{R}(\mathcal{G}_{\bar{J}}^*) = \mathcal{R}(\mathcal{G}_{\bar{J}}) = \mathcal{S}_{barJ}$. The dual problem can be expressed as follows

$$\begin{aligned} \mu_{R2} := \max \quad & -Y_{00} \\ \text{s.t.} \quad & \hat{V}^T(L_Q + Y)\hat{V} \succeq 0 \\ & Y \in \mathcal{S}_{\bar{J}}. \end{aligned}$$

4.3 Inequality Constraints

We now consider generic inequality constraints to further tighten the derived relaxations. These constraints come from the relaxation of the (0,1)-constraints of the original problem. For $Y = Y_X$, with $X \in \Pi$, the simplest inequalities are of the type

$$Y_{(i,j),(k,l)} \geq 0, \quad \text{since } x_{ij}x_{kl} \geq 0.$$

Helmberg et al. [18] show that the so called triangle inequalities of the general integer quadratic programming problem in the (-1,+1)-model are also generic inequalities for the (0,1)-formulation. Nevertheless, we are going to restrict ourselves to the simplest type of inequalities, which are facet defining for the QAP polytope, as shown in [21, 38]. Beside the nonnegativity constraints one can also impose nonpositivity constraints on the zero elements of \hat{Y} . Together with the gangster operator, these inequalities and the corresponding nonnegativity constraints are clearly redundant. But for the basic relaxation (QAP_{R1}) we can use both nonnegativity and nonpositivity constraints to approximate the gangster operator. This leads to the following semidefinite relaxation of QAP.

$$\begin{aligned} \mu_{R3} := \min \quad & \text{trace}(\hat{V}^T L_Q \hat{V})R \\ \text{s.t.} \quad & \text{b}^0 \text{diag}(\hat{V}R\hat{V}^T) = I, \quad \text{o}^0 \text{diag}(\hat{V}R\hat{V}^T) = I \\ & \text{arrow}(\hat{V}R\hat{V}^T) = e_0, \quad \hat{V}R\hat{V}^T \succeq 0 \\ & \mathcal{G}(\hat{V}R\hat{V}) \leq 0, \quad R \succeq 0 \end{aligned} \quad (4.7)$$

Note that this relaxation is stronger than (QAP_{R2}) because nonnegativity constraints are also imposed on elements which are not covered by the gangster operator. The advantage of this formulation is that the number of inequalities can be adapted so that the model is not too large. The larger the model is the better it approximates the original gangster operator.

4.4 A Comparison with Linear Relaxations

We now look at how our relaxations of QAP compare to relaxations based on linear programming. Adams and Johnson [2] derive a linear relaxation providing bounds which are at least as good as other lower bounds based on linear relaxations or reformulations of QAP. Using our notation, their continuous linear program can be written as

$$(QAP_{CLP}) \quad \mu_{CLP} := \min\{\text{trace} LZ : Z \in \mathcal{F}_{CLP}\} \quad (4.8)$$

where the feasible set is

$$\mathcal{F}_{CLP} := \left\{ \begin{aligned} Z \in \mathcal{N}; & \quad Z_{(i,j),(k,l)} = Z_{(k,l),(i,j)}, \quad 1 \leq i, j, k, l \leq n, i < k, j \neq l; \\ \sum_k Z_{(k,l),(k,l)} &= \sum_l Z_{(k,l),(k,l)} = 1; \\ \sum_{i \neq k} Z_{(i,j),(k,l)} &= Z_{(k,l),(k,l)}, \quad 1 \leq j, k, l \leq n, j \neq l; \\ \sum_{j \neq l} Z_{(i,j),(k,l)} &= Z_{(k,l),(k,l)}, \quad 1 \leq i, k, l \leq n, i \neq k \end{aligned} \right\}.$$

We now compare the feasible sets of relaxations (QAP_{R3}) and (QAP_{CLP}) . It is easy to see that the elements of Z which are not considered in \mathcal{F}_{CLP} are just the elements covered by the gangster operator, i.e. for which $\mathcal{G}(Y) = 0$. In (QAP_{R3}) the gangster operator is replaced by nonnegative and nonpositive constraints. The linear constraints in \mathcal{F}_{CLP} are just the lifted assignment constraints, but they are taken care of by the projection and the arrow operator in (QAP_{R3}) . The nonnegativity of the elements is enforced in both feasible sets. Hence the only difference is that we impose the additional constraint $Y \in \mathcal{P}$. We can summarize these observations in the following theorem.

Theorem 4.2 *Let μ_{R3} be the bound obtained by the semidefinite relaxation (QAP_{R3}) defined in (4.7), and let μ_{CLP} be the bound obtained by (QAP_{CLP}) , the linear relaxation of QAP defined in (4.8). Then*

$$\mu_{R3} \geq \mu_{CLP}.$$

□

5 PRIMAL-DUAL INTERIOR-POINT ALGORITHM

We now outline how to apply the primal-dual interior-point method of Helmsberg et al. [17, 19] to our semidefinite relaxations. First, we consider a generic SDP model. In Section 5.2 we discuss its application to (QAP_{R2}) , which we also call the *gangster model*; and in Section 5.3 we apply it to (QAP_{R3}) , which we call the *block model*. We also address practical and computational aspects for their solution.

5.1 Generic SDP Model

Let $\mathcal{A}(\cdot)$ and $\mathcal{B}(\cdot)$ be (symmetric) linear operators defined on \mathcal{S}_{n^2+1} , $a \in \mathbb{R}^{n_a}$ and $b \in \mathbb{R}^{n_b}$, where n_a and n_b are of appropriate size. Then, by identifying the equality constraints of the relaxations by $\mathcal{A}(\cdot)$ and a , and the inequality constraints by $\mathcal{B}(\cdot)$ and b , we get the following general (primal) semidefinite programming problem in the variable $R \in \mathcal{S}_{n^2+1}$

$$(P) \quad \begin{aligned} \mu^* := \min & \quad \text{trace } LR \\ \text{s.t.} & \quad \mathcal{A}(R) + a = 0 \\ & \quad \mathcal{B}(R) + b \geq 0 \\ & \quad R \succeq 0. \end{aligned}$$

The dual problem is

$$(D) \quad \begin{aligned} \nu^* &:= \max && w^T a - t^T b \\ &\text{s.t.} && L + \mathcal{A}^*(w) - \mathcal{B}^*(t) - Z = 0 \\ &&& t \geq 0 \\ &&& Z \succeq 0, \end{aligned}$$

where \mathcal{A}^* and \mathcal{B}^* denote the adjoint operators to \mathcal{A} and \mathcal{B} , respectively, and $w \in \mathfrak{R}^{n_a}$ and $t \in \mathfrak{R}^{n_b}$. Since, as we will prove in Section 5.4 the Slater constraint qualification holds for our primal (and dual) projected SDP relaxations, there is no duality gap, i.e. $\mu^* = \nu^*$.

The Karush-Kuhn-Tucker optimality conditions for the primal-dual pair are

$$(KKT) \quad \begin{aligned} F_P &:= \mathcal{A}(R) + a &= 0 \\ F_D &:= L + \mathcal{A}^*(w) - \mathcal{B}^*(t) - Z &= 0 \\ F_{tR} &:= -t \circ [\mathcal{B}(R) + b] + \mu e &= 0 \\ F_{ZR} &:= ZR - \mu I &= 0. \end{aligned}$$

The first and second equation are the primal and dual feasibility equations. The remaining equations take care of complementary slackness for the pairs $(t, [\mathcal{B}(R) + b])$, and (Z, R) , respectively.

We solve this system of equations with a Newton type method, which means we have to solve the following linearization for a search direction.

$$(\delta KKT) \quad \begin{aligned} \mathcal{A}(\delta R) &= -F_P \\ \mathcal{A}^*(\delta w) - \mathcal{B}^*(\delta t) - \delta Z &= -F_D \\ -(\delta t) \circ [\mathcal{B}(R) + b] - t \circ \mathcal{B}(\delta R) &= -F_{tR} \\ (\delta Z)R + Z(\delta R) &= -F_{ZR}. \end{aligned}$$

We first solve for δZ and eliminate the second equation of (δKKT)

$$\delta Z = \mathcal{A}^*(\delta w) - \mathcal{B}^*(\delta t) + F_D.$$

By defining t^{inv} as the vector having elements $(t^{inv})_i = \frac{1}{t_i}$ we get

$$(5.1) \quad \begin{aligned} \mathcal{A}(\delta R) &= -F_P \\ -t^{inv} \circ (\delta t) \circ [\mathcal{B}(R) + b] - \mathcal{B}(\delta R) &= -t^{inv} \circ F_{tR} \\ \mathcal{A}^*(\delta w)R - \mathcal{B}^*(\delta t)R + Z(\delta R) &= -F_{ZR} - F_D R \end{aligned}$$

Now solve for δR and eliminate the third equation of (5.1), i.e.

$$\delta R = -Z^{-1}\mathcal{A}^*(\delta w)R + Z^{-1}\mathcal{B}^*(\delta t)R - Z^{-1}F_{ZR} - Z^{-1}F_D R.$$

The system becomes

$$(5.2) \quad \begin{aligned} -\mathcal{A}(Z^{-1}\mathcal{A}^*(\delta w)R) + \mathcal{A}(Z^{-1}\mathcal{B}^*(\delta t)R) &= \mathcal{A}(Z^{-1}F_{ZR} + Z^{-1}F_D R) - F_P \\ +\mathcal{B}(Z^{-1}\mathcal{A}^*(\delta w)R) - \mathcal{B}(Z^{-1}\mathcal{B}^*(\delta t)R) - t^{inv} \circ (\delta t) \circ [\mathcal{B}(R) + b] &= \\ &= -\mathcal{B}(Z^{-1}F_{ZR} + Z^{-1}F_D R) - t^{inv} \circ F_{tR}. \end{aligned}$$

We can observe that the *final system* (5.2) is of size $(m + m_b)$, where m_b denotes by definition the number of inequality constraints. This final system is solved with respect to δw and δt and back substitution yields δR and δZ . Note that since δR cannot be assumed to be symmetric it is symmetrized; but, as shown in [24], this still yields polynomial time convergence of the interior-point method.

We point out that solving the final system is the most expensive part of the primal-dual algorithm. We are using two approaches for this purpose: a preconditioned conjugate gradient method for the gangster model; and a Cholesky factorization for the block model.

5.2 Application to the Gangster Model

Now we apply the above generic model to the SDP relaxation (QAP_{R2}) . The primal-dual pair is

$$(P) \quad \begin{aligned} \min \quad & \text{trace}(\hat{V}^T L_Q \hat{V}) R \\ \text{s.t.} \quad & \mathcal{G}_{\bar{J}}(\hat{V} R \hat{V}^T) = E_{00} \\ & R \succeq 0 \end{aligned}$$

and

$$(D) \quad \begin{aligned} \max \quad & -Y_{00} \\ \text{s.t.} \quad & \hat{V}^T (L_Q + Y) \hat{V} - Z = 0 \\ & Z \succeq 0 \\ & Y \in \mathcal{S}_{\bar{J}}. \end{aligned}$$

The Karush-Kuhn-Tucker conditions of the dual log-barrier problem are

$$\begin{aligned} F_P &:= \mathcal{G}_{\bar{J}}(\hat{V} R \hat{V}^T) - E_{00} &= 0 \\ F_D &:= \hat{V}^T (L_Q + Y) \hat{V} - Z &= 0 \\ F_{ZR} &:= ZR - \mu I &= 0, \end{aligned} \tag{5.3}$$

where $R \succ 0, Z \succ 0$ and $Y \in \mathcal{S}_{\bar{J}}$. The first equation is primal feasibility conditions, while the second is the dual feasibility conditions and the third takes care of complementary slackness for R and Z . After substituting for δZ and δR we obtain the following final system.

$$\mathcal{G}_{\bar{J}}(\hat{V} Z^{-1} \hat{V}^T \delta Y \hat{V} R \hat{V}^T) = F_P - \mathcal{G}_{\bar{J}}(\hat{V} (Z^{-1} F_D R + Z^{-1} F_{ZR}) \hat{V}^T). \tag{5.4}$$

The size of the above problem is $m = n^3 - 2n^2 + 1$. Therefore, to solve such a huge system of equations we have to use a conjugate gradient method. It is worthwhile to note that even if the above system of equations can be solved directly, it is very time consuming to create an explicit matrix representation.

5.2.1 The Preconditioned Conjugate Gradient Method

We use $\mathcal{K}(\delta y) = b$ to denote the above system (5.4). We solve the system inexactly by the conjugate gradient method. We use the square root of the size of the above linear system as a limit on the number of iterations of the conjugate gradient method. We choose the diagonal

of the matrix representation as the preconditioner. We approximate the angle θ between $\mathcal{K}(\delta y)$ and b by

$$\cos \theta \approx \frac{|b^T(b-r)|}{\|b\| \cdot \|b-r\|},$$

where r is the estimate of the residual of the linear system. We then choose $\sigma = 0.001$ and terminate the conjugate gradient algorithm when

$$1 - \cos \theta \leq \sigma.$$

(See e.g. [33].)

The special structure of the gangster operator makes it relatively cheap to construct a preconditioner. Let $\tilde{R} = \hat{V}R\hat{V}^T$ and $\tilde{Z} = \hat{V}Z^{-1}\hat{V}^T$. Then the linear operator system (5.4) becomes

$$\mathcal{G}_{\tilde{J}}(\tilde{Z}\delta Y\tilde{R}) = F_P^1 - \mathcal{G}_{\tilde{J}}(\hat{V}(Z^{-1}F_DR + Z^{-1}F_{ZR})\hat{V}^T).$$

For $1 \leq k, l \leq m$, let us try to calculate \mathcal{K}_{kl} , the (k, l) entry of \mathcal{K} . Note that we can always order the index set \tilde{J} . Let (k_i, k_j) and (l_i, l_j) be the index pairs from \tilde{J} corresponding to k and l , respectively. The l th column of \mathcal{K} is $\mathcal{K}(e_l)$, i.e.

$$\left(\mathcal{G}_{\tilde{J}}(\tilde{Z}(0.5e_{l_i}e_{l_j}^T + 0.5e_{l_j}e_{l_i}^T)\tilde{R}) \right).$$

Therefore,

$$\mathcal{K}_{kl} = (\tilde{Z}_{k_i l_j} \tilde{R}_{l_i k_j} + \tilde{Z}_{k_i l_i} \tilde{R}_{l_j k_j} + \tilde{Z}_{k_j l_i} \tilde{R}_{l_j k_i} + \tilde{Z}_{k_j l_j} \tilde{R}_{l_i k_i})/2.$$

The above formula allows for efficient calculation of the diagonal elements.

5.2.2 Stopping Criterion for the Interior-Point Method

Because of the primal infeasibility, we use the increasing rate of the dual objective value for the stopping criteria (instead of using the duality gap). The rate is defined as follows.

$$\delta t_k := \frac{t_{k+1} - t_k}{t_{k+1}},$$

where t_k is the dual objective value at the iteration k . At each iteration the dual objective value gives a lower-bound and the lower-bound increases as k increases. We terminate the algorithm when

$$\delta t_k < \epsilon,$$

where $\epsilon := 0.001$. In other words, when the gain for increasing the lower-bound is not worth the computation expense, we stop the algorithm. Since our goal is to find a lower-bound this stopping criterion is quite reasonable.

5.3 Application to the Block Model

In the case of the block model, i.e. (QAP_{R3}) and its special case (QAP_{R1}) , we apply the following primal-dual interior-point approach.

The linear operator $\mathcal{B}(\cdot)$ acting on $(n^2 + 1) \times (n^2 + 1)$ matrices is used to model the nonnegativity and nonpositivity constraints. Since the constraints used to approximate the gangster operator do not allow for a primal interior-point to exist, they are relaxed to $y_{ij} + \varepsilon \geq 0$ and $-y_{ij} + \varepsilon \geq 0$ with $\varepsilon > 0$. For these relaxed constraints the barycenter as given in Theorem 3.1 is strictly feasible. Now set $b = \varepsilon e$ and obtain as (relaxed) inequality constraints $\mathcal{B}(\hat{V}R\hat{V}^T) + b \geq 0$ in (QAP_{R3}) . In practice we set $\varepsilon = 10^{-3}$. Due to practicality, all nonnegativity constraints are relaxed as well. The primal program of the primal-dual pair for (QAP_{R3}) is now

$$(P) \quad \begin{aligned} \min \quad & \text{trace } LR \\ \text{s.t.} \quad & \text{arrow } (\hat{V}R\hat{V}^T) - e_0 = 0 \\ & \text{b}^0\text{diag } (\hat{V}R\hat{V}^T) - I = 0 \\ & \text{o}^0\text{diag } (\hat{V}R\hat{V}^T) - I = 0 \\ & \mathcal{B}(\hat{V}R\hat{V}^T) + b \geq 0 \\ & R \succeq 0. \end{aligned}$$

and the dual program is

$$(D) \quad \begin{aligned} \max \quad & -w_0 - b^T t \\ \text{s.t.} \quad & L + \hat{V}^T(\text{Arrow}(w) + \text{B}^0\text{Diag}(S_b) + \text{O}^0\text{Diag}(S_o) - \mathcal{B}^*(t))\hat{V} - Z = 0 \\ & Z \succeq 0, t \geq 0. \end{aligned}$$

Note that the dual variables S_b and S_o do not get into the objective function of (D) , since the main diagonal elements are not covered by the block-0-diag and off-0-diag operators. This follows from the considerations about the redundancies of certain parts of the operators in Section 3.2.

The left hand side of the final system corresponding to the solution of (KKT) is now a 4×4 block. The remaining variables are δw , δS_b , δS_o , and δt and the left hand side is

$$K(\cdot) := \begin{bmatrix} -\mathcal{A}(\tilde{Z}\mathcal{A}^*(\cdot)\tilde{R}) & \mathcal{A}(\tilde{Z}\mathcal{B}^*(\cdot)\tilde{R}) \\ \mathcal{B}(\tilde{Z}\mathcal{A}^*(\cdot)\tilde{R}) & -\mathcal{B}(\tilde{Z}\mathcal{B}^*(\cdot)\tilde{R}) - t^{inv} \circ (\cdot) \circ [\mathcal{B}(R) + b] \end{bmatrix}, \quad (5.5)$$

where we have $\tilde{Z} := VZ^{-1}V^T$ and $\tilde{R} := VRV^T$, and the operator $\mathcal{A}(\cdot)$ covers the equality constraints. Thus

$$\mathcal{A}(\cdot) = \begin{pmatrix} \text{arrow } (\cdot) \\ \text{b}^0\text{diag } (\cdot) \\ \text{o}^0\text{diag } (\cdot) \end{pmatrix}$$

makes up a 3×3 block in the left upper corner of $K(\cdot)$. This block is of size $m_a \times m_a$, where $m_a = 2n^2 - 3n + 1$. Recall that the dimension of the image space of the arrow operator is $n^2 + 1$ while the block-0-diag and off-0-diag operators both contain $(n^2 - 3n)/2$ linearly independent equalities.

In the block model we assume primal and dual feasibility from the beginning, and hence the right hand side of the final system is just

$$\begin{bmatrix} \mathcal{A}(R - \mu Z^{-1}) \\ b + \mu(Z^{-1} - t^{inv}) \end{bmatrix}. \quad (5.5)$$

For solving the final system we construct an $(m_a + m_b) \times (m_a + m_b)$ matrix which corresponds to $K(\cdot)$. A way for doing this is described in [22]. Building this matrix for the basic relaxation (QAP_{R1}) requires $\mathcal{O}(n^6)$ operations and its factorization is of the same complexity. Note that a conjugate gradient approach to solve the final system of the block model would require the same order of work in each iteration. Hence, solving (QAP_{R1}) employing a conjugate gradient method would be of similar expense as for solving (QAP_{R2}).

It should also be pointed out that the projections $\hat{V}^T Y \hat{V}$ and $\hat{V} R \hat{V}^T$ can be performed in order $\mathcal{O}(n^4)$ operations instead of $\mathcal{O}(n^6)$ steps if the special structure of \hat{V} is exploited, see [22].

5.3.1 Predictor Corrector Approach

We are now going to look at the change in the right hand side of the final system when we apply a predictor-corrector approach to the block model.

Predictor-corrector approaches prove to be very successful for linear programming, see e.g. [28, 9], and the concept can also be applied to semidefinite programming, see [3] and [17]. As shown in [17] the application of a predictor-corrector approach only changes the right hand side of the final system (5.2).

The main observation is that splitting up the search direction $\delta s = \delta s^p + \delta s^c$ yields an improved solution since it better solves the nonlinear complementarity conditions. Here we denote by δs the vector containing our search direction $(\delta w, \delta t, \delta R, \delta Z)$.

The predictor step δs^p is also called the affine scaling step ($\mu = 0$). It is just the solution of the final system (5.2) with right hand side

$$\begin{bmatrix} \mathcal{A}(R) \\ b \end{bmatrix}. \quad (5.6)$$

The result is the predictor step $\delta s^p = (\delta w^p, \delta t^p, \delta R^p, \delta Z^p)$. In the corrector step δs^c we solve for the correction to the central path. This results in the same final system (5.2) where the right hand side is now

$$\begin{bmatrix} \mathcal{A}[Z^{-1}(\delta Z^p)(\delta R^p)] - \mu \mathcal{A}[Z^{-1}] \\ -\mathcal{B}[Z^{-1}(\delta Z^p)(\delta R^p)] + t^{inv} \circ (\delta t^p) \circ \mathcal{B}(\delta R^p) + \mu \mathcal{B}[Z^{-1} - t^{inv}] \end{bmatrix}. \quad (5.7)$$

We now solve for $\delta s^c = (\delta w^c, \delta t^c, \delta R^c, \delta Z^c)$ and finally obtain $\delta s = \delta s^p + \delta s^c$.

5.3.2 A Cutting Plane Approach

The number of possibly violated inequalities can be of order $\mathcal{O}(n^4)$. In order to find a good approximation of the QAP with relatively few inequalities in the model we use a cutting plane approach.

We first solve the basic relaxation (QAP_{R1}) to optimality. Then we add the $m = \min\{n^2, 200\}$ most violated inequalities to the model and solve the new relaxation (QAP_{R3}). Before adding additional violated inequalities we check whether all inequality constraints are tight and remove those that have positive slack whose dual costs are close to zero. Here, we remove an inequality if its dual cost is smaller than $5 * 10^{-5} * t_{max}$ where t_{max} is the largest dual variable. We repeat

this process of removing and adding inequalities until one of the following stopping criterions for the cutting plane approach is met: we can prove optimality for the given instance, i.e. the lower bound is tight; there are no more violated inequalities; or a given upper bound for the number of inequalities that can be used, here $m_b \leq 2000$, is reached.

5.4 Strictly Feasible Points for Both Models

We still have to address the existence of strictly feasible points for our relaxations in order to satisfy Slater's constraint qualification. The following lemma gives interior points for the primal problems.

Lemma 5.1 *Define the $((n-1)^2 + 1) \times ((n-1)^2 + 1)$ matrix*

$$\hat{R} := \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \frac{1}{n^2(n-1)}(nI_{n-1} - E_{n-1}) \otimes (nI_{n-1} - E_{n-1}) \end{array} \right]$$

Then \hat{R} is positive definite and feasible for (QAP_{R1}) , (QAP_{R2}) , and (QAP_{R3}) .

Proof. First it is easy to check that \hat{R} is strictly positive definite since $nI_{n-1} - E_{n-1}$ is strictly positive definite.

We complete the proof by showing that

$$\hat{V} \hat{R} \hat{V}^T = \hat{Y},$$

where \hat{Y} is the barycenter.

$$\begin{aligned} \hat{V}^T \hat{R} \hat{V} &= \left[\begin{array}{c|c} 1 & 0 \\ \hline \frac{1}{n}e \otimes e & V \otimes V \end{array} \right] \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \frac{1}{n^2(n-1)}(nI - E) \otimes (nI - E) \end{array} \right] \left[\begin{array}{c|c} 1 & \frac{1}{n}e^T \otimes e^T \\ \hline 0 & V^T \otimes V^T \end{array} \right] \\ &= \left[\begin{array}{c|c} 1 & 0 \\ \hline \frac{1}{n}e \otimes e & V \otimes V \end{array} \right] \left[\begin{array}{c|c} 1 & \frac{1}{n}e^T \otimes e^T \\ \hline 0 & \frac{1}{n^2(n-1)}(nI - E) \otimes (nI - E)(V^T \otimes V^T) \end{array} \right] \\ &= \left[\begin{array}{c|c} 1 & \frac{1}{n}e^T \otimes e^T \\ \hline \frac{1}{n}e \otimes e & \frac{1}{n^2}E \otimes E + \frac{1}{n^2(n-1)}(nVV^T - VEV^T) \otimes (nVV^T - VEV^T) \end{array} \right]. \end{aligned}$$

Now it remains to show that $nVV^T - VEV^T = nI_n - E_n$. We have

$$\begin{aligned} nVV^T - VEV^T &= \left[\begin{array}{c|c} nI_{n-1} & -ne_{n-1}^T \\ \hline -ne_{n-1} & n(n-1) \end{array} \right] - \left[\begin{array}{c|c} E_{n-1} & -(n-1)e_{n-1}^T \\ \hline -(n-1)e_{n-1} & (n-1)^2 \end{array} \right] \\ &= \left[\begin{array}{c|c} nI_{n-1} - E_{n-1} & -e_{n-1}^T \\ \hline -e_{n-1} & n-1 \end{array} \right] \\ &= nI_n - E_n. \end{aligned}$$

□

The next lemma provides strictly dual-feasible points.

Lemma 5.2 1. Let

$$\hat{Y} = M \begin{bmatrix} n & 0 \\ 0 & I_n \otimes (I_n - E_n) \end{bmatrix}.$$

Then for M large enough, $\hat{Y} \succ 0$ and it is in the feasible set of the dual of (QAP_{R2}) .

2. Let $\hat{w} = \alpha(n^2/4 + \varepsilon, e_{n^2})^T$ with $\varepsilon > 0$ and α large enough, $\hat{S}_o = 0$, $\hat{S}_b = 0$, and let \hat{t} be arbitrary. Then the quartuple $(\hat{w}, \hat{S}_o, \hat{S}_b, \hat{t})$ is strictly feasible for the duals of (QAP_{R3}) , and of (QAP_{R1}) if $\hat{t} \equiv 0$.

Proof.

1. It is obvious that we only need to show that $\hat{V}(\mathcal{G}_j^*(\hat{Y}) + \hat{Y}_{00}e_0e_0^T)\hat{V}$ is positive definite.

$$\begin{aligned} \hat{V}(\mathcal{G}_j^*(\hat{Y}) + \hat{Y}_{00}e_0e_0^T)\hat{V} &= \begin{bmatrix} 1 & 0 \\ 0 & (V \otimes V)^T(I_n \otimes (I_n - E_n))V \otimes V \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & (V^T I_n V) \otimes (V^T (I_n - E_n) V) \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & V^T V \otimes V^T V \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & (I_{n-1} + E_{n-1}) \otimes (I_{n-1} + E_{n-1}) \end{bmatrix}. \end{aligned}$$

Since $I_{n-1} + E_{n-1}$ is positive definite, we have that

$$\begin{bmatrix} 1 & 0 \\ 0 & (I_{n-1} + E_{n-1}) \otimes (I_{n-1} + E_{n-1}) \end{bmatrix}$$

is positive definite.

2. Fixing \hat{S}_o , \hat{S}_b and \hat{t} , we only need to show that $\text{Arrow}(\hat{w}/\alpha) \succ 0$. Using Schur complements this is equivalent to showing that $(n^2 + \varepsilon)/4 > 0$ and $I_{n^2} \succ -\frac{1}{2}e_{n^2}(\frac{4}{n^2+\varepsilon})\frac{1}{2}e_{n^2}^T = \frac{1}{n^2+\varepsilon}E_n^2$. The first inequality is obvious and for the second we only need to observe that the largest eigenvalue of the right hand side is smaller than 1. Making α large enough provides an interior point for the dual of (QAP_{R3}) and also for (QAP_{R1}) for which $\hat{t} \equiv 0$.

□

6 NUMERICAL RESULTS

In this Section we present the results of our numerical experiments. The experiments are divided into two parts. First we investigate the quality of the new bounds compared to bounds from the literature. Then, we also look at their quality and growth rate in the first level of the branching tree, see Table 5.

The results of the comparisons are summarized in the following tables. Tables 1 and 2 contain instances from the current version of QAPLIB [8] while Table 3 consists of data of a previous version of the library. Note that all considered instances are pure quadratic, i.e. have no linear term, except the problems *Carxx*. The tables read as follows. The first column indicates the problem instance and its size, e.g. *Nugxx* refers to the Nugent example of size xx . For references of the problem instances we refer to QAPLIB [8]. The following columns contain the best known feasible solution (which is optimal for all $n \leq 24$); the Gilmore-Lawler bound GLB [13, 26]; the projection or elimination bound ELI of [16]; the linear programming bound RRD obtained in [37]; and an improved eigenvalue bound EVB3 from [36]. For EVB3 we performed 100 iterations of the underlying bundle trust code. The last three columns contain the bounds obtained in this paper, μ_{R1} , μ_{R2} and μ_{R3} . An ‘n.a.’ means that the value of the bound is not available.

The implementation of our bounds was done in MATLAB using CMEX interfaces. Even though there is still room for improvement with respect to implementational aspects, our running times are comparable to the ones for RRD [37]. For the *Nug20* problem instance, Resende et al. needed 60.19 minutes of CPU-time to obtain their bound on a Silicon Graphics Challenge computer (150-MHz with 1.5 Gbytes of RAM). The implementation of their bounding technique was done in FORTRAN and C. The calculation of μ_{R1} and μ_{R2} on DEC 3000-900 Alpha AXP computers (275-MHz with 256 Mbytes and 64 Mbytes of RAM) took 19.93 and 316.17 minutes of CPU-time, respectively.

We do not report μ_{R2} and μ_{R3} for instances larger than $n = 22$ (except for one instance of size $n = 30$ where μ_{R2} is given). The reasons therefore are the large running times for the gangster model (QAP_{R2}) and the restriction on the number of inequalities in the cutting plane approach to $m_b \leq 2000$ for (QAP_{R3}). Furthermore, this work is primarily concerned with the theoretical aspects of the application of semidefinite relaxations to the QAP. The issue of better and more efficient implementations will be part of subsequent work. Regarding (QAP_{R3}), one can observe that the restriction on the size of the model does not allow for large improvements within the cutting plane approach for instances of size $n \geq 15$. In this case the gangster model (QAP_{R2}) provides stronger bounds than (QAP_{R3}). But the block model provides at least a primal feasible approach from the beginning and the less expensive basic relaxation (QAP_{R1}) is competitive with respect to RRD for the *Nugxx* instances of dimension $n \geq 20$.

The comparison with bounds from the literature shows that our bounds compare favorable on instances *Hadxx*, *Nugxx*, *Rouxx*, and *Taixx*. These instances have in common that their matrices are rather dense. On the other hand, for sparse instances as most of *Escxx* and *Scrxx* are, RRD dominates the bounds based on semidefinite relaxation. ELI seems to be a good indicator of when to expect the semidefinite bounds to be stronger than the ones based on linear relaxation. It seems as if the nonnegativity constraints are more important than the semidefinite ones on sparse instances. On these instances ELI, μ_{R1} and μ_{R2} become even negative. Note that on the *Esc16x* problems ELI and μ_{R1} coincide.

Table 4 contains instances whose inherent symmetry was destroyed by introducing a linear term. For instance, the distance matrices of the *Nugxx* problems contain the distances of

	Sol.	GLB	ELI	RRD	EVB3	μ_{R1}	μ_{R2}	μ_{R3}
Esc16a	68	38	47	68	50	47	50	47
Esc16b	292	220	250	278	276	250	276	277
Esc16c	160	83	95	118	113	95	113	110
Esc16d	16	3	-19	4	-12	-19	-12	-6
Esc16e	28	12	6	14	13	6	13	9
Esc16g	26	12	9	14	11	9	11	10
Esc16h	996	625	708	704	708	708	909	806
Esc16i	14	0	-25	0	-21	-25	-21	-6
Esc16j	8	1	-6	2	-4	-6	-4	-4
Had12	1652	1536	1573	n.a.	1595	1604	1640	1648
Had14	2724	2492	2609	n.a.	2643	2651	2709	2703
Had16	3720	3358	3560	n.a.	3601	3612	3678	3648
Had18	5358	4776	5104	n.a.	5176	5174	5286	5226
Had20	6922	6166	6625	n.a.	6702	6713	6847	6758
Kra30a	88900	68360	63717	76003	n.a.	69736	–	–
Kra30b	91420	69065	63818	76752	n.a.	70324	–	–
Nug12	578	493	472	523	498	486	530	547
Nug14	1014	852	871	n.a.	898	903	959	967
Nug15	1150	963	973	1041	1001	1009	1060	1075
Nug16a	1610	1314	1403	n.a.	1455	1461	1527	1520
Nug16b	1240	1022	1046	n.a.	1081	1082	1138	1132
Nug17	1732	1388	1487	n.a.	1521	1548	1621	1604
Nug18	1930	1554	1663	n.a.	1707	1723	1801	1776
Nug20	2570	2057	2196	2182	2290	2281	2385	2326
Nug21	2438	1833	1979	n.a.	2116	2090	2252	2157
Nug22	3596	2483	2966	n.a.	3174	3140	3394	3234
Nug24	3488	2676	2960	n.a.	3074	3068	–	–
Nug25	3744	2869	3190	n.a.	3287	3305	–	–
Nug30	6124	4539	5266	4805	5448	5413	–	–

Table 1: QAPLIB instances 1

	Sol.	GLB	ELI	RRD	EVB3	μ_{R1}	μ_{R2}	μ_{R3}
Rou12	235528	202272	200024	224278	201337	208685	220991	227986
Rou15	354210	298548	296705	324869	297958	306833	323141	324900
Rou20	725522	599948	597045	643346	n.a.	615549	642448	631680
Scr12	31410	27858	4727	29872	n.a.	11117	24230	27183
Scr15	51140	44737	10355	49264	n.a.	17046	42094	40821
Scr20	110030	86766	16113	95113	n.a.	28535	83026	59780
Tai12a	224416	195918	193124	n.a.	195673	203595	215377	220938
Tai15a	388214	327501	325019	n.a.	327289	333437	349476	347908
Tai17a	491812	412722	408910	n.a.	410076	419619	441238	435675
Tai20a	703482	580674	575831	n.a.	n.a.	591994	618720	606228
Tai25a	1167256	962417	956657	n.a.	n.a.	974004	–	–
Tai30a	1818146	1504688	1500407	n.a.	n.a.	1529135	–	–
Tho30	149936	90578	119254	100784	n.a.	125972	–	–

Table 2: QAPLIB instances 2

	Sol.	GLB	ELI	RRD	EVB3	μ_{R1}	μ_{R2}	μ_{R3}
Car10ga	4954	3586	4079	n.a.	4541	4435	4853	4919
Car10gb	8082	6139	7211	n.a.	7617	7600	7960	8035
Car10gc	8649	7030	7837	n.a.	8233	8208	8561	8612
Car10gd	8843	6840	8006	n.a.	8364	8319	8666	8780
Car10ge	9571	7627	8672	n.a.	8987	8910	9349	9473
Car10pa	32835	28722	-4813	n.a.	n.a.	1583	12492	30359
Car10pb	14282	12546	-14944	n.a.	n.a.	-5782	9934	13361
Car10pc	14919	12296	-17140	n.a.	n.a.	-8040	2473	13655
Esc08a	2	0	-2	0	n.a.	-2	0	2
Esc08b	8	1	-2	2	n.a.	-2	3	6
Esc08c	32	13	8	22	n.a.	9	18	30
Esc08d	6	2	-2	2	n.a.	-2	2	6
Esc08e	2	0	-6	0	n.a.	-6	-4	1
Esc08f	18	9	8	18	n.a.	9	13	18
Nug05	50	50	47	50	50	49	50	50
Nug06	86	84	69	86	70	74	85	86
Nug07	148	137	125	148	130	132	144	148
Nug08	214	186	167	204	174	179	197	210

Table 3: Numerical Results for old instances

	Sol.	μ_{R1}	μ_{R2}	μ_{R3}
Nug12C	578	492	534	545
Nug15C	1150	1012	1075	1081
Nug20C	2570	2292	2396	2335
Nug30C	6124	5424	5648	–

Table 4: Instances for which symmetry is destroyed

rectangular grids. The grid on which the locations of Nug12 are placed is given by

$$G = \begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 4 \\ \hline 5 & 6 & 7 & 8 \\ \hline 9 & 10 & 11 & 12 \\ \hline \end{array}.$$

In this case, an assignment of any facility, say facility 1, to other locations but 1, 2, 5 and 6, can not result in a solution which is not obtained by a restricted solution, say $1 \rightarrow \{1, 2, 5, 6\}$. For restricting the solution set to such a subset, we introduce a linear cost matrix C whose elements are all 0 except $c_{1j}, j \in \{3, 4, 7, 8, 9, 10, 11, 12\}$. These nonzero entries of C are sufficiently large numbers. The resulting instances are marked with a ‘C’, e.g. Nug12C, and are equivalent to the originals. Table 4 shows that our bounds improve when this is done. We point out that symmetries can also be found in the other instances but we do not specify this here.

We also investigate whether the new bounds satisfy a necessary condition for their applicability within a branch and bound algorithm. Eigenvalue bounds show a relatively small growth rate in the branching tree and, therefore computationally more expensive variants are not well suited for branch and bound, see [10]. Here, we look at the quality of the new bounds in the first level of the branching tree, i.e. we want to see how fast the lower bounds increase after branching. Table 5 gives the results for the first level, when one partial assignment is made. As pointed out above, the Nug xx examples possess inherent symmetries due to their distance matrices, e.g. there are only four subproblems to be considered in the first level of Nug12. The partial assignments of facility 1 are indicated by the entry after the dot in the name of the instance. To measure the increasing rate (ir) of the lower bound (lb) by branching, we define the rate in percent as follows.

$$ir := \frac{lb_{\text{child}} - lb_{\text{parent}}}{lb_{\text{parent}}} * 100\%$$

In Table 5, the increasing rates are shown by the numbers in the brackets. The results of this table show that the lower bounds given by the SDP relaxations increase much faster than the Gilmore-Lawler bounds in the first level of the branching tree. Even though this does not allow a general conclusion on the applicability of the new bounds to exact solution methods, it does also not rule out the possibility that bounds based on semidefinite relaxations are good candidates for branch and bound methods.

	n	Sol.	GLB	(ir)	μ_{R1}	(ir)	μ_{R2}	(ir)	μ_{R3}	(ir)
Nug12	12	578	493		486		530		547	
Nug12.1	11	586	496	(0.6)	514	(5.4)	551	(3.9)	574	(4.9)
Nug12.2	11	578	495	(0.4)	514	(5.4)	553	(4.3)	571	(4.3)
Nug12.5	11	578	494	(0.2)	524	(7.8)	552	(4.1)	570	(4.2)
Nug12.6	11	586	499	(1.2)	530	(9.0)	561	(5.8)	578	(5.6)
Nug15	15	1150	963		1009		1060		1075	
Nug15.1	14	1150	967	(0.4)	1049	(4.0)	1104	(4.2)	1114	(3.6)
Nug15.2	14	1166	974	(1.1)	1076	(6.6)	1124	(6.0)	1135	(5.6)
Nug15.3	14	1200	987	(2.5)	1075	(6.5)	1133	(6.9)	1145	(6.5)
Nug15.6	14	1152	968	(0.5)	1056	(4.7)	1106	(4.3)	1118	(4.0)
Nug15.7	14	1166	979	(1.7)	1052	(4.3)	1112	(5.2)	1125	(4.7)
Nug15.8	14	1168	983	(2.1)	1063	(5.4)	1118	(5.5)	1133	(5.4)
Nug20	20	2570	2057		2281		2385		2326	
Nug20.1	19	2628	2082	(1.2)	2358	(3.4)	2449	(2.7)	2414	(3.8)
Nug20.2	19	2600	2130	(3.6)	2401	(5.3)	2489	(4.4)	2464	(6.0)
Nug20.3	19	2588	2067	(0.5)	2331	(2.2)	2428	(1.8)	2392	(2.8)
Nug20.6	19	2570	2064	(0.3)	2341	(2.6)	2431	(1.9)	2403	(3.3)
Nug20.7	19	2634	2105	(2.3)	2387	(4.6)	2479	(3.9)	2436	(4.7)
Nug20.8	19	2636	2127	(3.4)	2381	(4.4)	2485	(4.2)	2438	(4.8)

Table 5: Results for first level in branching tree

Finally, the tests in the first level of the search tree, where the subproblems contain linear parts, and the results for the *Carxx* data also show that the semidefinite bounds perform well for instances with linear terms.

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A Notation

\mathcal{M}_t	the space of $t \times t$ real matrices
\mathcal{S}_t	the space of $t \times t$ symmetric matrices
$t(n)$	$\frac{n(n+1)}{2}$, the dimension of \mathcal{S}_t
\mathcal{P}_t or \mathcal{P}	the cone of positive semidefinite matrices in \mathcal{S}_t
$M_1 \succeq M_2$	$M_1 - M_2$ is positive semidefinite
A^*	the adjoint of the linear operator A
K^+	the polar cone of K , $K^+ = \{\phi : (\phi, k) \geq 0, \forall k \in K\}$
$A \circ B$	the Hadamard product of A and B
$A \otimes B$	the Kronecker product of A and B
$\text{vec}(X)$	the vector formed from the columns of the matrix X
$\text{Mat}(x)$	the matrix formed, columnwise, from the vector x
$\text{Diag}(v)$	the diagonal matrix formed from the vector v
$\text{diag}(M)$	the vector of the diagonal elements of the matrix M
E	the matrix of ones
e	the vector of ones
e_i	the i -th unit vector
E_{ij}	the matrix $E_{ij} := e_i e_j^T$
$\mathcal{R}(M)$	the range space of the matrix M
$\mathcal{N}(M)$	the null space of the matrix M

\mathcal{E}	the set of matrices with row and column sums one, $\mathcal{E} := \{X : Xe = X^T e = e\}$
\mathcal{Z}	the set of (0,1)-matrices, $\mathcal{Z} := \{X : X_{ij} \in \{0, 1\}\}$
\mathcal{N}	the set of nonnegative matrices, $\mathcal{N} := \{X : X_{ij} \geq 0\}$
\mathcal{O}	the set of orthogonal matrices, $\mathcal{O} := \{X : XX^T = X^T X = I\}$
Y_X	the lifting of the matrix X , with $x = \text{vec}(X)$,

$$Y_X := \begin{bmatrix} 1 & x^T \\ x & xx^T \end{bmatrix}$$

$\mathcal{G}_J(Y)$	Gangster operator, an operator that “shoots” holes or zeros in the matrix Y , (4.1)
$\mathcal{PG}(Y)$	Gangster operator projected onto its range space, (4.6)
Arrow (\cdot)	the Arrow operator, (2.11)
$B^0\text{Diag}(\cdot)$	the Block Diag operator, (2.12)
$O^0\text{Diag}(\cdot)$	the Off Diag operator, (2.13)
arrow (\cdot)	the arrow operator, (2.15)
$b^0\text{diag}(\cdot)$	the block diag operator, (2.16)
$o^0\text{diag}(\cdot)$	the off diag operator, (2.17)
$QAP_{\mathcal{E}}$	an equivalent formulation of QAP, Section 2
$QAP_{\mathcal{O}}$	an equivalent formulation of QAP, Section 2.2

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