Chapter 1

SEMIDEFINITE PROGRAMMING APPROACHES TO THE QUADRATIC ASSIGNMENT PROBLEM

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Contents

Abstract The Quadratic Assignment Problem, QAP, is arguably the hardest of the NP-hard problems. One of the main reasons is that it is very difficult to get good quality bounds for branch and bound algorithms. We show that many of the bounds that have appeared in the literature can be ranked and put into a unified Semidefinite Programming, SDP, framework. This is done using redundant quadratic constraints and Lagrangian relaxation. Thus, the final SDP relaxation ends up being the strongest.

Keywords: Quadratic Assignment Problem, Semidefinite Programming, Lagrangian Relaxation, Redundant Constraints.

1. INTRODUCTION

The Quadratic Assignment Problem, QAP, can be considered to be the hardest of the NP-hard problems. This is an area where dimension $n = 30$ is considered to be large scale, and more often than not, is too hard to solve to optimality. One of the main reasons is that it is very difficult to get good lower bounds for fathoming partial solutions in branch and bound algorithms. In this chapter we consider several different bounding strategies. We show that these can be put into a Semidefinite Programming, SDP, framework.

Bounds for QAP can be classified into four types: Gilmore-Lawler type; eigenvalue based; reformulation or linear programming type; and semidefinite programming based. A connection between the reformulation type bounds and the Gilmore-Lawler type bounds has been made using Lagrangian relaxation, see [16, 1]. The connection between Lagrangian and semidefinite relaxations is now well known, see e.g. [39, 33, 43]. In this chapter we unify many of the bounds in the literature using the Lagrangian relaxation approach. Our main theme is to show that with the correct choice of redundant constraints, we can illustrate the equivalence of many of the bounds with Lagrangian relaxations and therefore show in a transparent way how the bounds rank against each other.

The following (1.1) is the trace (Koopmans-Beckmann [25]) formulation of the QAP (see e.g. [30, 31] for various formulations and many useful applications), where the variable X is a permutation matrix and e is the vector of ones. As a model for facility location problems, where there are n facilities (locations), the matrix B represents distances between locations, the matrix A represents flows between facilities, and the matrix C represents fixed costs. We use the fact that assignment problems can be modelled using permutation matrices, and permutation matrices are 0,1 matrices with row and column sums 1. This formulation illustrates the quadratic nature of the objective function.

$$
QAP \qquad \begin{array}{lll} \mu^* := & \max & q(X) \quad \left(= \text{Trace}\,(AXB - 2C)X^T\right) \\ & \text{subject to} & Xe = e \\ & & X^T e = e \\ & & X_{ij} \in \{0,1\} \quad \forall i,j. \end{array} \tag{1.1}
$$

Rather than restricting the data to being the product of flows and distances, a more general formulation was given in [27]; see also [1].

1.1 PRELIMINARIES

1.1.1 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 $\mathcal{S}_t$

$\langle A, B \rangle$ Trace $A^T B$, the trace inner product of two matrices, § 1.1.2

$\mathcal{P}^t$ **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, (1.2)

$A \circ B$ $(A_{ij} B_{ij})$, the Hadamard (elementwise) 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

u the normalized vector of ones, $u = e/||e||$

V the orthogonal matrix to u, so $[u \mid V]$ is orthogonal

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

$\mathcal{E}$ $\{X : Xe = X^T e = e\}$, the set of matrices with row and column sums one

$\mathcal{Z}$ $\{X : X_{ij} \in \{0,1\}\}$, the set of (0,1)-matrices

$\mathcal{N}$ $\{X : X_{ij} \geq 0\}$, the set of nonnegative matrices

$\mathcal{O}$ $\mathcal{O} := \{X : XX^T = X^T X = I\}$, the set of orthogonal matrices

Π the set of permutation matrices, (1.3)

$\langle x, y \rangle_-$ $\min_{P \in \Pi} \langle x, Py \rangle$, the minimal scalar product of two vectors

$r(A)$ Ae, the vector of row sums of A

$s(A)$ $e^T Ae$, the sum of elements of A

Y_X the lifting of the matrix X, with $x = \mathrm{vec}\,(X)$,

$$Y_X := \begin{bmatrix} x_0 & x^T \\ x & xx^T \end{bmatrix}, \quad x_0^2 = 1$$

$\mathcal{G}_J(Y)$ Gangster operator, an operator that "shoots" holes or zeros in the matrix Y, (1.44)

$\mathcal{P}G(Y)$ Gangster operator projected onto its range space, (1.47)

$\mathrm{Arrow}\,(\cdot)$ the Arrow operator, (1.34)

$\mathrm{B^0Diag}\,(\cdot)$ the Block Diag operator, (1.35)

$\mathrm{O^0Diag}\,(\cdot)$ the Off Diag operator, (1.36)

$\mathrm{arrow}\,(\cdot)$ the arrow operator, (1.38)

$\mathrm{b^0diag}\,(\cdot)$ the block diag operator, (1.39)

$\mathrm{o^0diag}\,(\cdot)$ the off diag operator, (1.40)

QAP The trace formulation of QAP, (1.1)

LAP The linear assignment problem (QAP with no quadratic term)

$QAP_{\mathcal{E}}$ an equivalent formulation of QAP, (1.27)

$QAP_{\mathcal{O}}$ an equivalent formulation of QAP, (1.28)

1.1.2 Background. We work with $n \times n$ real matrices and use the trace inner product $\langle A, B \rangle = \text{Trace}\, A^T B$. We also work with several linear operators and their adjoints. Though linear operators in finite dimensions are equivalent to matrices, we find that using adjoints, rather than the transposes of the equivalent matrix representations, simplifies things in the long run. Note that for a linear operator $\mathcal{A}$, the adjoint operator, $\mathcal{A}^*$, satisfies

$$\langle \mathcal{A}x, y \rangle = \langle x, \mathcal{A}^* y \rangle, \quad \forall x, y. \tag{1.2}$$

The bounds we discuss involve relaxations of QAP. The constraints in QAP can be expressed in several ways, e.g. the permutation matrices satisfy

$$\Pi = \mathcal{O} \cap \mathcal{E} \cap \mathcal{N} = \mathcal{O} \cap \mathcal{N} = \mathcal{O} \cap \mathcal{Z} = \mathcal{E} \cap \mathcal{Z}. \tag{1.3}$$

Relaxations can be interpreted to mean that we ignore part of the definitions of permutation matrices. Usually we ignore the hard (or combinatorial) parts, e.g. $\mathcal{N}$ and/or $\mathcal{Z}$.

In [28], the authors present a review of three categories of existing bounds: first is Gilmore-Lawler (GLB) related bounds [18, 27] and the authors' new lower bounds (see also [37]); second is eigenvalue related bounds [15, 35, 21, 20]; third is reformulation type bounds e.g. [7, 11, 12, 1]. In [1], the authors present a new lower bound based on a mixed 0-1 linear formulation which is derived by constructing redundant quadratic inequalities and then defining additional continuous variables to replace all product terms. They show that this technique provides a strengthened version of the majority of lower bounding techniques. The major tool that they use is Lagrangian relaxation.

A seemingly independent category appears to be bounds based on semidefinite programming relaxations, e.g. [44]. In this chapter we show how these SDP type bounds can fit into and unite the eigenvalue type bounds and, in fact, the other bounds as well. The main theme of this chapter is to show how the SDP bounds arise using Lagrangian relaxation and thus provide strengthened versions of the other bounds. Indeed, we follow a similar approach to [1] in that we use many redundant quadratic constraints. However, the linearization that we do is different. Rather than defining additional continuous variables to replace product terms, we use the hidden (semidefinite) constraint that: *a quadratic function bounded below must be convex (positive semidefinite Hessian).* We see that the addition of the correct redundant constraints can be a very powerful tool in strengthening relaxations. In fact, in §3.4.1, we show that our SDP bound is always stronger than the one in [1].

Due to the equivalence between Lagrangian and SDP relaxations, we often do not differentiate between the two in this chapter.

1.1.3 Outline. This chapter is organized as follows. In §2. we present various eigenvalue bounds and their duality properties. This includes the hierarchical structure: the basic eigenvalue bound §2.1; the eigenvalue bounds using transformations (perturbations) §2.2; and the projected eigenvalue bound 2.3.

We then study the SDP relaxation for QAP in §3.. We derive the relaxation studied in [44] using Lagrangian relaxation, i.e. the relaxation is the Lagrangian dual of the Lagrangian dual of the quadratic model of the QAP obtained after adding redundant quadratic constraints. We discuss the geometry of the relaxation in §3.2 including the so-called *gangster operator* that results in a simplified relaxation at the end. Concluding remarks are given in §4..

2. EIGENVALUE TYPE BOUNDS

Linear bounds such as the Gilmore-Lawler bound deteriorate quickly as the dimension increases, e.g. [15, 20]. One of the earliest nonlinear bounds for QAP was based on eigenvalue techniques. We now look at several different eigenvalue bounds for QAP in increasing improvement, viewed using the SDP and Lagrangian relaxations. In §2.1 we look at the basic eigenvalue bound on the homogeneous QAP. Then §2.2 looks at improvements to this bound using transformations (perturbations) of the data. An improved bound is the projected bound in §2.3 which avoids one class of the perturbations. It is quite interesting to see how this bound can also be viewed using Lagrangian relaxation and adding redundant constraints. This view allows one to easily see that one class of the transformations (perturbations) are not helpful, i.e. the Lagrangian relaxation finds the best of these transformations automatically, see §2.4.

2.1 HOMOGENEOUS QAP

The first eigenvalue bounds for QAP are based on ignoring all but the orthogonality constraints, see e.g. [15, 20] and the survey article [30]. This was applied to the homogeneous QAP, i.e. the case where $C = 0$.

The bounds were based on a generalization of the eigenvalue problem. Let D be an $n \times n$ symmetric matrix. By abuse of notation, we define the quadratic function $q(x) = x^T Dx$. Then the Rayleigh Principle yields the following formulation of the smallest eigenvalue.

$$\lambda_{\min}(D) = \min_{x^T x=1} q(x) \quad (= x^T Dx).$$

This result can be proved easily using Lagrange multipliers, i.e. the optimum x must be a stationary point of the Lagrangian $q(x)+\lambda\left(1-x^Tx\right)$. We can get an equivalent SDP problem using Lagrangian duality and relaxation. Note that

$$\begin{aligned}
\lambda_{\min}(A) &= \min_{x^Tx=1} x^TAx \\
&= \min_x \max_\lambda x^TAx+\lambda\left(1-x^Tx\right) && (1.4)\\
&\geq \max_\lambda \min_x x^TAx+\lambda\left(1-x^Tx\right) && (1.5)\\
&= \max_{A-\lambda I\succeq 0} \min_x x^TAx+\lambda\left(1-x^Tx\right) && (1.6)\\
&= \max_{A-\lambda I\succeq 0} \min_x x^T(A-\lambda I)x+\lambda && (1.7)\\
&= \max_{A-\lambda I\succeq 0} \lambda=\lambda_{\min}(A). && (1.8)
\end{aligned}$$

The second equality (1.4) follows from the hidden constraint on the inner maximization problem, i.e. if $x^Tx\neq 1$ is chosen then the inner maximization is $+\infty$. If we add this hidden constraint $x^Tx=1$ to the minimization problem, then we recover the Rayleigh Principle. The next inequality (1.5) comes from interchanging min and max. The following equality (1.6) (and equivalently (1.7)) comes again from a hidden constraint, i.e. the quadratic function $x^T(A-\lambda I)x$ must be convex or the inner minimization is $-\infty$. This then yields the equivalence to the smallest eigenvalue problem (1.8) again. Thus we see the equivalence of this norm 1 problem with an SDP and with its Lagrangian dual. The trick to getting the equivalence was to use the hidden constraints.

Note that the above strong duality result still holds if the quadratic objective function $q(x)$ has a linear term. In this case the problem is called *the Trust Region Subproblem, TRS.* (See [40, Theorem 5.1] for the strong duality theorem.) However, strong duality can fail if there are two constraints, i.e. the so-called CDT problem [13]. Thus we see that going from one to two constraints, even if both constraints are convex, can result in a duality gap. Therefore, the following strong duality result in Theorem 2..2 below is very surprising.

We now relax the QAP to a quadratic problem over orthogonal constraints by ignoring both the nonnegativity and row and column sum constraints in (1.3), i.e. we consider the constraints

$$X^TX=I, \qquad X\in\mathcal{M}_n.$$

(The set of such X is sometimes known as the Stiefel manifold, e.g. [14, 41].) Because of the similarity of the orthogonality constraint to the norm constraint $x^Tx = 1$, the result of this section can be viewed as a matrix generalization of the strong duality result for the Rayleigh Principle given above. Thus we consider the homogeneous version of the QAP and its orthogonal relaxation

$$\text{QAP}_{\mathcal{O}} \qquad \mu^O := \begin{array}{ll} \min & \text{Trace}\, AXBX^T \\ \text{s.t.} & XX^T = I. \end{array} \tag{1.9}$$

Though this is a nonconvex problem with many nonconvex constraints, this problem can be solved efficiently using Lagrange multipliers and eigenvalues, see e.g. [21], or using the classical Hoffman-Wielandt inequality, e.g. [9]. The optimal value is the minimal scalar product of the eigenvalues of A and B. We include a simple proof for completeness using Lagrange multipliers. As was done for the ordinary eigenvalue problem above, we note that Lagrange multipliers can be used in two ways. First, one can use them in the necessary conditions (Karush-Kuhn-Tucker) for optimality, i.e. in the stationarity of the Lagrangian. This is how we apply them now. (The other use is in Lagrangian duality or Lagrangian relaxation where the Lagrangian is positive semidefinite. This is done below.) Also, the Lagrange multipliers here are symmetric matrices since the image of the constraint $X^TX - I$ is a symmetric matrix.

Proposition 2..1 *Suppose that the orthogonal diagonalizations of A, B are $A = V\Sigma V^T$ and $B = U\Lambda U^T$, respectively, where the eigenvalues in Σ are ordered nonincreasing, and the eigenvalues in Λ are ordered nondecreasing. Then the optimal value of* $\text{QAP}_{\mathcal{O}}$ *is* $\mu^O = \text{Trace}\, \Sigma\Lambda$, *and the optimal solution is obtained using the orthogonal matrices that yield the diagonalizations, i.e. $X^* = VU^T$.*

Proof. The constraint $G(X) := XX^T - I$ maps $\mathcal{M}_n$ to $\mathcal{S}_n$. The Jacobian of the constraint at X acting on the direction h is $J(X)(h) = Xh^T + hX^T$. (This can be found by simply expanding and neglecting the second order term.) The adjoint of the Jacobian acting on $S \in \mathcal{S}_n$ is $J^*(X)(S) = 2SX$, since

$$\text{Trace}\, SJ(X)(h) = \text{Trace}\, h^T J^*(X)(S).$$

But $J^*(X)(S) = 0$ implies $S = 0$, i.e. J^* is one-one for all X orthogonal. Therefore J is onto, i.e. the standard constraint qualification holds at the optimum. It follows that the necessary conditions for optimality are that the gradient of the Lagrangian

$$L(X, S) = \text{Trace}\, AXBX^T - \text{Trace}\, S(XX^T - I), \tag{1.10}$$

is 0, i.e.

$$AXB - SXI = 0.$$

Therefore,

$$AXBX^T = S = S^T,$$

i.e. $AXBX^T$ is symmetric which means that A and XBX^T commute and so are mutually diagonalizable by the orthogonal matrix U. Therefore, we can assume that both A and B are diagonal and we choose X to be a product of permutations that gives the correct ordering of the eigenvalues. ■

The second use of Lagrange multipliers is in forming the Lagrangian dual. The Lagrangian dual of $\text{QAP}_{\mathcal{O}}$ is

$$\max_{S=S^T} \min_{X} \operatorname{Trace} AXBX^T - \operatorname{Trace} S(XX^T - I). \tag{1.11}$$

However, there can be a nonzero duality gap for the Lagrangian dual, see [44, 6] and Example 3..2 below. The inner minimization in the dual problem (1.11) is an unconstrained quadratic minimization in the variables $\operatorname{vec}(X)$, with Hessian

$$B \otimes A - I \otimes S.$$

We apply the hidden semidefinite constraint again. This minimization is unbounded only if the Hessian is not positive semidefinite. In order to close the duality gap, we need a larger class of quadratic functions. Here is where our theme comes in, i.e. we find some redundant quadratic constraints to add. Note that in $\text{QAP}_{\mathcal{O}}$ the constraints $XX^T = I$ and $X^TX = I$ are equivalent. We add the redundant constraints $X^TX = I$ and arrive at

$$\begin{array}{llll} \text{QAP}_{\mathcal{O}\mathcal{O}} & \mu^O := & \min & \operatorname{Trace} AXBX^T \qquad (1.12) \\ & & \text{s.t.} & XX^T = I,\ X^TX = I. \qquad (1.13) \end{array}$$

Using symmetric matrices S and T to relax the constraints $XX^T = I$ and $X^TX = I$, respectively, we obtain a dual problem

$$\begin{array}{llll} \text{DQAP}_{\mathcal{O}\mathcal{O}} & \mu^O \geq \mu^D := & \max & \operatorname{Trace} S + \operatorname{Trace} T \\ & & \text{s.t.} & (I \otimes S) + (T \otimes I) \preceq (B \otimes A) \\ & & & S = S^T,\ T = T^T. \end{array}$$

We now prove the strong duality presented in [6]. We include two proofs. The first proof is from [6]; it uses the well known strong duality for LAP, the linear assignment problem; and, it uses the fact that we know the optimal value from Proposition 2..1. The second proof exploits the LAP duality results from the first proof; but, it illustrates where convexity and complementary slackness arise without using Proposition 2..1.

Theorem 2..2 *Strong duality holds for* $\mathrm{QAP}_{\mathcal{OO}}$ *and* $\mathrm{DQAP}_{\mathcal{OO}}$, *i.e.* $\mu^D = \mu^O$ *and both primal and dual are attained.*

Proof I. Let $A = V\Sigma V^T$, $B = U\Lambda U^T$, where V and U are orthonormal matrices whose columns are the eigenvectors of A and B, respectively, σ and λ are the corresponding vectors of eigenvalues, and $\Sigma = \operatorname{diag}(\sigma)$, $\Lambda = \operatorname{diag}(\lambda)$. Then for any S and T,

$$(B \otimes A) - (I \otimes S) - (T \otimes I) = (U \otimes V)\left[(\Lambda \otimes \Sigma) - (I \otimes \bar{S}) - (\bar{T} \otimes I)\right](U^T \otimes V^T),$$

where $\bar{S} = V^T S V$, $\bar{T} = U^T T U$. Since $U \otimes V$ is nonsingular, $\operatorname{Trace} S = \operatorname{Trace} \bar{S}$ and $\operatorname{Trace} T = \operatorname{Trace} \bar{T}$, the dual problem $\mathrm{DQAP}_{\mathcal{OO}}$ is equivalent to

$$\begin{array}{rll} \mu^D = & \max & \operatorname{Trace} S + \operatorname{Trace} T \\ & \text{s.t.} & (\Lambda \otimes \Sigma) - (I \otimes S) - (T \otimes I) \succeq 0 \\ & & S = S^T,\ T = T^T. \end{array} \tag{1.14}$$

However, since Λ and Σ are diagonal matrices, (1.14) is equivalent to the ordinary linear program:

$$\begin{array}{lll} \text{LD} & \max & e^T s + e^T t \\ & \text{s.t.} & \lambda_i \sigma_j - s_j - t_i \geq 0, \quad i,j = 1,\ldots,n. \end{array}$$

But LD is the dual of the linear assignment problem:

$$\begin{array}{lll} \text{LP} & \min & \sum_{i,j} \lambda_i \sigma_j y_{ij} \\ & \text{s.t.} & \sum_{j=1}^n y_{ij} = 1, \quad i = 1,\ldots,n \\ & & \sum_{i=1}^n y_{ij} = 1, \quad j = 1,\ldots,n \\ & & y_{ij} \geq 0, \quad i,j = 1,\ldots,n. \end{array}$$

Assume without loss of generality that $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$, and $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n$. Then LP can be interpreted as the problem of finding a permutation $\pi(\cdot)$ of $\{1,\ldots,n\}$ so that $\sum_{i=1}^n \lambda_i \sigma_{\pi(i)}$ is minimized. But the minimizing permutation is then $\pi(i) = i$, $i = 1,\ldots,n$, and from Proposition 2..1 the solution value μ^D is exactly μ^O.

Proof II. Using the above notation in Proof I, we diagonalize A and B. We can write (1.12) with diagonal matrices, i.e.

$$\mathrm{QAP}_{\mathcal{OO}} \qquad \mu^O := \begin{array}{ll} \min & \mathrm{Trace}\, V\Sigma V^T X U \Lambda U^T X^T \\ \text{s.t.} & XX^T = I,\ X^TX = I. \end{array}$$

With

$$Y = V^T X U, \tag{1.15}$$

we get the equivalent problem

$$\mathrm{QAP}_{\mathcal{OO}} \qquad \mu^O := \begin{array}{ll} \min & \mathrm{Trace}\, \Sigma Y \Lambda Y^T \\ \text{s.t.} & YY^T = I,\ Y^TY = I. \end{array} \tag{1.16}$$

The Lagrangian for this problem is

$$L(Y,S,T) = \mathrm{Trace}\, \Sigma Y \Lambda Y^T - \mathrm{Trace}\, S(YY^T - I) - \mathrm{Trace}\,(YTY^T - T).$$

Stationarity for the Lagrangian is

$$0 = \nabla L(Y,S,T) = \Sigma Y \Lambda - SYI - IYT.$$

As shown in Proof I, the dual program is equivalent to the ordinary linear program LD which is the dual of the LAP, LP above. Let Y be the optimal permutation of LP above and let S,T be the optimal solutions of LD above. Then the constraints of LD guarantee that the Hessian of the Lagrangian $L(Y,S,T)$ is positive semidefinite, i.e. the Lagrangian is convex in Y. In addition, complementary slackness between LD and LP is equivalent to the stationarity condition. Therefore, we have feasibility (and so complementary slackness), stationarity and convexity of the Lagrangian, i.e. these are the ingredients needed to guarantee optimality. Therefore Y is optimal for (1.16). After using the transformation (1.15), we get the optimal X for the original problem. ■

Remark 2..3 *Though we have strong duality between the above dual pairs, it is not known what happens if a linear term ($C \neq 0$) exists. The second proof of the above theorem could be used to study this case, i.e. one needs to use the optimal solution found from the dual LD to obtain an optimal solution for the original problem. To prove optimality one needs to use the following* necessary conditions for sufficiency to hold*: primal feasibility; stationarity of the Lagrangian (equivalently complementary slackness between the dual and the dual of the dual); and convexity of the Lagrangian.*

In [42], it is shown that a duality gap can *occur, for this orthogonal relaxation, if* $C \neq 0$. *This becomes clear once one notices that the optimal value of the dual is independent of the signs of the individual elements of* C. *Whereas, in the pure linear case, the optimal value is found using the sum of the singular values of* C, *see e.g. [42, Proposition 2.3]. However, one can close this duality gap, in the pure linear case, by using the objective function* $\text{Trace}\, YCX^T$ *and relaxing the constraints to* $XX^T + YY^T = I$, *see [42]. Thus, instead of doubling the number of constraints, we double the number of variables.*

2.2 PERTURBATIONS

Though the eigenvalue bound may be better then the linear type bounds, it still deteriorates very quickly as the dimension grows. One approach to improve this bound is to perform perturbations (transformations) on A and B that do not change the objective value but reduce the influence of the quadratic part of the objective function.

Note that the quadratic part can be bounded using Proposition 2..1, while the linear part is solved independently as a linear assignment problem, LAP. We let QAP(A,B,C) denote the optimal objective function value of the QAP defined by matrices A, B, C, and we let LAP(C) denote the optimal value of the LAP defined by C. The following eigenvalue related bound was proposed in [15].

$$QAP(A, B, C) \geq \langle \lambda(A), \lambda(B) \rangle_- + LAP(C). \tag{1.17}$$

To improve the bound in (1.17), transformations are applied to A, B and C that leave $q(X)$ unchanged over Π, but move a part of the quadratic over to the linear part. (The advantage for this is that the linear part is solved exactly.) Two types of transformations are known to have this property:

1. adding a constant to A or B either row or column-wise and appropriately modifying C;
2. changing the main diagonal of A or B and appropriately modifying C.

To be more specific, suppose $g, f, r, s \in \Re^n$. We define

$$\begin{aligned}
A(g,r) &:= A + ge^T + eg^T + \text{diag}\,(r) \\
B(f,s) &:= B + fe^T + ef^T + \text{diag}\,(s) \\
C(g,f,r,s) &:= C + 2Aef^T + 2ge^TB - 2ngf^T - 2\sum_k g_k ef^T
\end{aligned}$$

$$+\,\mathrm{diag}\,(A)s^T + r\ \mathrm{diag}\,(B)^T - 2gs^T - 2rf^T - rs^T.$$

Then it can easily be verified, see [15, 16], that

$$\begin{array}{rcl}\text{Trace }(AXB^T + C)X^T & = & \text{Trace }(A(g,r)XB^T(f,s) + C(g,f,r,s))X^T \\ & & \forall g,f,r,s \in \Re^n,\ \forall X \in \Pi.\end{array} \tag{1.18}$$

Relation (1.18) shows that we may choose any transformation $d := (g, f, r, s) \in \Re^{n\times 4}$ to derive bounds for QAP. There are several strategies for making reasonable choices for the transformations, [15, 35]. However, we will see below that these transformations actually come about from adding redundant constraints and taking the Lagrangian dual. Therefore, the best transformations are automatically chosen when using the semidefinite relaxation and there is no need for choosing any transformations.

2.3 PROJECTED EIGENVALUE BOUND

We saw above that we can solve the orthogonal relaxation of the homogeneous QAP using Lagrangian duality. We can then improve the resulting bound using perturbations. However, this results in a linear term. The next obvious question is how to handle this linear term. In addition, can we improve the bound by including the linear row and column sum constraints?

Since Lagrangian duality was so successful, it appears to make sense to use this now. However, The linear constraints have to be handled in a special way. We cannot just bring them into the Lagrangian with Lagrange multipliers as they will be ignored, since they have a zero contribution to the Hessian of the Lagrangian, see [33]. There are several ways to overcome this problem. One way is to eliminate the linear constraint. However, one would then drastically change the orthogonality constraint. Instead, we can use a special substitution and elimination. Let V be an $n \times (n-1)$ orthogonal matrix with e in the null space of V^T, i.e.

$$V^Te = 0, \quad V^TV = I.$$

Let $u := e/||e||$. Therefore

$$P := [u \mid V] \tag{1.19}$$

is a square orthogonal matrix. Then the following holds, see [21].

Lemma 2..4 *Let P be defined as in (1.19); let X be $n \times n$ and Y be $(n-1) \times (n-1)$. Suppose that X and Y satisfy*

$$X = P \begin{pmatrix} 1 & 0 \\ 0 & Y \end{pmatrix} P^T. \tag{1.20}$$

Then, the following three statements hold.

1. $X \in \mathcal{E}$;
2. $X \in \mathcal{N} \iff VYV^T \geq -uu^T$;
3. $X \in \mathcal{O}_n \iff Y \in \mathcal{O}_{n-1}$.

Conversely, if $X \in \mathcal{E}$, then there is a Y such that (1.20) holds.

■

Lemma 2..4 let's us substitute for X and the linear equality constraints without damaging the orthogonality constraints.

$$\begin{array}{rcl} q(X) & = & \text{Trace}\,[A(vv^T + VYV^T)B^T + C](vv^T + VY^TV^T) \\ & = & \text{Trace}\,\{Avv^TB^Tvv^T + Avv^TB^TVY^TV^T + AVYV^TB^Tvv^T + \\ & & \quad AVYV^TB^TVY^TV^T + Cvv^T + CVY^TV^T\} \\ & = & \text{Trace}\,\{(V^TAV)Y(V^TB^TV) + V^TCV + \frac{2}{n}V^Tr(A)r^T(B)V\}Y^T + \\ & & \quad \frac{s(A)s(B)}{n^2} + \frac{s(C)}{n}. \end{array}$$

Let $\hat{A} := V^TAV$, $\hat{B} := V^TBV, \hat{C} := V^TCV$ and $\hat{D} := \frac{2}{n}V^Tr(A)r^T(B)V + \hat{C}$. We now define the *projected* problem PQAP.

$$\text{PQAP} \quad \begin{array}{ll} \min & \text{Trace}\,\hat{A}Y\hat{B}^TY^T + \text{Trace}\,D[vv^T + VY^TV^T] \\ & \qquad\qquad\qquad -\frac{1}{n^2}s(A)s(B) \\ \text{s.t.} & Y \in \mathcal{O}, VYV^T \geq -vv^T, \end{array} \tag{1.21}$$

i.e. we have a very similar problem to QAP. The variable is still a square matrix,Y (though one dimension smaller). The constraints are still orthogonality and nonnegativity, though the nonnegativity is not just on the matrix variable Y itself.

We have derived the following equivalence and bound from [21].

Theorem 2..5 *Let X and Y be related by (1.20). Then X solves QAP $\iff$ Y solves PQAP.*

Theorem 2..6 *Let a symmetric QAP with matrices A,B and C be given. Then, using the notation from above*

$$QAP(A,B,C) \geq \left\langle \lambda(\hat{A}), \lambda(\hat{B}) \right\rangle_- + LAP(D) - s(A)s(B)/n^2.$$

■

Though there are special cases where one can minimize both the quadratic and the resulting term together, this is not true in general. This results in the deterioration of the bound since we are using the sum of the minimum of two functions rather than the minimum of the sum. However, this bound is a definite improvement over the eigenvalue bound without increasing the evaluation cost. We First note that the constant row and column transformations are not needed.

Proposition 2..7

$$PB(A,B,C) = PB(A(g,0),B(f,0),C(g,f,0,0)) \quad \forall g,f \in \Re^n.$$

■

2.4 STRENGTHENED PROJECTED EIGENVALUE BOUND

The above bound and proposition are proved in [21]. In [3] (numerical tests in [4]), a strengthened version of the projected eigenvalue bound is presented. This bound is an attempt to handle both the quadratic and linear terms together while maintaining convexity, or equivalently, tractability of the bound. We now look at a Lagrangian dual approach.

As mentioned above, we have to be careful how we handle linear constraints when taking the Lagrangian dual. Above, we substituted for X and eliminated the linear constraints. Another, equivalent, approach is to change the linear constraint to a quadratic constraint, e.g. to $||X^Te - e||^2 + ||Xe - e||^2 = 0$. This was the approach used in [44]. We now look at the Lagrangian dual of the problem with orthogonal and linear constraints, i.e.

$$\text{QAP}_{\mathcal{E}\mathcal{E}} \qquad \mu^O := \begin{array}{ll} \min & \text{Trace}\, AXBX^T - 2CX^T \\ \text{s.t.} & X^TX = I, XX^T = I, \\ & Xe = e, X^Te = e. \end{array} \tag{1.22}$$

In the case that $C = 0$, if we take the Lagrangian dual of this, then we get the bound that is equivalent to the projected eigenvalue bound. However, if we do the elimination or use the form $||X^Te - e||^2 + ||Xe - e||^2 = 0$ for the linear constraints, then the relaxation is equivalent to the elimination. Therefore, we can add redundant constraints that involve the linear constraints and not change the bound. For example, we can add the constraint, $XBX^Te = XBe$. After adding a Lagrange multiplier, we get $\text{Trace}\, ev^T\left(XBX^T - XB\right) = 0$. This is equivalent to the constant row transformation $A + ev^T$ which results in a linear term $\text{Trace}\, ev^T XB = \text{Trace}\, r(B)v^T X$. Similarly, we get the other constant row and column sum transformations. So we see that the reason for the lack of improvement is due to the considerations of adding redundant constraints in the Lagrangian dual. In fact, we can get many other transformations (perturbations) in this way, though they are no longer needed.

2.5 TRUST REGION TYPE BOUND

The Rayleigh quotient result for the minimum eigenvalue can be expressed using inequality, i.e.

$$\lambda_{\min}(A) = \min_{x^T x \leq 1} x^T A x.$$

Just as above, this can be expressed using strong duality and semidefinite programming. (In fact, we can add a linear term here as well and get the TRS.) The extension to matrices for QAP would involve the constraint $XX^T \preceq I$. A further relaxation of the above orthogonal relaxation is the trust region relaxation studied in [24, 5],

$$\begin{array}{rll} \mu^T := & \min & \text{Trace}\, AXBX^T \\ & \text{s.t.} & XX^T \preceq I. \end{array} \tag{1.23}$$

Though using the constraints $XX^T \preceq I$ in place of $XX^T = I$ weakens the bound on QAP; i.e. $\mu^T \leq \mu^O$, the constraints $XX^T \preceq I$ are convex, and so it is hoped that solving this problem would be useful in obtaining bounds for QAP and improve eigenvalue bounds in the case that $C \neq 0$. We first present the solution to the problem.

Theorem 2..8 *Let $V^T AV = \Sigma$, $U^T BU = \Lambda$, where $U, V \in \mathcal{O}$, $\Sigma = \text{Diag}\,(\sigma)$, $\Lambda = \text{Diag}\,(\lambda)$, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then for any X with $XX^T \preceq I$ we have*

$$\sum_{i=1}^{n} \min\{0, \lambda_i \sigma_{n-i+1}\} \leq \text{Trace}\, AXBX^T \leq \sum_{i=1}^{n} \max\{0, \lambda_i \sigma_i\}.$$

The upper bound is attained for $X = V\text{Diag}\,(\epsilon)U^T$, where $\epsilon_i = 1$ if $\sigma_i \lambda_i \geq 0$, and $\epsilon_i = 0$ otherwise. The lower bound is attained for $X = V\text{Diag}\,(\epsilon)JU^T$, where $\epsilon_i = 1$ if $\sigma_i \lambda_{n+1-i} \leq 0$, and $\epsilon_i = 0$ otherwise, $J = (e_n, e_{n-1}, \cdots, e_1)$ and e_i is the ith element unit vector.

■

As above we use the following problem with the redundant constraint added.

$$\text{QAPT} \qquad \begin{array}{rll} \mu^T = & \min & \operatorname{Trace} AXBX^T \\ & \text{s.t.} & XX^T \preceq I, \quad X^TX \preceq I. \end{array}$$

The dual program is

$$\text{DQAPT} \qquad \begin{array}{rll} \mu^T \geq \mu^{DT} := & \max & -\operatorname{Trace} S - \operatorname{Trace} T \\ & \text{s.t.} & (B \otimes A) + (I \otimes S) + (T \otimes I) \succeq 0 \\ & & S \succeq 0, \ T \succeq 0. \end{array}$$

The following strong duality result is presented in [5].

Theorem 2..9 *Strong duality holds for $QAPT$ and $DQAPT$, i.e. $\mu^T = \mu^{DT}$ and both primal and dual values are attained.*

No numerical tests have yet been done with this relaxation. However, it is interesting to observe that strong duality holds in this case even though the objective function is not convex. It is still unknown what happens if the objective function is not homogeneous.

3. SDP RELAXATIONS

We now present the SDP relaxation of QAP studied in [44]. (The missing details can be found there.) This relaxation arose by adding many redundant constraints and taking the Lagrangian dual of the Lagrangian dual and then removing redundant constraints at the end. Since we add many redundant constraints at the start, it can be shown that this is the strongest of the bounds that we have looked at so far. In addition, the final bound is greatly simplified by the application of a so-called *gangster operator*. This illustrates the strength of the Lagrangian dual approach to finding the SDP relaxation. One can add many redundant constraints at the start which contribute to the final SDP relaxation. This appears to create a very large SDP relaxation. However, many linear constraints can be shown to be redundant in the final relaxation.

Additional strengthening can be obtained by adding linear inequalities. This is discussed below in §3.4.

The QAP can be *lifted* into a higher dimensional space of symmetric matrices so as to obtain a tractable (convex) relaxation. (See e.g. [19, 29].) Suppose we represent the QAP using binary vectors $x := \operatorname{vec}(X)$. Then the embedding in $\mathcal{S}^{n^2+1}$ is obtained by

$$Y_X := \begin{pmatrix} x_0 \\ \operatorname{vec}(X) \end{pmatrix} (x_0, \operatorname{vec}(X)^T), \ x_0^2 = 1,$$

which results in Y_X being a symmetric and positive semidefinite matrix.

We now outline this for the quadratic constraints that arise from the fact that X is a $(0,1)$, orthogonal matrix . Let $X \in \Pi$ be a permutation matrix and, again, let $x = \text{vec}\,(X)$, $x_0^2 = 1$, and $c = \text{vec}\,(C)$. Then the objective function for QAP (by abuse of notation we add x_0) is

$$\begin{aligned} q(X, x_0) &= \text{Trace}\, AXBX^T - 2CX^T x_0 \\ &= x^T (B \otimes A) x - 2c^T x x_0 \\ &= \text{Trace}\, xx^T (B \otimes A) - 2c^T x x_0 \\ &= \text{Trace}\, L_Q Y_X, \end{aligned}$$

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

$$L_Q := \begin{bmatrix} 0 & -\text{vec}\,(C)^T \\ -\text{vec}\,(C) & B \otimes A \end{bmatrix}, \tag{1.24}$$

and

$$Y_X := \begin{bmatrix} 1 & x^T \\ x & xx^T \end{bmatrix}. \tag{1.25}$$

This shows how the objective function of QAP is transformed into a linear function in the SDP relaxation. 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 $X_{ij}^2 - X_{ij} = 0$ 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 (1.38) below. Similarly, the orthogonality constraint, $XX^T = I, X^T X = I$ can be written using the block diagonal constraint, see (1.39). and the block off diagonal constraints, see (1.40). The SDP relaxation with these constraints, as well as the ones arising from the row and column sums equal 1, is given below in (1.37).

3.1 LAGRANGIAN RELAXATION

Though we can derive the SDP relaxations directly as above, 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.

In the process we see several of the interesting operators that arise in the relaxation and add the gangster operator which results in a great simplification of the relaxation.

Remark 3..1 *Note that it could be 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 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 e.g. [26, 17].*

As we saw above (and also in [33, 44, 6, 5, 2]), adding, possibly redundant, quadratic constraints often tightens the SDP relaxation obtained through the Lagrangian dual. Using the fact that Π can be characterized as the intersection of (0,1)-matrices with $\mathcal{E}$ and $\mathcal{O}$, i.e.

$$\Pi = \mathcal{E} \cap \mathcal{Z} = \mathcal{O} \cap \mathcal{Z}, \tag{1.26}$$

we can rewrite QAP as

$$(QAP_{\mathcal{E}}) \qquad \begin{array}{rll} \mu^* := & \min & \text{Trace}\, AXBX^T - 2CX^T \\ & \text{s.t.} & XX^T = X^TX = I \\ & & Xe = X^Te = e \\ & & X_{ij}^2 - X_{ij} = 0, \quad \forall i,j. \end{array} \tag{1.27}$$

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 $i \neq j$. This is equivalent to the fact that the Hadamard products

$$(XP) \circ X = 0,$$

for all permutations P that do not leave any of the columns not permuted, i.e. the permutation does not have a 1-cycle. This latter constraint implies that there are a lot of zeros in the lifted matrices. This is essentially the ingredient for the gangster operator.

We now apply the recipe for the relaxations. We have added the, possibly redundant, constraints to the model. We now continue with the homogenization and taking Lagrangian duals. After changing the row and column sum constraints into $||Xe - e||^2 + ||X^Te - e||^2 = 0$, we consider the following equivalent problem to QAP.

$$(QAP_{\mathcal{O}}) \qquad \begin{array}{rll} \mu_{\mathcal{O}} := & \min & \operatorname{Trace} AXBX^T - 2CX^T \\ & \text{s.t.} & XX^T = I \\ & & X^TX = I \\ & & \|Xe - e\|^2 + \|X^Te - e\|^2 = 0 \\ & & X_{ij}^2 - X_{ij} = 0, \quad \forall i,j. \end{array} \tag{1.28}$$

We used the approach that changes the linear constraint to a quadratic constraint e.g. to $\|Xe - e\|^2 = 0$. This was the approach used in [44]. The result is an SDP relaxation where the Slater constraint qualification (strict feasibility) fails. (To overcome this problem, in order to successfully apply interior point methods, one projects the problem onto the so-called minimal face of the problem. Following this one can also remove redundant constraints. This is outlined below in §3.2.)

$$\begin{array}{rl} \mu_{\mathcal{O}} \geq \mu_{\mathcal{L}} := & \max\limits_{W,u_0} \min\limits_{XX^T=X^TX=I, x_0^2=1} \{\operatorname{Trace}[AXBX^T + W(X\circ X)^T \\ & \quad + u_0(\|Xe\|^2 + \|X^Te\|^2) - x_0(2C+W)X^T] \\ & \quad - 2x_0u_0e^T(X+X^T)e + 2nu_0x_0^2\}. \end{array} \tag{1.29}$$

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 $X^TX = I$, we get the lower bound μ_R

$$\begin{array}{l} \mu_{\mathcal{O}} \geq \mu_{\mathcal{L}} \geq \mu_R := \\ \quad \max\limits_{W,S_b,S_o,u_0,w_0} \min\limits_{X,\ x_0} \{\operatorname{Trace}[AXBX^T + u_0(\|Xe\|^2 + \|X^Te\|^2) \\ \qquad + W(X\circ X)^T + w_0x_0^2 + S_bXX^T + S_oX^TX] \\ \qquad - \operatorname{Trace} x_0(2C+W)X^T - 2x_0u_0e^T(X+X^T)e \\ \qquad - w_0 - \operatorname{Trace} S_b - \operatorname{Trace} S_o + 2nu_0x_0^2\}. \end{array} \tag{1.30}$$

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 (see [44]).

Example 3..2 *Consider the the pure quadratic, orthogonally constrained problem*

$$\begin{array}{rll} \mu^* := & \min & \operatorname{Trace} AXBX^T \\ & s.t. & XX^T = I, \end{array} \tag{1.31}$$

with 2×2 *matrices*

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

The dual problem is

$$\begin{array}{rcc}\mu^D := & \max & -\text{Trace}\, Ss \\ & s.t. & (B \otimes A + I \otimes Ss) \succeq 0 \\ & & S = S^T.\end{array} \qquad (1.32)$$

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* $-\text{Trace}\, Ss = 9$ *in the optimum. Thus we have a duality gap for this simple example.*

One can also easily construct a counterexample in the pure linear case, i.e. the case where $A = B = 0$. *The* 2×2 *example with* $C = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ *provides such an example, see [42].*

In (1.30), 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

$$\begin{array}{l}\mu_R = \\ \max\limits_{w, S_b, S_o, u_0} \min\limits_y \{ y^T \left[L_Q + \text{Arrow}\,(w) + \text{B}^0\text{Diag}\,(S_b) + \text{O}^0\text{Diag}\,(S_o) + u_0 D \right] y \\ \qquad\qquad - w_0 - \text{Trace}\, S_b - \text{Trace}\, S_o \},\end{array} \qquad (1.33)$$

where L_Q is as above and the linear operators

$$\text{Arrow}\,(w) := \begin{bmatrix} w_0 & -\frac{1}{2} w_{1:n^2}^T \\ -\frac{1}{2} w_{1:n^2} & \text{Diag}\,(w_{1:n^2}) \end{bmatrix}, \qquad (1.34)$$

$$\text{B}^0\text{Diag}\,(S) := \begin{bmatrix} 0 & 0 \\ 0 & I \otimes S_b \end{bmatrix}, \qquad (1.35)$$

$$\text{O}^0\text{Diag}\,(S_o) := \begin{bmatrix} 0 & 0 \\ 0 & S_o \otimes I \end{bmatrix}, \qquad (1.36)$$

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 (1.33), 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.

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

We now obtain our desired SDP relaxation of $(QAP_{\mathcal{O}})$ as the Lagrangian dual of $(D_{\mathcal{O}})$. This dual is derived just as in linear programming. The similarities are very noticeable. We introduce the $(n^2+1)\times(n^2+1)$ dual matrix variable $Y \succeq 0$ and derive the dual program to the SDP $(D_{\mathcal{O}})$.

$$(SDP_{\mathcal{O}}) \quad \begin{array}{lll} \min & \operatorname{Trace} L_Q Y & \\ \text{s.t.} & \mathrm{b}^0\mathrm{diag}(Y) = I, & \mathrm{o}^0\mathrm{diag}(Y) = I \\ & \operatorname{arrow}(Y) = e_0, & \operatorname{Trace} DY = 0 \\ & Y \succeq 0, & \end{array} \tag{1.37}$$

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

$$\operatorname{arrow}(Y) := \operatorname{diag}(Y) - \left(0, (Y_{0,1:n^2})^T\right), \tag{1.38}$$

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

$$\mathrm{b}^0\mathrm{diag}(Y) := \sum_{k=1}^{n} Y_{(k,\cdot),(k,\cdot)} \tag{1.39}$$

and

$$\mathrm{o}^0\mathrm{diag}(Y) := \sum_{k=1}^{n} Y_{(\cdot,k),(\cdot,k)}. \tag{1.40}$$

These are the adjoint operators of $\mathrm{B}^0\mathrm{Diag}(\cdot)$ and $\mathrm{O}^0\mathrm{Diag}(\cdot)$, 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 $X^TX = I$, respectively.

We have expressed the orthogonality constraints with both $XX^T = I$ and $X^TX = I$. 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.

3.2 GEOMETRY OF THE RELAXATION

Proposition 3..3 *Suppose that Y is feasible for the SDP relaxation (1.37). Then Y is singular.*

Proof. Note that $D \neq 0$ and both D, Y are positive semidefinite. Therefore Y has to be singular in order to satisfy the constraint $\text{Trace}\, DY = 0$. ■

Thus the feasible set of the primal problem $(SDP_{\mathcal{O}})$ has no strictly feasible points. However, it is easy to see that the dual problem $(D_{\mathcal{O}})$, does satisfy the Slater's constraint qualification (strict feasibility). This means that there is no duality gap between this SDP dual pair but, interior-point algorithms will have difficulty because, as formulated in this way, we have an ill-posed problem, e.g. the dual may not be attained. (See Example 3..4 below.) Fortuitously, one can use this to advantage, i.e. when Slater's condition fails one can project onto the so-called minimal face of the problem, see [10] and also [34]. Moreover, in our case here we can do this analytically and gain advantages without losing anything to numerical instability.

Example 3..4 *Consider the SDP pair*

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

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.

3.2.1 The Minimal Face. In order to overcome the above difficulties, we need to explore the geometrical structure of $F_{\mathcal{O}}$. We project the feasible set into a smaller dimensional space so that strict feasibility is satisfied. To do this we need to characterize the so-called minimal face of the problem, see [10].

The points

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

are feasible. Moreover, these points are rank-one matrices and are, therefore, contained in the set of extreme points of $F_{\mathcal{O}}$, see e.g. [32]. We need only consider faces of $F_{\mathcal{O}}$ which contain all of these extreme points. To do this, we 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..7 below.)

Define the following $(n^2+1) \times ((n-1)^2+1)$ matrix.

$$\hat{V} := \left[\begin{array}{c|c} 1 & 0 \\ \hline \frac{1}{n}(e \otimes e) & V \otimes V \end{array} \right], \tag{1.41}$$

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

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

The following theorem characterizes the minimal face by finding the barycenter of the convex hull of the permutation matrices and using the fact that a face of $\mathcal{P}$ can be characterized using the null space (or range space) of any point in its relative interior. We now see that the barycenter has a very simple and elegant structure.

Theorem 3..5 *Define the barycenter*

$$\hat{Y} := \frac{1}{n!} \sum_{X \in \Pi} Y_X. \tag{1.42}$$

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*

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

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

$$(2, \frac{1}{n-1}e^T_{(n-1)^2}, 0e^T_{2n-1})^T.$$

4. The null space and range space are

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

■

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..6 *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..7 *Consider the constraints*

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

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.

3.2.2 The Projected SDP Relaxation. In Theorem 3..5, we presented explicit expressions for the range and null space of the barycenter, denoted $\hat{Y}$. It is well known, see e.g. [8], 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

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

where S is a given subspace. In particular, if $\hat{X} \in \operatorname{relint} \mathcal{K}$, 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..5, we can project the SDP relaxation $(SDP_{\mathcal{O}})$ onto the minimal face. The projected problem is

$$(QAP_{R1}) \quad \begin{array}{rll} \mu_{R1} := & \min & \operatorname{Trace}(\hat{V}^T L_Q \hat{V}) R \\ & \text{s.t.} & \mathrm{b}^0\mathrm{diag}\,(\hat{V} R \hat{V}^T) = I, \qquad \mathrm{o}^0\mathrm{diag}\,(\hat{V} R \hat{V}^T) = I \\ & & \operatorname{arrow}(\hat{V} R \hat{V}^T) = e_0, \qquad R \succeq 0. \end{array} \tag{1.43}$$

Note that the constraint $\operatorname{Trace}(\hat{V}^T D \hat{V}) R = 0$ can be dropped since it is always satisfied, i.e. $D\hat{V} = 0$.

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.

3.3 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. (These entries are easy to handle with a linear operator constraint.) The relaxation is obtained from

$$\begin{aligned} Y_X &= \begin{pmatrix} 1 \\ \operatorname{vec}(X) \end{pmatrix} (1 \;\; \operatorname{vec}(X)^T) \\ &= \begin{pmatrix} 1 \\ X_{:1} \\ X_{:2} \\ \vdots \\ X_{:n} \end{pmatrix} (1 \;\; X_{:1}^T \;\; X_{:2}^T \;\; \vdots \;\; X_{:n}^T) \end{aligned}$$

which contains the n^2 blocks

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

We then have

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

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, i.e. for $J \subset \{(i,j) : 1 \leq i,j \leq n^2+1\}$. $\mathcal{G}_J : \mathcal{S}^{n^2+1} \to \mathcal{S}^{n^2+1}$ is called the *Gangster* operator if

$$(\mathcal{G}_J(Y))_{ij} := \begin{cases} Y_{ij} & \text{if } (i,j) \in J \\ 0 & \text{otherwise.} \end{cases} \tag{1.44}$$

Denote the subspace of matrices

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

Then the range and null space of $\mathcal{G}_J$ satisfy

$$\mathcal{R}(\mathcal{G}_J) = \mathcal{S}^J$$

and

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

where $-J$ denotes the complement of the set J. Let $J := \{(i,j) : \hat{Y}_{ij} = 0\}$, be the zeros found above using the Hadamard product; we have

$$\mathcal{G}_J(\hat{Y}) = 0. \tag{1.45}$$

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 (1.45), we have

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

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

$$\mathcal{G}_J(Y) = 0. \tag{1.46}$$

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.

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

3.3.1 The Gangster Operator and Redundant Constraints.

The addition of the gangster operator allows makes many constraints redundant. Define the subset $\hat{J}$ of J, of indices of Y, (a union of two sets)

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

These are the indices for the 0 elements of the barycenter. (We do not include (up to symmetry) the off-diagonal block $(n-2, n-1)$ or the last column of off-diagonal blocks.) After removing redundant constraints, this results in the following simple projected relaxation.

$$(QAP_{R2}) \qquad \begin{array}{rll} \mu_{R2} := & \min & \text{Trace}\,(\hat{V}^T L_Q \hat{V})R \\ & \text{s.t.} & \mathcal{G}_{\bar{J}}(\hat{V}R\hat{V}^T) = E_{00} \\ & & R \succeq 0. \end{array} \tag{1.47}$$

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

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

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

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

3.4 INEQUALITY CONSTRAINTS

An important technique that is used to further tighten the derived relaxations is to add generic linear inequality constraints. 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

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

see e.g. [23, 38]. In addition, in [22] the authors 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. The basic relaxation (QAP_{R1}) can use both nonnegativity and nonpositivity constraints to approximate the gangster operator, e.g.

$$\mathcal{G}_J(\hat{V}R\hat{V}^T) \leq 0. \tag{1.48}$$

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.

Further strengthening can be done using a second lifting, see [2].

3.4.1 A Comparison with Linear Relaxations. We now look at how our relaxations of QAP compare to relaxations based on linear programming. Adams and Johnson [1] 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

$$(QAP_{CLP}) \quad \mu_{CLP} := \min\{\operatorname{Trace} LZ : Z \in \mathcal{F}_{CLP}\} \tag{1.49}$$

where the feasible set is

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

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 $\mathcal{G}_J(Y) = 0$. 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 $Y \in \mathcal{P}$.

4. CONCLUSION

In this chapter we have derived and ranked many of the known bounds for QAP. The comparisons between the bounds was done using Lagrangian relaxation. Bounds were derived by using relaxed quadratic models of QAP and taking the Lagrangian relaxation. Thus, stronger quadratic models resulted in stronger bounds. The strongest of these bounds was the SDP relaxation studied in §3.2.2. This relaxation had a surprisingly simple form after the addition of the gangster operator. A primal-dual interior-point algorithm that solves this SDP relaxation, along with numerical tests, can be found in [44]. Further testing for these bounds as well as new bounds based on trust region methods is being done in [36].

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