ADMM for the **SDP** relaxation of the **QAP***

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Abstract

Semidefinite programming, SDP, relaxations have proven to be extremely strong for many hard discrete optimization problems. This is in particular true for the quadratic assignment problem, QAP, arguably one of the hardest NP-hard discrete optimization problems. There are several difficulties that arise in efficiently solving the SDP relaxation, e.g., increased dimension; inefficiency of the current primaldual interior point solvers in terms of both time and accuracy; and difficulty and high expense in adding cutting plane constraints.

We propose using the alternating direction method of multipliers ADMM in combination with facial reduction, FR, to solve the SDP relaxation. This first order approach allows for: inexpensive iterations, a method of cheaply obtaining low rank solutions; and a trivial way of exploiting the FR for adding cutting plane inequalities. In fact, we solve the doubly nonnegative, **DNN**, relaxation that includes both the SDP and all the nonnegativity constraints. When compared to current approaches and current best available bounds we obtain robustness, efficiency and improved bounds.¹

Keywords: Quadratic assignment problem, semidefinite programming relaxation, alternating direction method of multipliers, facial reduction, doubly nonnegative, large scale.

Classification code: 90C22, 90B80, 90C46, 90C06, 90-08

Introduction 1

The quadratic assignment problem, QAP, in the trace formulation [11] is

$$(\mathbf{QAP}) \qquad p^* := \min_{X \in \Pi_n} \langle AXB - 2C, X \rangle, \tag{1.1}$$

where $A, B \in \mathbb{S}^n$ are real symmetric $n \times n$ matrices, C is a real $n \times n$ matrix, $\langle \cdot, \cdot \rangle$ denotes the trace inner product, i.e., $\langle Y, X \rangle = \operatorname{trace} Y X^{\top}$, and Π_n denotes the set of $n \times n$ permutation matrices. A typical application of the \mathbf{QAP} is to assign n facilities to n locations while minimizing total cost. This total cost uses the flow A_{ij} between a pair of facilities i, j multiplied by the distance B_{st} between their assigned locations s,t, respectively. Included is the location cost C_{is} of placing facility i in location s. The **QAP** was first introduced as a model for analyzing the location of economic activities [17,18]. Further applications include: various layout problems, e.g., hospitals, airports, circuit boards, VLSI keyboards; bandwith minimization of a graph; image processing; molecular conformations in chemistry; scheduling; supply chains; manufacturing

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¹The code can be downloaded from the author's webpage https://xu-yangyang.github.io/ADMM_QAP/

lines. Moreover, many well known discrete optimization problems are a special case of \mathbf{QAP} , e.g., the traveling salesman problem and the maximum cut problem; see e.g., [3, 20, 21].

It is well known that the \mathbf{QAP} is an NP-hard problem and that problems with size as moderate as n=30 still remain difficult to solve, e.g., [1]. Solution techniques rely on efficiently calculating lower and upper bounds. An important tool for finding lower bounds is the work in [28] that provides a semidefinite programming (\mathbf{SDP}), relaxation of (1.1). In particular, this relaxation uses facial reduction (\mathbf{FR}) to guarantee strict feasibility for both the relaxation and its dual and thus providing robustness; and \mathbf{FR} greatly simplifies the constraints by making many of them redundant. The methods of choice for \mathbf{SDP} are based on a primal-dual interior-point, p-d i-p, approach. These methods cannot solve large problems, have difficulty in obtaining high accuracy solutions, and cannot properly exploit sparsity. Moreover, it is very expensive to add on nonnegativity and other cutting plane constraints. The current state for finding bounds and solving \mathbf{QAP} is given in e.g., [1, 2, 6, 9, 23, 24].

1.1 Contributions

In this paper we apply the alternating direction method of multipliers (ADMM) for solving the facially reduced SDP relaxation of the QAP where we add additional elementwise nonnegativity constraints to the SDP constraints, i.e., an ADMM method for solving a doubly nonnegative (DNN) problem. Our model takes particular advantage of the facial reduction by doubling the number of variables so that the ADMM approach can take advantage of separate simplified subproblems for the semidefinite constraints and the elementwise nonnegativity constraints. The recent papers [16,27] also present algorithms for solving the DNN relaxation of QAP, and their methods turn out to be very efficient for finding strong lower bounds of many QAP instances. However, they do not use the FR technique, and our lower bounds are stronger on many of our tested instances.

We compare our upper and lower bounds with: the best known results given in [24]; the best known bounds found at SDPLIB [7]; and with a p-d i-p methods based on the so-called HKM direction. We tested all symmetric instances from QAPLIB [7] with sizes up to n=100. We find that our bounds strictly improve on the existing bounds in the literature and provably solve many instances to optimality. Moreover, we see that the **ADMM** method is significantly faster, and can often easily obtain medium-accuracy solutions, that are sufficient to provide strong lower bounds for **QAP**. This is partly due to the ability of obtaining low rank **SDP** solutions, as well as being able to solve the subproblems within the **ADMM** method fast and accurately. Finally, by exploiting low rank projections, we also obtain strong upper bounds.

1.2 Related works

A survey for various eigenvalue and **SDP** type lower bounds for **QAP** is given in [1]. Included are exact solution techniques as well. A copositive program, **CP**, is formulated in [23] and is shown to be equivalent to the **QAP**. Although the **CP** is convex, it is still intractable. Starting with the **CP**, several relaxations of **QAP** are presented in [23]. A review and a comparison with several other **SDP** relaxations is included.

Since the submission of our paper, we have become aware of the results in [15, 16, 27]. The work [15] studies optimization over permutation matrices. It shows that a penalized problem with the ℓ_0 seminorm can recover the solution to the original one if the penalty parameter is sufficiently large. Based on that observation, [15] uses an $\ell_p, p \in (0, 1)$ seminorm to replace the ℓ_0 term. In addition, an ℓ_p regularization algorithm is used to find KKT points of a sequence of smoothed ℓ_p regularized problems. The algorithm is guaranteed to return a permutation matrix in a finite number of steps. Applied to the **QAP**, it will give a feasible solution and thus provide an upper bound.

General quadratic optimization with linear and also binary constraints is studied in [16]. This includes **QAP** as a special case. A Lagrangian-DNN relaxation is solved. Based on a formulation given in [23], lower bounds for some **QAP** instances are reported in [16]. It is demonstrated that the Lagrangian-DNN approach can be significantly faster than a Newton-CG **SDP** method (SDPNAL) [29], and comparable lower bounds

are obtained. In contrast, our method yields the same or even better lower bounds on all the common tested instances except for Char20c, even though a small tolerance 10^{-12} was set in [16]. This is most likely due to the fact that FR was not used.

An improved version of SDPNAL, called SDPNAL+, is given in [27]. Using a good initial point found with an **ADMM** type method, SDPNAL+ applies a semismooth Newton-CG to subproblems in the augmented Lagrangian method framework. It is shown to be superior to several other other **SDP** solvers and can solve many difficult **SDP**s from **QAP** instances to tolerance of order 10⁻⁶. When compared to our appraoch, [27] obtains a better lower bound only on the instance **Tai25a**, and for many other tested instances, our results turn out to be strictly better. As noted above, this is possibly due to the use of **FR**.

More recently, [13] introduced a MATLAB based software package BBCPOP, that appears to improve further on [27] for solving the **DNN** relaxation of **QAP**. It applies the solver on the same relaxation used in [16]. It obtained a stronger lower bound than our approach on the single instance Char20c, while our lower bounds were strictly better on many tested instances.

We note that previous success of **ADMM** for solving **SDP** is presented in e.g., [26]. Convincing results on a few combinatorial optimization problems were obtained.. A detailed survey for **ADMM** can be found in [5].

1.3 Outline

We continue in Section 2 with a new derivation of the facially reduced **SDP** relaxation of the **QAP** from [28]. This derivation is novel in that it directly includes the so-called *gangster constraints*. The new **ADMM** approach is presented in Section 3, where details of the **ADMM** subproblems are included, as well as details for obtaining the lower bounds from possibly inaccurate solutions of the **SDP**, and obtaining the upper bounds efficiently. Our numerics are presented in Section 4 with several tables. We conclude in Section 5.

2 A New Derivation for the SDP Relaxation

In this section we present a new derivation of the facially reduced **SDP** relaxation of the **QAP** obtained in [28]. The derivation is new in that the *gangster constraints* are obtained directly. We first briefly introduce **FR** and then derive the **SDP** relaxation from the dual of the Lagrangian dual.

2.1 Original FR for SDP relaxation of QAP

The **SDP** relaxation of the **QAP** in [28] begins with a set of quadratic constraints that represent the permutation matrices. Then, the Lagrangian relaxation (Lagrangian dual) is formed and shown to be equivalent to an **SDP**. The dual of this Lagrangian dual is then the **SDP** relaxation of the **QAP**. However, it is then shown in [28] that strict feasibility fails for this **SDP** relaxation. But one can find the barycenter, \hat{Y} , of the feasible set and use the spectral decomposition

$$\widehat{Y} = \begin{bmatrix} \widehat{V} & \widehat{U} \end{bmatrix} \begin{bmatrix} D \succ 0 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \widehat{V} & \widehat{U} \end{bmatrix}^T$$

to obtain the facial reduction, minimal face \mathcal{F} , of all feasible Y for the **SDP** relaxation,

$$Y \in \mathcal{F} := \widehat{V} \mathbb{S}_{+}^{(n-1)^2 + 1} \widehat{V}^T \leq \mathbb{S}^{n^2 + 1},$$

where \leq denotes face. Using the substitution $Y = \hat{V}R\hat{V}^T$ results in a smaller dimensional problem and moreover, this substitution and the addition of the gangster constraints, makes many of the original constraints redundant. The result is an elegant, much simplified, stable **SDP** relaxation.

2.2 The new derivation

We now provide the new derivation of the facially reduced **SDP** relaxation in [28]. We start with the following equivalent quadratically constrained quadratic problem for **QAP**

$$\min_{X} \langle AXB - 2C, X \rangle
\text{s.t. } X_{ij} X_{ik} = 0, \ X_{ji} X_{ki} = 0, \ \forall i, \ \forall j \neq k,
X_{ij}^2 - X_{ij} = 0, \ \forall i, j,
\sum_{i=1}^n X_{ij}^2 - 1 = 0, \ \forall j, \ \sum_{i=1}^n X_{ij}^2 - 1 = 0, \ \forall i.$$
(2.1)

Remark 2.1. Note that the quadratic orthogonality constraints $X^{\top}X = I$, $XX^{\top} = I$, and the linear row and column sum constraints Xe = e, $X^{\top}e = e$, can all be represented using linear combinations of those in (2.1). This observation avoids the need for adding all the redundant quadratic constraints and then removing redundant linear constraints in the **SDP**. Here e is the vector of all ones.

In addition, the first set of constraints, the elementwise orthogonality of the row and columns of X, are referred to as the gangster constraints. They are particularly strong constraints and enable many of the other constraints to be redundant. In fact, after the $\mathbf{F}\mathbf{R}$ is done, many of these gangster constraints also become redundant.

The Lagrangian for (2.1) is

$$\mathcal{L}_{0}(X, U, V, W, u, v) = \langle AXB - 2C, X \rangle + \sum_{i=1}^{n} \sum_{j \neq k} U_{jk}^{(i)} X_{ij} X_{ik} + \sum_{i=1}^{n} \sum_{j \neq k} V_{jk}^{(i)} X_{ji} X_{ki} + \sum_{i,j} W_{ij} (X_{ij}^{2} - X_{ij}) + \sum_{j=1}^{n} u_{j} \left(\sum_{i=1}^{n} X_{ij}^{2} - 1 \right) + \sum_{i=1}^{n} v_{i} \left(\sum_{j=1}^{n} X_{ij}^{2} - 1 \right).$$

The dual problem is a maximization of the dual functional d_0 ,

$$\max \ d_0(U, V, W, u, v) := \min_X \mathcal{L}_0(X, U, V, W, u, v). \tag{2.2}$$

To simplify the dual problem, we homogenize \mathcal{L}_0 by multiplying the degree-one terms in X by a scalar variable x_0 and adding the single constraint $x_0^2 = 1$ to the dual functional. We add the additional dual variable w_0 and let

$$\mathcal{L}_{1}(X, x_{0}, U, V, W, w_{0}, u, v) = \langle AXB - 2x_{0}C, X \rangle + \sum_{i=1}^{n} \sum_{j \neq k} U_{jk}^{(i)} X_{ij} X_{ik} + \sum_{i=1}^{n} \sum_{j \neq k} V_{jk}^{(i)} X_{ji} X_{ki}$$

$$+ \sum_{i,j} W_{ij} (X_{ij}^{2} - x_{0}X_{ij}) + \sum_{j=1}^{n} u_{j} \left(\sum_{i=1}^{n} X_{ij}^{2} - 1 \right)$$

$$+ \sum_{i=1}^{n} v_{i} \left(\sum_{j=1}^{n} X_{ij}^{2} - 1 \right) + w_{0} (x_{0}^{2} - 1).$$

This homogenization technique is the same as that in [28]. The new dual problem is

$$\max \ d_1(U, V, W, w_0, u, v) := \min_{X, x_0} \mathcal{L}_1(X, x_0, U, V, W, w_0, u, v). \tag{2.3}$$

Note that the dual functionals satisfy $d_1 \leq d_0$. Hence, our relaxation still yields a lower bound to (2.1). In fact, the relaxations give the same lower bound. This follows from strong duality of the trust region subproblem as shown in [28].

Let x = vec(X), $y = [x_0; x]$, and w = vec(W), where vec(X) denotes the columnwise vectorization of X. Then

 $\mathcal{L}_{1}(X, x_{0}, U, V, W, w_{0}, u, v) = y^{\top} \left[L_{Q} + \mathcal{B}_{1}(U) + \mathcal{B}_{2}(V) + \operatorname{Arrow}(w, w_{0}) + \mathcal{K}_{1}(u) + \mathcal{K}_{2}(v) \right] y - e^{\top}(u + v) - w_{0},$ where

$$\begin{split} \mathcal{K}_1(u) &= \mathrm{blkdiag}(0, u \otimes I), \quad \mathcal{K}_2(v) = \mathrm{blkdiag}(0, I \otimes v), \\ \mathcal{B}_1(U) &= \mathrm{blkdiag}(0, \widetilde{U}), \quad \mathcal{B}_2(V) = \mathrm{blkdiag}(0, \widetilde{V}), \\ L_Q &= \left[\begin{array}{cc} 0 & -\mathrm{vec}(C)^\top \\ -\mathrm{vec}(C) & B \otimes A \end{array} \right], \quad \mathrm{Arrow}(w, w_0) = \left[\begin{array}{cc} w_0 & -\frac{1}{2}w^\top \\ -\frac{1}{2}w & \mathrm{Diag}(w) \end{array} \right]. \end{split}$$

Here, \otimes denotes the *Kronecker product*, and \widetilde{U} and \widetilde{V} are $n \times n$ block matrices. \widetilde{U} has zero diagonal blocks and the (j,k)-th off-diagonal block is the diagonal matrix $\mathrm{Diag}(U_{jk}^{(1)},\ldots,U_{jk}^{(n)})$, for all $j \neq k$. \widetilde{V} has zero

off-diagonal blocks and the *i*-th diagonal block is $\begin{bmatrix} 0 & V_{12}^{(i)} & \cdots & V_{1n}^{(i)} \\ V_{21}^{(i)} & 0 & \cdots & V_{2n}^{(i)} \\ \vdots & \vdots & \ddots & \vdots \\ V_{n1}^{(i)} & V_{n2}^{(i)} & \cdots & 0 \end{bmatrix}.$ We use blkdiag (A_1, A_2) to denote the block diagonal matrix with principal diagonal matrix.

denote the block diagonal matrix with principal diagonal blocks A_1, A_2 , cf. the same command in MATLAB. Hence, the dual problem (2.3) is equivalent to the **SDP**

$$\max - e^{\top}(u+v) - w_0$$
s.t. $L_Q + \mathcal{B}_1(U) + \mathcal{B}_2(V) + \text{Arrow}(w, w_0) + \mathcal{K}_1(u) + \mathcal{K}_2(v) \succeq 0.$ (2.4)

To obtain the **SDP** relaxation of (2.1), we further take the dual of (2.4). Before presenting the relaxation, we give a few definitions.

Definition 2.2 (block matrix $Y \in \mathbb{S}^{n^2+1}$). Given n^2 matrices \widetilde{Y}_{ij} for i = 1, ..., n and j = 1, ..., n that satisfy $\widetilde{Y}_{ij} = \widetilde{Y}_{ji}^{\top}$, let \overline{Y} be the $n \times n$ block matrix with \widetilde{Y}_{ij} as the (i, j)-th block. We form the symmetric block matrix

$$Y = \begin{bmatrix} y_{00} & y_0^{\top} \\ y_0 & \bar{Y} \end{bmatrix}, \tag{2.5}$$

where y_{00} is a scalar, and y_0 is a vector in \mathbb{R}^{n^2} .

Definition 2.3 (Gangster index set). The gangster index set, J is defined to be the union of the top left index (00) and the set of indices i < j in the matrix \bar{Y} in (2.5) corresponding to:

- 1. the off-diagonal elements in the n diagonal blocks;
- 2. the diagonal elements in the off-diagonal blocks.

Definition 2.4 (Gangster operator). The gangster operator, \mathcal{G}_J : $\mathbb{S}^{n^2+1} \to \mathbb{S}^{n^2+1}$ is defined by

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

By abuse of notation, we let the same symbol denote the projection onto $\mathbb{R}^{|J|}$, and thus for $y \in \mathbb{R}^{|J|}$, the adjoint yields $Y = \mathcal{G}_J^*(y) \in \mathbb{S}^{n^2+1}$ obtained by symmetrization and filling in the missing elements with zeros.

Now, taking the dual of (2.4), we have the **SDP** relaxation of (2.1):

min
$$\langle L_Q, Y \rangle$$

s.t. $\mathcal{G}_J(Y) = E_{00}$
 $\operatorname{diag}(\bar{Y}) = y_0$
 $\operatorname{trace}(\tilde{Y}_{ii}) = 1, \, \forall i$
 $\sum_{i=1}^n \tilde{Y}_{ii} = I$
 $Y \succeq 0,$ (2.6)

where $E_{00} = e_0 e_0^T$ is the outer product of the first unit vector, the block matrix Y is defined in Definition 2.2 and the gangster index set J and the gangster operator \mathcal{G}_J are defined in Definitions 2.3 and 2.4. Note that the variable Y in (2.6) is in a higher dimensional space compared to the original variable X in (2.1). This can be motivated from the lifting $Y = \begin{pmatrix} 1 \\ \text{vec}(X) \end{pmatrix} \begin{pmatrix} 1 \\ \text{vec}(X) \end{pmatrix}^{\top}$. We apply **ADMM** to an equivalent, more

Remark 2.5. If one more feasible quadratic constraint q(X) can be added to (2.1), and q(X) cannot be linearly represented by those in (2.1), the relaxation following the same derivation as above can be tighter. We conjecture that no more such q(X) exists, and thus (2.6) is the tightest among all Lagrange dual relaxations from a quadratically constrained program like (2.1). However, this does not mean that more linear inequality constraints cannot be added, i.e., linear cuts.

2.3 Strict feasibility by FR

As above, let e be the vector of all ones of appropriate dimension, and let $V \in \mathbb{R}^{n \times (n-1)}$ be full column rank with $V^T e = 0$, and

$$\widehat{V} = \begin{bmatrix} 1 & 0 \\ \frac{1}{n}e & V \otimes V \end{bmatrix}. \tag{2.7}$$

FR is applied in [28] by using the substitution

succinct, modification of (2.6). (See (3.1) and Theorem 3.1, below.)

$$Y = \widehat{V}R\widehat{V}^{\top} \in \mathbb{S}^{n^2+1}. \tag{2.8}$$

This way, it is shown that (2.6) is equivalent to

$$p_R^* := \min_R \quad \langle \widehat{V}^\top L_Q \widehat{V}, R \rangle$$
s.t.
$$\mathcal{G}_J(\widehat{V} R \widehat{V}^\top) = E_{00}$$

$$R \succeq 0,$$
(2.9)

a greatly simplified **SDP**. This simplification arising from **FR** allows for the **ADMM** to be applied efficiently for the **DNN** problem, i.e., we use the equivalence in (2.8) to relate Y, R and apply the gangster constraints and nonnegativity on Y while applying the semidefinite constraint on R.

Note that after \mathbf{FR} , many constraints in (2.6) become redundant, and also we can remove redundant indices in J: the diagonal (zero) constraints in the last column of off-diagonal blocks and in the (n-2, n-1) off-diagonal block. By abuse of notation, we use the same notation J and \mathcal{G}_J after removing these indices. Another advantage of (2.9) is that strict feasibility holds, i.e., there exists a feasible R > 0, as shown in Lemma 2.6. In addition, strict feasibility holds for its dual problem, see Lemma 2.7. Both lemmas are from [28].

Lemma 2.6. The matrix \hat{R} defined by

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

is (strictly) feasible for (2.9).

We note that the gangster operator is self-adjoint, $\mathcal{G}_J^* = \mathcal{G}_J$. Therefore, the dual of (2.9) can be written as the following:

$$d_Y^* := \max_{Y} \quad \langle E_{00}, Y \rangle \qquad (=Y_{00})$$

s.t. $\hat{V}^{\top} \mathcal{G}_J(Y) \hat{V} \preceq \hat{V}^{\top} L_Q \hat{V}.$ (2.10)

Again by abuse of notation, using the same symbol twice, we get the two equivalent dual constraints:

$$\hat{V}^{\top} \mathcal{G}_J(Y) \hat{V} \preceq \hat{V}^{\top} L_Q \hat{V}; \qquad \hat{V}^{\top} \mathcal{G}_J^*(y) \hat{V} \preceq \hat{V}^{\top} L_Q \hat{V}.$$

As above, the dual variable for the first form is $Y \in \mathbb{S}^{n^2+1}$ and for the second form is $y \in \mathbb{R}^{|J|}$. We have used \mathcal{G}^* for the second form to emphasize that only the first form is self-adjoint.

Lemma 2.7. Define matrices \hat{Y} , \hat{Z} , with M > 0 sufficiently large, by

$$\widehat{Y} := M \left[\begin{array}{c|c} n & 0 \\ \hline 0 & I_n \otimes (I_n - E_n) \end{array} \right] \in \mathbb{S}_{++}^{(n-1)^2 + 1}, \quad \widehat{Z} := \widehat{V}^\top L_Q \widehat{V} - \widehat{V}^\top \mathcal{G}_J(\widehat{Y}) \widehat{V} \in \mathbb{S}_{++}^{(n-1)^2 + 1}.$$

Then they are (strictly) feasible variable and slack for (2.10).

3 A New ADMM Algorithm for the SDP Relaxation

We can write (2.9) equivalently as

$$\min_{R,Y} \langle L_Q, Y \rangle \text{ s.t. } \mathcal{G}_J(Y) = E_{00}, Y = \widehat{V} R \widehat{V}^\top, R \succeq 0.$$
(3.1)

The following theorem from [28] shows the equivalence between (2.6) and (3.1).

Theorem 3.1. A matrix Y is feasible for
$$(2.6)$$
 if, and only if, it is feasible for (3.1) .

Therefore we can work with (3.1). The augmented Lagrange of (3.1) is

$$\mathcal{L}_A(R, Y, Z) = \langle L_Q, Y \rangle + \langle Z, Y - \widehat{V}R\widehat{V}^{\top} \rangle + \frac{\beta}{2} \|Y - \widehat{V}R\widehat{V}^{\top}\|_F^2.$$
(3.2)

Recall that (R, Y, Z) are the primal reduced, primal, and dual variables respectively. We denote (R, Y, Z) as the *current iterate*. Our new algorithm, an application of **ADMM**, uses the augmented Lagrangian in (3.2) and performs the following updates to obtain a new iterate (R_+, Y_+, Z_+) :

$$R_{+} = \underset{R \in \mathbb{S}_{+}}{\operatorname{arg\,min}} \mathcal{L}_{A}(R, Y, Z), \tag{3.3a}$$

$$Y_{+} = \underset{Y \in \mathcal{P}_{+}}{\operatorname{arg\,min}} \, \mathcal{L}_{A}(R_{+}, Y, Z), \tag{3.3b}$$

$$Z_{+} = Z + \gamma \cdot \beta (Y_{+} - \widehat{V} R_{+} \widehat{V}^{\top}), \tag{3.3c}$$

where the simplest case for the polyhedral constraints \mathcal{P}_i is the linear manifold from the gangster constraints:

$$\mathcal{P}_1 = \{ Y \in \mathbb{S}^{n^2 + 1} : \mathcal{G}_J(Y) = E_{00} \}.$$

We use this notation as we add additional simple polyhedral constraints. The second case is the polytope:

$$\mathcal{P}_2 = \mathcal{P}_1 \cap \{0 \le Y \le 1\}.$$

Let \hat{V} be normalized such that $\hat{V}^{\top}\hat{V} = I$. Then the R-subproblem can be explicitly solved by

$$\begin{split} R_{+} &= \arg\min_{R\succeq 0} \langle Z, Y - \widehat{V}R\widehat{V}^{\top}\rangle + \frac{\beta}{2}\|Y - \widehat{V}R\widehat{V}^{\top}\|_{F}^{2} \\ &= \arg\min_{R\succeq 0} \left\|Y - \widehat{V}R\widehat{V}^{\top} + \frac{1}{\beta}Z\right\|_{F}^{2} \\ &= \arg\min_{R\succeq 0} \left\|R - \widehat{V}^{\top}(Y + \frac{1}{\beta}Z)\widehat{V}\right\|_{F}^{2} \\ &= \mathcal{P}_{\mathbb{S}_{+}}\left(\widehat{V}^{\top}(Y + \frac{1}{\beta}Z)\widehat{V}\right), \end{split} \tag{3.4}$$

where \mathbb{S}_+ denotes the **SDP** cone, and $\mathcal{P}_{\mathbb{S}_+}$ is the orthogonal projection onto \mathbb{S}_+ . For any symmetric matrix W, we have

$$\mathcal{P}_{\mathbb{S}_+}(W) = U_+ \Sigma_+ U_+^\top,$$

where (U_+, Σ_+) contains the positive eigenpairs of W; we let (U_-, Σ_-) be for the negative eigenpairs. If i = 1 in (3.3b), the Y-subproblem also has a closed-form solution:

$$Y_{+} = \underset{\mathcal{G}_{J}(Y)=E_{00}}{\operatorname{arg \, min}} \langle L_{Q}, Y \rangle + \langle Z, Y - \widehat{V}R_{+}\widehat{V}^{\top} \rangle + \frac{\beta}{2} \|Y - \widehat{V}R_{+}\widehat{V}^{\top}\|_{F}^{2}$$

$$= \underset{\mathcal{G}_{J}(Y)=E_{00}}{\operatorname{arg \, min}} \left\| Y - \widehat{V}R_{+}\widehat{V}^{\top} + \frac{L_{Q} + Z}{\beta} \right\|_{F}^{2}$$

$$= E_{00} + \mathcal{G}_{J^{c}} \left(\widehat{V}R_{+}\widehat{V}^{\top} - \frac{L_{Q} + Z}{\beta} \right). \tag{3.5}$$

One major advantage of using **ADMM** is that the complexity increases marginally when we add constraints to (2.9) and tighten the **SDP** relaxation. If $0 \le \hat{V}R\hat{V}^{\top} \le 1$ is added in (2.9), then we simply add the constraints $0 \le Y \le 1$ to (3.1). This yields the new problem

$$p_{RY}^* := \min_{R, Y} \{ \langle L_Q, Y \rangle : \mathcal{G}_J(Y) = E_{00}, \ 0 \le Y \le 1, \ Y = \widehat{V}R\widehat{V}^\top, \ R \succeq 0 \}.$$
 (3.6)

The **ADMM** for solving (3.6) has the same R-update and Z-update as those in (3.3). The Y-update is changed to

$$Y_{+} = E_{00} + \min\left(1, \max\left(0, \mathcal{G}_{J^{c}}(\widehat{V}R_{+}\widehat{V}^{\top} - \frac{L_{Q} + Z}{\beta})\right)\right). \tag{3.7}$$

The nonnegativity constraint means that the ≤ 1 constraint is redundant. But the inclusion makes the algorithm converge faster and avoid roundoff error. We emphasize again that it is the **FR** that allows for the splitting into polyhedral and semidefinite constraints. The update for R_+ is a nearest semidefinite problem and we can efficiently *cheat* and reduce the number of eigenvalues we allow to be positive by using the Eckart-Young Theorem, [10]. The update for Y_+ is a projection onto a simple polyhedral set and is very efficient and accurate.

3.1 Lower bound

If we solve (3.6) to high accuracy, we get a lower bound for the original **QAP**. However, the problem size of (3.6) can be extremely large, and it would be very expensive to obtain a highly accurate solution. In the following, we provide an inexpensive way to get a valid lower bound from the output of our algorithm that solves (3.6) to a moderate accuracy. Our method is to find a feasible solution of the dual problem of (3.6). The lemma below shows that any feasible dual solution provides a valid lower bound to (3.6) and thus the original **QAP**.

Lemma 3.2 (Lagrangian dual problem). Let

$$\mathcal{R} := \{R : R \succeq 0\}, \quad \mathcal{Y} := \{Y : \mathcal{G}_J(Y) = E_{00}, \ 0 \le Y \le 1\}, \quad \mathcal{Z} := \{Z : \widehat{V}^\top Z \widehat{V} \le 0\}.$$

Define

$$g(Z) := \min_{Y \in \mathcal{Y}} \langle L_Q + Z, Y \rangle.$$

Then the dual problem of (3.6) is $d_Z^* := \max_{Z \in \mathcal{Z}} g(Z)$, and the weak duality holds, i.e, $d_Z^* \leq p_{RY}^*$, where p_{RY}^* is the optimal objective value of (3.6).

Proof. The dual problem of (3.6) can be derived as

$$\begin{split} d_Z^* &:= \max_{Z} \min_{R \in \mathcal{R}, Y \in \mathcal{Y}} \langle L_Q, Y \rangle + \langle Z, Y - \widehat{V} R \widehat{V}^\top \rangle \\ &= \max_{Z} \min_{Y \in \mathcal{Y}} \langle L_Q, Y \rangle + \langle Z, Y \rangle + \min_{R \in \mathcal{R}} \langle Z, -\widehat{V} R \widehat{V}^\top \rangle \\ &= \max_{Z} \min_{Y \in \mathcal{Y}} \langle L_Q, Y \rangle + \langle Z, Y \rangle + \min_{R \in \mathcal{R}} \langle \widehat{V}^\top Z \widehat{V}, -R \rangle \\ &= \max_{Z} \min_{Y \in \mathcal{Y}} \langle L_Q + Z, Y \rangle \\ &= \max_{Z \in \mathcal{Z}} \max_{Y \in \mathcal{Y}} \langle L_Q + Z, Y \rangle \\ &= \max_{Z \in \mathcal{Z}} g(Z), \end{split}$$

where the fourth equality holds because if $Z \notin \mathcal{Z}$, then $\min_{R \in \mathcal{R}} \langle \hat{V}^{\top} Z \hat{V}, -R \rangle = -\infty$. Weak duality follows in the usual way by exchanging the max and min.

For any $Z \in \mathcal{Z}$, we have $g(Z) \leq d_Z^*$. Hence, from the above lemma, it follows that g(Z) is a lower bound of (3.6) and thus of the original **QAP**. In addition, note that g(Z) is easy to evaluate. Let $(R^{out}, Y^{out}, Z^{out})$ be the output of the **ADMM** for (3.6). We use the dual function value at the projected point $\mathcal{P}_{\mathcal{Z}}(Z^{out})$, namely $g(\mathcal{P}_{\mathcal{Z}}(Z^{out}))$, as the lower bound. Below we show how to get $\mathcal{P}_{\mathcal{Z}}(\widetilde{Z})$ for any symmetric matrix \widetilde{Z} .

Let \widehat{V}_{\perp} be the orthonormal basis of the null space of \widehat{V} . Then $\overline{V} = (\widehat{V}, \widehat{V}_{\perp})$ is an orthogonal matrix. Given any $Z \in \mathcal{Z}$, let $W = \overline{V}^{\top} Z \overline{V}$, and we write W into the 2×2 block matrix $\begin{bmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{bmatrix}$. We have

$$Z \in \mathcal{Z} \Leftrightarrow \widehat{V}^{\top} Z \widehat{V} \preceq 0 \Leftrightarrow \widehat{V}^{\top} Z \widehat{V} = \widehat{V}^{\top} \bar{V} W \bar{V}^{\top} \widehat{V} = W_{11} \preceq 0.$$

Hence,

$$\mathcal{P}_{\mathcal{Z}}(\widetilde{Z}) = \operatorname*{arg\,min}_{Z \in \mathcal{Z}} \|Z - \widetilde{Z}\|_F^2 = \bar{V} W^* \bar{V}^\top,$$

where

$$\begin{split} W^* &= \underset{W_{11} \preceq 0}{\arg\min} \, \| \bar{V} W \bar{V}^\top - \widetilde{Z} \|_F^2 \\ &= \underset{W_{11} \preceq 0}{\arg\min} \, \| W - \bar{V}^\top \widetilde{Z} \bar{V} \|_F^2 \\ &= \left[\begin{array}{cc} \mathcal{P}_{\mathbb{S}_-}(\widetilde{W}_{11}) & \widetilde{W}_{12} \\ \widetilde{W}_{21} & \widetilde{W}_{22} \end{array} \right], \end{split}$$

where \mathbb{S}_{-} denotes the negative semidefinite cone, and we have assumed $\bar{V}^{\top} \widetilde{Z} \bar{V} = \begin{bmatrix} \widetilde{W}_{11} & \widetilde{W}_{12} \\ \widetilde{W}_{21} & \widetilde{W}_{22} \end{bmatrix}$. Note that $\mathcal{P}_{\mathbb{S}_{-}}(W_{11}) = -\mathcal{P}_{\mathbb{S}_{+}}(-W_{11})$.

3.2 Upper bound from feasible solution

Let $(R^{out}, Y^{out}, Z^{out})$ be the output of the **ADMM** for (3.6). Assume the largest eigenvalue and the corresponding eigenvector of Y are λ and v, respectively. Then λvv^{\top} is a best rank-one approximation of Y. We let X^{out} be the square matrix reshaped from the second through the last elements of the first column of λvv^{\top} . This is our approximation to (a multiple of) the optimal permutation matrix. Note that for any permutation matrix X we have trace $X^TX = n$. This implies that

$$\|X^{out} - X\|_F^2 = -2\operatorname{trace} X^T X^{out} + \text{ constant}.$$

Thus to find the nearest permutation matrix to our approximation, we can take advantage of the Birkoff-von Neumann Theorem e.g., [4], that the permutation matrices are the extreme points of the doubly stochastic matrices. We only need to solve the *linear program*

$$\max_{X} \left\{ \langle X^{out}, X \rangle : Xe = e, X^{\top}e = e, X \ge 0 \right\}$$
 (3.8)

by a simplex method that gives a basic feasible optimal solution, i.e., a permutation matrix.

3.3 Low-rank solution

Instead of finding a feasible solution with (3.8), we can directly get one by restricting R to a rank-one matrix, i.e., rank(R) = 1 and $R \succeq 0$. With this constraint, the R-update can be modified to

$$R_{+} = \mathcal{P}_{\mathbb{S}_{+} \cap \mathcal{R}_{1}} \left(\widehat{V}^{\top} \left(Y + \frac{Z}{\beta} \right) \widehat{V} \right), \tag{3.9}$$

where $\mathcal{R}_1 = \{R : \operatorname{rank}(R) = 1\}$ denotes the set of rank-one matrices. For a symmetric matrix W with largest eigenvalue $\lambda > 0$ and corresponding eigenvector w, we have

$$\mathcal{P}_{\mathbb{S}_+ \cap \mathcal{R}_1} = \lambda w w^\top.$$

Despite of the nonconvexity of the rank-one constraint, we observed empirically that our algorithm almost always converged to a solution satisfying all the constraints in (3.6). Therefore, we obtained a permutation matrix from the lower bound.

3.4 Different choices for V, \widehat{V}

The matrix \widehat{V} is essential in the steps of the algorithm, see e.g., (3.4). A sparse \widehat{V} helps in the projection if one is using a sparse eigenvalue code. We have compared several. One is based on applying a QR algorithm to the original simple V from the definition of \widehat{V} in (2.7). The other two are based on the approach in [22] and we present the most successful here. The orthogonal V we use is

$$V = \begin{bmatrix} \begin{bmatrix} I_{\lfloor \frac{n}{2} \rfloor} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \end{bmatrix} \begin{bmatrix} I_{\lfloor \frac{n}{4} \rfloor} \otimes \frac{1}{2} \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix} \end{bmatrix} [\dots] \begin{bmatrix} \widehat{V} \end{bmatrix} \\ 0_{(n-2\lfloor \frac{n}{2} \rfloor), \lfloor \frac{n}{2} \rfloor} \end{bmatrix}_{n \times n-1}$$

i.e., the block matrix consisting of t blocks formed from Kronecker products along with one block \widehat{V} to complete the appropriate size so that $V^{\top}V = I_{n-1}, V^{\top}e = 0$. We take advantage of the 0, 1 structure of the Kronecker blocks and delay the scaling for the normalization till the end. The main work in the low rank projection part of the algorithm is to evaluate one (or a few) eigenvalues of $W = \widehat{V}^{\top}(Y + \frac{1}{\beta}Z)\widehat{V}$ to obtain the update R_+ . Here

$$Y + \frac{1}{\beta}Z = \begin{bmatrix} \rho & w^\top \\ w & \bar{W} \end{bmatrix}.$$

We let

$$K:=V\otimes V,\quad \alpha=1/\sqrt{2},\quad v=rac{1}{\sqrt{2}n}e,\quad x=egin{pmatrix}x_1\ ar{x}\end{pmatrix}.$$

The structure for \hat{V} in (2.7) means that we can evaluate the product for Wx as

structure for
$$V$$
 in (2.7) means that we can evaluate the product for Wx as
$$\begin{bmatrix} \alpha & 0 \\ v & K \end{bmatrix}^{\top} \begin{bmatrix} \rho & w^{\top} \\ w & \bar{W} \end{bmatrix} \begin{bmatrix} \alpha & 0 \\ v & K \end{bmatrix} x = \begin{bmatrix} \alpha & 0 \\ v & K \end{bmatrix}^{\top} \begin{bmatrix} \rho & w^{\top} \\ w & \bar{W} \end{bmatrix} \begin{pmatrix} \alpha x_1 \\ x_1 v + K \bar{x} \end{pmatrix}$$

$$= \begin{bmatrix} \alpha & v^{\top} \\ 0 & K^{\top} \end{bmatrix} \begin{pmatrix} \rho \alpha x_1 + w^{\top} (x_1 v + K \bar{x}) \\ \alpha x_1 w + \bar{W} (x_1 v + K \bar{x}) \end{pmatrix}$$

$$= \begin{pmatrix} \rho \alpha^2 x_1 + \alpha w^{\top} (x_1 v + K \bar{x}) + v^{\top} (\alpha x_1 w + \bar{W} (x_1 v + K \bar{x})) \\ K^{\top} (\alpha x_1 w + \bar{W} (x_1 v + K \bar{x}) + v^{\top} (\alpha x_1 w) \\ K^{\top} (\alpha x_1 w + \bar{W} (x_1 v + K \bar{x})) \end{pmatrix}.$$

We emphasize that $V \otimes V = (\bar{V} \otimes \bar{V})(D \otimes D)^{-1}$, where \bar{V} denotes the unscaled V, and D is the diagonal matrix of scale factors to obtain the orthogonality in V. Therefore, we can evaluate

$$K^{\top} \bar{W} K = (V \otimes V)^{\top} \bar{W} (V \otimes V) = (\bar{V} \otimes \bar{V})^{\top} \left[(D \otimes D)^{-1} \bar{W} (D \otimes D)^{-1} \right] (\bar{V} \otimes \bar{V}).$$

4 Numerical Experiments

In this section we present the results of extensive numerical tests using our proposed methods. We used MATLAB version 2018a. All **QAP** symmetric instances from [7,8] with size up to n = 100 were used in our tests, while the instances bur26a-bur26h are not symmetric and not used. We divided them into two sets: QAPLIB instances I and QAPLIB instances II. All the instances were tested on an Intel Xeon Gold 6130 2.10 Ghz PC with 32 cores and 64 Gigabyte memory and running on 64-bit Ubuntu system.

4.1 Parameter settings

The parameters β and γ in the updates (3.3) play important roles on the speed of the **ADMM** method. Running the algorithm on a few small-sized problems, we heuristically set $\gamma = 1.618$ and $\beta = \frac{n}{3}$. Unless specified, the algorithm was terminated if it reached a maximum number of iterations or the following conditions hold in 5 consecutive iterations:

$$\max\left(\frac{\|Y^{k} - \widehat{V}R^{k}\widehat{V}\|_{F}}{\|Y^{k}\|_{F}}, \beta\|Y^{k+1} - Y^{k}\|\right) \le \text{tol},\tag{4.1}$$

where "tol" is a specified tolerance. In (4.1), the first term on the left hand side measures the residual of primal feasibility while the second term measures the dual feasibility; see [5, Sect. 3.3]. Although we have the rank-1 constraint, the stopping conditions in (4.1) were still met for most instances.

4.2 Results on QAPLIB instances I

Two stopping tolerances 10^{-5} and 10^{-12} were used for **ADMM** on QAPLIB instances I, and the maximum number of iterations was set to 40,000. Solving the **SDP** to the higher accuracy rarely improved the bounds. The results of lower and upper bounds are listed in Table 4.1; and the CPU times and iteration numbers of the algorithm for both tolerances are in Table 4.2. Failure of an algorithm is marked by -1111.

- In Table 4.1 the columns are:
 - 0. Instance name;
 - 1. Opt value: the globally optimal value of each instance, except for problem Tai30a, where optimality of the value is still not known;
 - 2. Bundle LowBnd: current best known lower bound from [24];

- 3. HKM-FR LowBnd: the lower bound found using the p-d i-p approach with facial reduction and the HKM search direction and the code SDPT3 [25];²
- 4. Tol5 ADMM LowBnd: the lower bound found by running **ADMM** without the rank-1 constraint, with the tolerance 10^{-5} , and evaluating the dual objective using the approach in Section 3.1;
- 5. Tol5 feas UpBnd: the stronger upper bound found by running **ADMM** with the rank-1 constraint and tolerance 10⁻⁵, and also by running **ADMM** without the rank-1 constraint, with tolerance 10⁻⁵, and then using the approach in Section 3.2;
- 6. Tol12 ADMM LowBnd: the lower bound found by running **ADMM** without rank-1 constraint to the tolerance 10^{-12} and then evaluating the dual objective through the approach discussed in section 3.1;
- 7. Tol12 feas UpBnd: the stronger upper bound found by **ADMM** with the rank-1 constraint and tolerance 10^{-12} , and also **ADMM** without the rank-1 constraint with tolerance 10^{-12} and then using Section 3.2;
- 8. Tol5 ADMM % gap: the percentage gap between the lower and upper bounds found by our proposed approach with tolerance 10^{-5} ;
- 9. ADMM Tol5 vs Boundle %Impr LowBnd: the percentage improvement by our proposed approach with tolerance 10^{-5} over the current best known lower bound from [24].

Remark 4.1 (Table 4.1). From column 9, we see that our approach improves the currently best-known bounds for every instance. In addition, we have provably found the global optimal solution for the seven instances:

Esc16j, Had12, Had14, Had16, Had18, Rou12, Tai12a.

This is mainly due to the inclusion of all the nonnegativity constraints and the projection onto [0,1], all with essentially zero extra computational cost, see (3.7). Note that adding the nonnegativity constraints would be too expensive within an interior point approach. In addition, the bounds rarely improved when using the smaller tolerance 10^{-12} .

- In Table 4.2 the columns are:
 - 0. Instance name:
 - 1. Tol5 cpusec HighRk: CPU times (in seconds) of **ADMM** without the rank-1 constraint and with tolerance 10^{-5} :
 - 2. Tol5 cpusec LowRk: CPU times (in seconds) of **ADMM** with the rank-1 constraint and with tolerance 10^{-5} :
 - 3. HKM cpuratio Tol 9: the ratio between the CPU times by the p-d i-p approach and **ADMM** without the rank-1 constraint and with tolerance 10^{-5} ;
 - Tol5 iterations HighRk: iteration numbers of ADMM without the rank-1 constraint and with tolerance 10⁻⁵;
 - 5. Tol5 iterations LowRk: iteration numbers of \mathbf{ADMM} with the rank-1 constraint and with tolerance 10^{-5} ;
 - 6. Tol12 iterations HighRk: iteration numbers of **ADMM** without the rank-1 constraint and with tolerance 10^{-12} :
 - 7. Tol12 residual HighRk: residual of the output measured as in (4.1) of **ADMM** without the rank-1 constraint and with tolerance 10^{-12} ;
 - 8. ADMM Tol12 iterations LowRk: the iteration numbers of **ADMM** with the rank-1 constraint and with tolerance 10^{-12} .

Remark 4.2 (Table 4.2). We see that ADMM with rank-1 constraint is much faster than that without the rank-1 constraint to reach the same tolerance. In addition, we notice that for all instances, ADMM can reach an accuracy of 10^{-5} . However, for most instances, it cannot reach the accuracy of 10^{-12} even though running to 40.000 iterations.

²We do not include the times as they were much greater than those by the ADMM approach, e.g., hours instead of minutes and a day instead of an hour.

Problem	1	2	3	4 Tol5	5 Tol5	6 Tol12	7 Tol12	8 Tol5	9 ADMM Tol5
	Opt	Bundle [24]	HKM-FR	ADMM	feas	ADMM	feas	ADMM	vs Bundle
	value	LowBnd	LowBnd	LowBnd	UpBnd	LowBnd	UpBnd	%gap	%Impr LowBnd
Esc16a	68	59	50	64	78	64	78	20.59	7.35
Esc16b	292	288	276	290	294	290	294	1.37	0.68
Esc16c	160	142	132	154	170	154	170	10.00	7.50
Esc16d	16	8	-12	13	20	13	20	43.75	31.25
Esc16e	28	23	13	27	34	27	34	25.00	14.29
Esc16g	26	20	11	25	34	25	34	34.62	19.23
Esc16h	996	970	909	977	1012	977	1012	3.51	0.70
Esc16i	14	9	-21	12	14	12	14	14.29	21.43
Esc16j	8	7	-4	8	8	8	8	0.00	12.50
Had12	1652	1643	1641	1652	1652	1652	1652	0.00	0.54
Had14	2724	2715	2709	2724	2724	2724	2724	0.00	0.33
Had16	3720	3699	3678	3720	3720	3720	3720	0.00	0.56
Had18	5358	5317	5287	5358	5358	5358	5358	0.00	0.77
Had20	6922	6885	6848	6922	6930	6922	6930	0.12	0.53
Kra30a	88900	77647	-1111	86838	104050	86838	105900	19.36	10.34
Kra30b	91420	81156	-1111	87858	114950	87858	114950	29.63	7.33
Kra32	88700	79659	-1111	85775	111450	85775	111450	28.95	6.90
Nug12	578	557	530	568	654	568	654	14.88	1.90
Nug14	1014	992	960	1011	1022	1011	1022	1.08	1.87
Nug15	1150	1122	1071	1141	1196	1141	1196	4.78	1.65
Nug16a	1610	1570	1528	1600	1610	1600	1610	0.62	1.86
Nug16b	1240	1188	1139	1219	1438	1219	1438	17.66	2.50
Nug17	1732	1669	1622	1708	1756	1708	1756	2.77	2.25
Nug18	1930	1852	1802	1894	2160	1894	2160	13.78	2.18
Nug20	2570	2451	2386	2507	2732	2507	2732	8.75	2.18
Nug21	2438	2323	2386	2382	2672	2382	2672	11.89	2.42
Nug22	3596	3440	3396	3529	3856	3529	3856	9.09	2.47
Nug24	3488	3310	-1111	3402	3658	3402	3658	7.34	2.64
Nug25	3744	3535	-1111	3626	4052	3626	4052	11.38	2.43
Nug27	5234	4965	-1111	5130	5602	5130	5602	9.02	3.15
Nug28	5166	4901	-1111	5026	5534	5026	5534	9.83	2.42
Nug30	6124	5803	-1111	5950	6578	5950	6578	10.25	2.40
Rou12	235528	223680	221161	235528	235528	235528	235528	0.00	5.03
Rou15	354210	333287	323235	350217	367782	350217	367782	4.96	4.78
Rou20	725522	663833	642856	695181	765390	695181	765390	9.68	4.32
Scr12	31410	29321	23973	31410	44360	31410	44360	41.23	6.65
Scr15	51140	48836	42204	51140	58304	51140	58304	14.01	4.51
Scr20	110030	94998	83302	106803	149038	106803	149038	38.38	10.73
Tai12a	224416	222784	215637	224416	224416	224416	224416	0.00	0.73
Tai15a	388214	364761	349586	377101	412760	377101	412760	9.19	3.18
Tai17a	491812	451317	441294	476525	546366	476525	546366	14.20	5.13
Tai20a	703482	637300	619092	671675	750450	671676	750450	11.20	4.89
Tai25a	1167256	1041337	-1111	1096657	1271696	1096658	1271696	15.00	4.74
*Tai30a	1818146	1652186	-1111	1706871	1942086	1706872	1942086	12.94	3.01
Tho30	149936	136059	-1111	143576	169958	143576	169958	17.60	5.01

Table 4.1: Results of lower and upper bounds for each instance in **QAPLIB** Instances I. Failure of an algorithm is marked by -1111, and the optimal value of the instance marked by * is still unknown.

4.3 Results on QAPLIB instances II

Since the tests on QAPLIB instances I show now improvement from the smaller tolerance 10^{-12} , we simply set the tolerance to 10^{-5} for the tests on QAPLIB instances II. For the instances with size n < 60, we set the maximum number of iterations to 40,000. For larger instances, to reduce cputime, we simply run **ADMM** with the rank-1 constraint and **ADMM** without rank-1 constraint, but each to a maximum 2,000 iterations. For the former, at every 100 iterations, we found a feasible solution (thus an upper bound) by the method in Section 3.2. For the latter, at every 100 iterations we obtain a lower bound and also an upper bound by the methods in Sections 3.1 and 3.2. We reported the best lower and upper bounds that we obtained. The results are shown in Table 4.3 for instances of size n < 60 and in Table 4.4 for instances of size $n \ge 60$. The columns used are similar to those in Tables 4.1 and 4.2.

Remark 4.3. From Tables 4.3 and 4.4, we see that our method provably found exact optimal solutions for the 15 instances:

	1 Tol5	2 Tol5	3 HKM	4 Tol5	5 Tol5	6 Tol12	7 Tol12	8 Tol12
	cpusec	cpusec	cpuratio	iterations	iterations	iterations	residual	iterations
	HighRk	LowRk	Tol 9	HighRk	LowRk	HighRk	HighRk	LowRk
Esc16a	20.14	2.64	9.37	2053	280	7309	9.87e-13	305
Esc16b	3.10	2.93	8.08	338	311	641	3.94e-13	334
Esc16c	8.44	3.68	4.88	961	403	3751	9.69e-13	592
Esc16d	17.39	2.18	10.22	1889	236	7812	9.87e-13	270
Esc16e	24.04	2.63	8.79	2719	288	11784	9.93e-13	310
Esc16g	33.54	2.61	8.63	3839	285	9096	9.87e-13	304
Esc16h	4.01	2.73	10.60	433	300	886	8.47e-13	354
Esc16i	100.79	2.26	8.76	11653	290	27106	9.96e-13	323
Esc16j	56.90	2.67	7.93	6898	306	29743	9.95e-13	338
Had12	8.39	0.53	5.91	2682	157	2845	8.64e-13	178
Had14	23.07	0.99	10.46	3919	169	4747	2.35e-13	181
Had16	111.92	1.88	12.51	14179	210	14362	6.80e-13	228
Had18	268.58	3.57	13.28	18068	259	40000	2.07e-06	271
Had20	196.70	6.17	14.53	9038	309	40000	5.55e-07	321
Kra30a	988.47	62.61	-1111	8466	632	40000	2.08e-07	654
Kra30b	1481.32	63.31	-1111	12882	623	40000	8.73e-07	645
Kra32	1355.11	92.43	-1111	9020	720	40000	5.28e-07	737
Nug12	22.27	0.53	5.93	5813	146	40000	3.82e-09	163
Nug14	49.76	1.01	8.43	7667	167	40000	2.94e-07	186
Nug15	53.68	1.49	7.79	6547	200	40000	2.11e-07	221
Nug16a	117.57	1.76	12.24	11591	193	40000	1.46e-06	208
Nug16b	62.72	1.98	11.83	6410	207	40000	5.87e-10	234
Nug17	135.80	2.31	13.13	10727	204	40000	9.12e-07	215
Nug18	250.85	3.22	15.23	15862	226	40000	1.79e-06	240
Nug20	238.68	5.82	14.35	9786	276	40000	4.55e-07	289
Nug21	651.15	8.27	14.95	22465	322	40000	3.62e-06	340
Nug22	942.50	9.84	13.90	27839	325	40000	5.69e-06	338
Nug24	572.04	13.47	-1111	12148	335	40000	7.55e-07	346
Nug25	1308.41	18.38	-1111	24051	375	40000	5.05e-06	386
Nug27	1875.89	30.54	-1111	25201	454	40000	4.16e-06	465
Nug28	1658.48	34.50	-1111	18417	447	40000	2.73e-06	461
Nug30	2584.42	48.92	-1111	22613	469	40000	3.06e-06	478
Rou12	23.19	0.44	6.90	6327	127	6360	2.02e-13	142
Rou15	19.00	1.27	9.46	2219	170	19769	6.08e-13	184
Rou20	88.20	5.60	16.08	3684	263	40000	2.08e-07	275
Scr12	3.71	0.48	5.79	1135	142	2878	6.65e-13	160
Scr15	8.06	1.14	10.75	1061	158	2023	8.11e-13	176
Scr20	858.08	5.94	17.96	34679	264	40000	7.68e-06	276
Tai12a	1.56	0.50	6.70	421	127	454	1.38e-13	145
Tai15a	17.01	1.22	10.34	1955	157	29673	5.41e-13	170
Tai17a	39.60	2.31	12.04	2997	216	22276	7.29e-13	234
Tai20a	66.02	5.62	15.85	2755	252	40000	1.72e-08	267
Tai25a	128.14	17.20	-1111	2244	350	12809	6.33e-13	362
Tai30a	433.54	55.82	-1111	3698	527	39288	3.74e-13	539
Tho30	2045.32	51.37	-1111	17854	522	40000	2.23e-06	533

Table 4.2: CPU times (in seconds) and iteration numbers by different approaches on **QAPLIB** Instances I. Failure of an algorithm is marked by -1111.

chr12a, chr12b, chr12c, chr15a, chr15b, chr15c, chr18a, chr20a, chr20b, chr22a, chr22b, chr25a, Esc16f, Esc32e, Esc32f.

For the rest of the instances, our method yielded a relative gap smaller than 20% for 26 instances, between 20% to 40% for 8 instances, and greater than 40% for only 1 instance. In addition, the **ADMM** with the rank-1 constraint reached the same stopping tolerance in much less time.

4.4 Influence of the nonnegativity constraints

To highlight the importance of the nonnegativity constraints in strengthening the bounds, i.e., in using a **DNN** model, we now compare results with and without the restriction $0 \le Y \le 1$, i.e., Y is updated according to (3.5) or (3.7). For the instances in Table 4.1 with $n \le 24$, we obtained the same lower bounds as those from the HKM p-d i-p approach by updating Y according to (3.5). The upper and lower bounds

Problem	1.	2.	3.	4.	5 Tol5	6 Tol5	7 ADMM	8 ADMM
	opt	ADMM	feas	ADMM	cpusec	cpusec	iterations	iterations
	value	LowBnd	UpBnd	%gap	HighRk	LowRk	HighRk	LowRk
Chr12a	9552	9552	9552	0.00	6.53e + 01	4.08e-01	21061	117
Chr12b	9742	9742	9742	0.00	3.32e+01	4.11e-01	10592	119
Chr12c	11156	11156	11156	0.00	7.42e + 01	3.96e-01	23982	115
Chr15a	9896	9896	9896	0.00	2.07e + 02	1.28e + 00	31937	173
Chr15b	7990	7990	7990	0.00	2.69e + 01	9.84e-01	3976	133
Chr15c	9504	9504	9504	0.00	1.54e + 01	1.06e + 00	2192	147
Chr18a	11098	11098	11098	0.00	4.94e + 02	2.86e + 00	40000	198
Chr18b	1534	1534	2264	32.24	5.72e + 01	3.08e + 00	3843	243
Chr20a	2192	2192	2192	0.00	7.40e + 02	4.31e+00	40000	217
Chr20b	2298	2298	2298	0.00	1.42e + 02	5.31e+00	6355	243
Chr20c	14142	14139	14142	0.02	7.28e + 02	5.03e+00	40000	232
Chr22a	6156	6156	6156	0.00	4.02e+02	9.37e + 00	14051	310
Chr22b	6194	6194	6194	0.00	3.80e + 02	9.45e + 00	11418	304
Chr25a	3796	3796	3796	0.00	3.06e + 02	1.70e + 01	6164	355
Els19	17212548	17209789	17212548	0.02	6.17e + 02	4.48e + 00	40000	269
Esc16f	0	0	0	0.00	3.22e+02	3.39e + 02	40000	40000
Esc32a	130	104	168	38.10	2.89e + 03	9.16e + 01	20398	700
Esc32b	168	132	264	50.00	2.52e + 03	8.31e+01	17920	658
Esc32c	642	616	686	10.20	4.48e + 02	1.01e + 02	3177	780
Esc32d	200	191	228	16.23	8.68e + 02	1.09e + 02	6334	825
Esc32e	2	2	2	0.00	1.81e + 03	1.05e + 02	13040	836
Esc32f	2	2	2	0.00	1.80e + 03	1.07e + 02	13040	836
Esc32g	6	6	8	25.00	6.04e + 02	1.06e + 02	4405	855
Esc32h	438	425	482	11.83	3.02e+03	1.00e+02	21515	795
*Sko42	15812	15335	17086	10.25	1.06e + 04	3.87e + 02	21013	911
*Sko49	23386	22653	25076	9.66	3.03e + 04	1.18e + 03	28771	1316
*Sko56	34458	33390	36580	8.72	3.90e + 04	2.68e + 03	21106	1664
Ste36a	9526	9259	13866	33.23	1.02e + 04	1.87e + 02	40000	851
Ste36b	15852	15668	25878	39.45	1.01e + 04	1.56e + 02	40000	700
Ste36c	8239110	8134720	11152926	27.06	1.01e + 04	1.69e + 02	40000	798
*Tai35a	2422002	2216645	2599924	14.74	7.40e+02	1.33e+02	3225	661
*Tai40a	3139370	2843312	3392692	16.19	1.94e + 03	2.99e+02	4665	852
*Tai50a	4938796	4390976	5332790	17.66	6.36e + 03	1.33e+03	5393	1348
*Tho40	240516	226522	269452	15.93	8.52e + 03	2.90e + 02	21131	828
*Wil50	48816	48125	50040	3.83	1.73e + 04	1.43e+03	15370	1473

Table 4.3: Results of lower and upper bounds, iteration numbers, and also CPU times (in seconds) by **ADMM** for each instance in **QAPLIB** Instances II with size no larger than 64. Optimal values of the instances marked by * are still unknown.

for the remaining 10 instances by **ADMM** with updates (3.5) and (3.7) are shown in Table 4.5. We see that for all those 10 problems, **ADMM** using (3.7) obtained better lower bounds. **ADMM** with the rank-1 constraint can hardly achieve the tolerance 10^{-5} if the bound constraint is not enforced. In addition, except for Kra30b, Kra32, and Nug28, better upper bounds were also obtained by using (3.7).

Moreover, for the instances in Table 4.3 that were solved to optimality, if we update Y according to (3.5), the generated solution will not be optimal any more. For most of these 15 instances, **ADMM** with update (3.5) yielded the trivial lower bound 0. In Table 4.6, we present the 6 instances, for which **ADMM** with (3.7) improved the relative gap significantly over that with (3.5).

4.5 Improved lower bounds

For the problems marked with * in Tables 4.1, 4.3, and 4.4, their optimal values are still unknown, and we obtained better lower bounds than those given in [7]. In Table 4.7, the fourth column shows the improvement percentage of the lower bounds for those 23 instances. Its last two columns list the gap between current lower bound and the best known feasible solutions according to Tables 4.1, 4.3, and 4.4, and also the improved gap by the proposed approach. We note that around 10% improvement has been achieved on instances Tai60a, Tai80a, and Tai100a, 2% on 6 instances, and less than 0.01% improvement on the other 4 instances.

Problem	1.	2.	3.	4.	5 Tol5	6 Tol5
	opt	ADMM	feas	ADMM	cpusec	cpusec
	value	LowBnd	UpBnd	%gap	HighRk	LowRk
Esc64a	116	98	120	18.33	1.64e + 04	1.11e+04
*Sko64	48498	46888	50840	7.77	1.56e + 04	1.13e+04
*Sko72	66256	64205	70672	9.15	3.01e + 04	2.07e + 04
*Sko81	90998	87756	96456	9.02	5.94e + 04	3.77e + 04
*Sko90	115534	111300	121390	8.31	9.32e + 04	6.72e + 04
*Sko100a	152002	145775	160794	9.34	1.38e + 05	9.37e + 04
*Sko100b	153890	147332	162004	9.06	1.38e + 05	9.45e + 04
*Sko100c	147862	142018	156230	9.10	1.38e + 05	9.46e + 04
*Sko100d	149576	143205	157100	8.84	1.39e + 05	9.53e + 04
*Sko100e	149150	142977	155858	8.26	1.38e + 05	9.51e + 04
*Sko100f	149036	142413	156088	8.76	1.40e + 05	9.70e + 04
*Tai60a	7205962	6319630	7759332	18.55	1.34e + 04	1.01e + 04
Tai64c	1855928	1809370	1917484	5.64	1.65e + 04	1.14e + 04
*Tai80a	13499184	11613474	14618694	20.56	5.17e + 04	3.08e + 04
*Tai100	21052466	17704527	22641778	21.81	1.53e + 05	9.33e + 04
*Wil100	273038	267469	278898	4.10	$1.41\mathrm{e}{+05}$	9.67e + 04

Table 4.4: Results of lower and upper bounds and also CPU times (in seconds) by **ADMM** for each instance in **QAPLIB** Instances II with size at least 64. Optimal values of the instances marked by * are still unknown.

Problem	ADMM feas. Y as in (3.7)					ADMM feas. Y as in (3.5)				
	LowBnd	UpBnd	Iter.HighRk	Iter.LowRk	LowBnd	UpBnd	Iter.HighRk	Iter.LowRk		
Kra30a	86838	104050	8466	632	78687	104050	25974	40000		
Kra30b	87858	114950	12882	623	79510	108550	21248	40000		
Kra32	85775	111450	9020	720	77130	105500	3904	40000		
Nug24	3402	3658	12148	335	3235	3844	4629	39616		
Nug25	3626	4052	24051	375	3454	4078	8974	40000		
Nug27	5130	5602	25201	454	4922	5708	20763	40000		
Nug28	5026	5534	18417	447	4813	5466	15916	40000		
Nug30	5950	6578	22613	469	5694	6630	10524	40000		
Tai30a	1706871	1942086	3698	527	1578074	1963808	1072	40000		
Tho30	143576	169958	17854	522	136004	170390	34289	40000		

Table 4.5: Lower and upper bounds by **ADMM** for solving **SDP** relaxation with or without the restriction $0 \le Y \le 1$ on certain instances in **QAPLIB** Instances I

Problem		ADMM	feas. Y as in (3	.7)	ADMM feas. Y as in (3.5)			
	LowBnd	UpBnd	Iter.HighRk	Iter.LowRk	LowBnd	UpBnd	Iter.HighRk	Iter.LowRk
Chr18b	1534	2264	3843	243	477	2446	19642	21302
Esc32c	616	686	3177	780	529	692	2460	40000
Esc32h	425	482	21515	795	330	522	1685	40000
Tai35a	2216645	2599924	3225	661	2030958	2728422	1222	40000
Tai40a	2843312	3392692	4665	852	2594394	3475274	1433	40000
Tho40	226522	269452	21131	828	215639	290124	40000	40000

Table 4.6: Lower and upper bounds by **ADMM** for solving **SDP** relaxation with or without the restriction $0 \le Y \le 1$ on certain instances in **QAPLIB** Instances II.

5 Conclusion

In this paper we have shown the efficiency of using the **ADMM** approach for solving the *facially reduced* **SDP** relaxation of the **QAP** problem with added nonnegativity constraints, i.e., the usually hard-to-solve

Problem	QAPLIB	ADMM	% Impr	QAPLIB	New
	LowBnd	LowBnd	LowBnd	%gap	%gap
Sko42	14934	15335	2.61	5.55	3.02
Sko49	22004	22653	2.86	5.91	3.13
Sko56	32610	33390	2.34	5.36	3.10
Sko64	45736	46888	2.46	5.70	3.32
Sko72	62691	64205	2.36	5.38	3.10
Sko81	86072	87756	1.92	5.41	3.56
Sko90	109030	111300	2.04	5.63	3.66
Sko100a	143846	145775	1.32	5.37	4.10
Sko100b	145522	147332	1.23	5.44	4.26
Sko100c	139881	142018	1.50	5.40	3.95
Sko100d	141289	143205	1.34	5.54	4.26
Sko100e	140893	142977	1.46	5.54	4.14
Sko100f	140691	142413	1.21	5.60	4.44
Tai30a	1706855	1706871	< 0.01	6.12	6.12
Tai35a	2216627	2216645	< 0.01	8.48	8.48
Tai40a	2843274	2843312	< 0.01	9.43	9.43
Tai50a	4390920	4390976	< 0.01	11.09	11.09
Tai60a	5578356	6319630	11.73	22.59	12.30
Tai80a	10501941	11613474	9.57	22.20	13.97
Tai100	15844731	17704527	10.50	24.74	15.90
Tho40	224414	226522	0.93	6.69	5.82
Wil50	47098	48125	2.13	3.52	1.42
Wil100	264442	267469	1.13	3.15	2.04

Table 4.7: New lower bounds by the proposed approaches for **QAPLIB** unsolved instances.

DNN relaxation. We exploited the **FR** relation $Y = VRV^T$ by applying the polyhedral constraints to Y and the positive semidefinite and rank constraints to R. The addition of the nonnegativity constraints to Y causes essentially no extra cost but significantly improves the bounds. For most instances in QAPLIB, we have improved both lower and upper bounds for the **QAP**, and in several instances, the bounds provably find the optimal permutation matrix.

In a forthcoming study, begun in [19], we propose to include this in a branch and bound framework and implement it in a parallel programming approach, see e.g., [14]. In addition, we propose to test the possibility of using warm starts in the branching/bounding process and test it on the larger test sets such as used in e.g., [9].

The most expensive steps of our code was the matrix multiplication $W = V \bar{W} V^T$ and the eigenvalue decomposition of W. We hope that a more efficient approach for this special matrix multiplication can be found. Moreover, since only a few eigenvalues of W are needed it is hoped that a more efficient algorithm can be used, e.g., the MATLAB code *eigifp* based on [12].

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