REGULAR-SS12: A new matrix splitting based relaxation for the quadratic assignment problem

Marko Lange

Institute for Reliable Computing, Hamburg University of Technology

Abstract. Nowadays, the quadratic assignment problem (QAP) is widely considered as one of the hardest of the NP-hard problems. One of the main reasons for this consideration can be found in the enormous difficulty of computing good quality bounds for branch-and-bound algorithms. The practice shows that even with the power of modern computers QAPs of size $n > 30$ are typically recognized as huge computational problems. In this work, we are concerned with the design of a new low-dimensional semidefinite programming relaxation for the computation of lower bounds of the QAP. We discuss ways to improve the bounding program upon its semidefinite relaxation base and give numerical examples to demonstrate its applicability.

Keywords: quadratic assignment problem, semidefinite programming, relaxation

1 Introduction

The quadratic assignment problem (QAP) was introduced by Koopmans and Beckmann [12] in 1957 as a mathematical model for problems in the allocation of indivisible resources. The class of QAPs entails a great number of applications from different scenarios in the topic of combinatorial optimization. This includes problems arising in location theory, facility layout, VLSI design, communications and various other fields. For extensive lists of applications of QAPs, we refer to the survey works by Pardalos et al. [19], Burkard et al. [4], Çela [5], Loiola et al. [15] and most recently Burkard et al. [3].

In this work, we are concerned with the computation of lower bounds for QAPs which can be formulated in Koopmans-Beckmann trace formulation [8]:

$$\inf_{X \in \Pi^n} \quad \mathrm{tr}(AXBX^T + CX^T), \qquad \text{(KBQAP)}$$

where $A, B, C \in \mathbb{R}^{n \times n}$ are the parameter matrices of the QAP, Π^n denotes the set of $n \times n$ permutation matrices, and tr() terms the trace function. More precisely, our concern is a new technique for the construction of a low-dimensional semidefinite programming (SDP) relaxation for (KBQAP).

Our main contribution is the introduction of a new relaxation approach based on interrelated matrix splitting. The derivation of the corresponding framework can be found in Subsection 2.2. Subsequently, we discuss additional cuts which are based on techniques introduced by Mittelmann and Peng in [17]. In Subsection 3.1, we propose a way to tighten the respective constraints by exploiting a degree of freedom that is present in the original versions of these cuts.

1.1 Notation and preliminaries

Unless otherwise stated, we assume that both matrices A and B are symmetric. Furthermore, without loss of generality, it is assumed that the diagonal elements of A and B are equal to zero. If this is not the case, the corresponding costs can be shifted to the linear term by setting $C_{\text{new}} := C + \operatorname{diag}(A)\operatorname{diag}(B)^T$, where $\operatorname{diag}(A)$ denotes a column vector formed of the diagonal elements of A. Throughout this paper, $B = \sum_{i=1}^{n} \lambda_i q_i q_i^T$ shall denote the eigenvalue decomposition of B.

If not stated otherwise, $\|\cdot\|$ is used for the spectral norm. The trace inner product of two real matrices G, H is denoted by $\langle G, H\rangle := \operatorname{tr}(G^T H)$. Furthermore, we write $H^\dagger$ for the Moore-Penrose pseudoinverse of H [18, 22]. If H is an operator, $\mathcal{R}(H)$ denotes its range in the sense of its image. In the case that H is a matrix, we use the same notation referring to its column space.

The cone of symmetric positive semidefinite matrices is of major importance for every discussion about SDP problems. We denote the space of $n \times n$ symmetric matrices by $\mathbb{S}^n$ and its positive semidefinite subset by $\mathbb{S}^n_+$. In this context, we also utilize the relation sign '$\succeq$' to denote a Loewner's partial ordering, i.e. $H \succeq G$ is used to note the positive semidefiniteness of $H - G$. In addition to the already mentioned sets, we consider the space of $m \times n$ matrices $\mathbb{M}^{m,n}$ and the set of $n \times n$ double stochastic matrices $\mathbb{D}^n$. By e we denote the n dimensional column vector of all ones and $I := [e_1, \ldots, e_n]$ is used for the $n \times n$ identity matrix. Generally, we spare redundant informations on matrix dimensions. For instance, we write $\mathbb{M}^m$ instead of $\mathbb{M}^{m,m}$. Moreover, in cases where the dimension is evident from the context, the accompanying indicators may be discarded completely.

Complementary to the diag-operator, $\operatorname{off}(H)$ denotes a column vector that contains all off-diagonal elements of the matrix H. This vector is obtained by vertical concatenation of the columns of H, but without its diagonal elements. Another considered linear transformation is the triangular vectorization of a matrix; $\operatorname{tri}(H)$ denotes the vector obtained from the vertical concatenation of the columns of H taking solely its lower triangular elements (without matrix diagonal) into account. These operators may also be used in combination with relations, for instance $\{=_{\text{off}}, \geqslant_{\text{off}}, \leqslant_{\text{off}} \ldots\}$. In case of the subscript $_{\text{off}}$, the respective relations apply only to the off-diagonal elements of the corresponding matrices, hence $A \geqslant_{\text{off}} B$ is the short form for $\operatorname{off}(A) \geqslant \operatorname{off}(B)$.

2 QAP relaxations based on matrix splitting

Relaxation is a fundamental approach for the computation of lower or upper bounds of intractable programming problems. It can be used directly as an approximation of the original problem, for bound computations in branch-&-bound

and branch-&-cut approaches, or as a tool to measure the quality of other bounding algorithms. In regard to the form of the given optimization problem the first step of a relaxation process requires the reformulation of the original problem. The second step comprises the removal or replacement of constraints that are the cause for intractability.

One of the most popular relaxation approaches for quadratic programming problems is based on vector lifting. A good source for relaxations of this kind is given by Zhao et al. in [26]. Compared to newer low-dimensional SDP relaxations for the QAP, relaxation frameworks based on vector lifting have their strength in the computation of tighter bounds. Their major drawbacks are the large number of $\mathcal{O}(n^4)$ variables and the accompanying computational costs.

There are some efforts to reduce the computational costs of these high dimensional SDP relaxations, see for instance [23, 2, 25, 10]. Nevertheless, regarding QAP instances of size $n > 30$ and with little symmetry, the computational costs for solving SDP relaxation frameworks based on vector lifting remain too high for practical usage.

2.1 Non-redundant positive semidefinite matrix splitting

For a special class of QAPs - instances which are associated with Hamming and Manhatten distances - Mittelmann and Peng [17] pursued the idea of another low-dimensional SDP relaxation framework. The presented bounds not only involve a less expensive computational process, they are also provably tighter than the ones proposed in [6] by Ding and Wolkowicz. In [20] and [21], Peng et al. generalized the matrix splitting approach for other classes of the QAP.

If the parameter matrix B is positive semidefinite, the equality $Y = XBX^T$ can be relaxed to the convex semidefinite relation $Y \succeq XBX^T$. The implementation of the latter is usually realized by utilization of the Schur complement inequality [1], here

$$\begin{bmatrix} B & BX^T \\ XB & Y \end{bmatrix} = \begin{bmatrix} B^{\frac{1}{2}} \\ XB^{\frac{1}{2}} \end{bmatrix} \begin{bmatrix} B^{\frac{1}{2}} & B^{\frac{1}{2}} X^T \end{bmatrix} \in \mathbb{S}_+^{2n}. \tag{1}$$

In general, however, B does not satisfy any definiteness property. Peng et al. [20, 21] dealt with this case by applying a non-redundant positive semidefinite matrix splitting scheme.

Definition 1. *For a given matrix B a matrix pair (B_1, B_2) is called a positive semidefinite matrix splitting of B if it satisfies*

$$B = B_1 - B_2, \quad B_1, B_2 \in \mathbb{S}_+. \tag{2}$$

The splitting is said to be redundant if there exists a nonzero positive semidefinite matrix R, such that

$$B_1 - R \in \mathbb{S}_+, \quad B_2 - R \in \mathbb{S}_+. \tag{3}$$

If $R \equiv 0$ is the only feasible matrix that is positive semidefinite and satisfies (3), we say that the splitting is non-redundant.

For the relaxation framework *F-SVD* introduced in [20], the authors used the following non-redundant splitting:

$$B_+ = \sum_{i:\ \lambda_i > 0} \lambda_i q_i q_i^T \qquad \text{and} \qquad B_- = \sum_{i:\ \lambda_i < 0} -\lambda_i q_i q_i^T. \tag{4}$$

Together with (1) and the observations that

$$\forall X \in \Pi^n, B \in \mathbb{M}^n: \quad \operatorname{diag}(XBX^T) = X \operatorname{diag}(B), \quad XBX^T e = XBe, \tag{5}$$

we derive the SDP basis of their framework, here referred to as *B-SVD*:

$$\begin{aligned}
\inf_{X \in \mathbb{D}^n,\ Y_+, Y_- \in \mathbb{S}^n} \quad & \langle A, Y_+ - Y_- \rangle + \langle C, X \rangle && \text{(6a)}\\
\text{s. t.} \quad & \begin{bmatrix} B_+ & B_+X^T \\ XB_+ & Y_+ \end{bmatrix} \in \mathbb{S}_+, \quad \begin{bmatrix} B_- & B_-X^T \\ XB_- & Y_- \end{bmatrix} \in \mathbb{S}_+, && \text{(6b)}\\
& \operatorname{diag}(Y_+) = X \operatorname{diag}(B_+), \quad \operatorname{diag}(Y_-) = X \operatorname{diag}(B_-), && \text{(6c)}\\
& Y_+ e = XB_+ e, \quad Y_- e = XB_- e, && \text{(6d)}
\end{aligned}$$

where the variables Y_+ and Y_- are used to relax the quadratic terms XB_+X^T and XB_-X^T, respectively.

In regard to a matrix splitting based SDP relaxation such as (6), Peng et al. demonstrated the general advantage of non-redundant matrix splittings over redundant ones, see [21, Theorem 1]. Roughly speaking the theorem states that for any redundant positive semidefinite matrix splitting there exists a non-redundant splitting which leads to a tighter relaxation. Even though additional constraints on the respective variables may change this circumstance, the absence of redundancies in the positive semidefinite matrix splitting is a good indicator for a beneficial splitting scheme.

2.2 Interrelated matrix splitting

A particularly beautiful property of the positive semidefinite matrix splitting defined in (4) is that the ranges of the matrices B_+,B_- are not overlapping, i.e. $\mathcal{R}(B_+) \cap \mathcal{R}(B_-) = \varnothing$ or $B_+B_- \equiv 0$. As an immediate consequence of this circumstance, B_+ and B_- are simultaneously diagonalizable. It would be a great advantage if we could make use of these interrelations in the actual relaxation. Unfortunately, it is quite difficult to exploit the corresponding properties in form of beneficial SDP constraints. For the design of new relaxation strategies, we need a different kind of interrelation. In this subsection, we say goodbye to the idea of redundancy free positive semidefinite matrix splitting pairs (B_+, B_-) and present a new splitting scheme.

$$B = B_\vartriangle - B_\triangledown \quad \text{with additional conditions on } (B_\vartriangle, B_\triangledown). \tag{7}$$

By the introduction of specific redundancies, we induce the presence of artificial correlations between the respective splitting parts. These interrelations shall be used to construct new types of constraints which are applicable in the corresponding QAP relaxations.

A beneficial interrelation property for the relaxation of QAP is the semidefinite inverse relation

$$B_\vartriangle \succeq B_\triangledown^{-1} \succeq 0. \tag{8}$$

The existence of the inverse $B_\triangledown^{-1}$ implies the regularity of $B_\triangledown$ and thereby also the regularity of $B_\vartriangle$. By the matrix equality

$$B_\triangledown - B_\vartriangle^{-1} = B_\vartriangle^{-1}(\underbrace{B_\vartriangle - B_\triangledown^{-1}}_{\succeq 0})B_\vartriangle^{-1} + (I - B_\triangledown^{-1}B_\vartriangle^{-1})^T \underbrace{B_\triangledown}_{\succeq 0}(I - B_\triangledown^{-1}B_\vartriangle^{-1}),$$

it is furthermore apparent that (8) implies the validity of

$$B_\triangledown \succeq B_\vartriangle^{-1} \succeq 0 \tag{9}$$

Indeed, it is straightforward to show that the conditions (8) and (9) are equivalent.

The discussed interrelation property can be exploited by transferring the same to the relaxation variables for the quadratic terms $Y_\vartriangle = XB_\vartriangle X^T$ and $Y_\triangledown = XB_\triangledown X^T$. The orthogonality of permutation matrices $X \in \Pi$ gives

$$XB_\triangledown^{-1}X^T = (XB_\triangledown X^T)^{-1}.$$

Relation (8) therefore requires $XB_\vartriangle X^T \succeq (XB_\triangledown X^T)^{-1} \succeq 0$ providing the basis for the constraint $Y_\vartriangle \succeq Y_\triangledown^{-1} \succeq 0$. The latter condition can be realized by utilization of the Schur complement inequality [1]:

$$\begin{bmatrix} Y_\vartriangle & I \\ I & Y_\triangledown \end{bmatrix} \in \mathbb{S}_+^{2n}. \tag{10}$$

For the attainment of tight SDP conditions, we are looking for matrices $B_\vartriangle$ and $B_\triangledown$ with minimal traces. This is the case for the splitting that satisfies the identity $B_\vartriangle = B_\triangledown^{-1}$.

Theorem 1. *Let $B \in \mathbb{S}^n$ be given and consider the minimization problem*

$$\begin{aligned} \inf_{B_\vartriangle, B_\triangledown \in \mathbb{S}^n} \quad & \operatorname{tr}(B_\vartriangle) + \operatorname{tr}(B_\triangledown) \\ \text{s.t.} \quad & B_\vartriangle \succeq B_\triangledown^{-1} \succeq 0, \\ & B_\vartriangle - B_\triangledown = B. \end{aligned} \tag{11}$$

A solution to this program is given by the matrix pair $(B_\vartriangle, B_\triangledown)$ defined as

$$B_\vartriangle := \frac{1}{2}\left(B + \sqrt{B^2 + 4I}\right), \qquad B_\triangledown := B_\vartriangle - B. \tag{12}$$

This pair satisfies the identity $B_\vartriangle = B_\triangledown^{-1}$.

Proof. The multiplication of the matrices defined in (12) gives

$$B_\vartriangle B_\triangledown = \frac{1}{2}\left(B + \sqrt{B^2+4I}\right)\frac{1}{2}\left(\sqrt{B^2+4I} - B\right) = \frac{1}{4}\left(B^2 + 4I - B^2\right) = I$$

and proves $B_\vartriangle = B_\triangledown^{-1}$. It is also straightforward to check that $(B_\vartriangle, B_\triangledown)$ satisfies the constraints of problem (11), hence states a feasible point. For now, let us assume that there is some solution $(\hat{B}_\vartriangle, \hat{B}_\triangledown)$ that accompanies a smaller objective value than the matrix pair from (12), thus $\operatorname{tr}(\hat{B}_\vartriangle) < \operatorname{tr}(B_\vartriangle)$. By definition, the matrices B, $B_\vartriangle$ and $B_\triangledown$ are all three simultaneously diagonalizable. Let $\{q_1, \ldots, q_n\}$ denote the set of the corresponding orthonormal eigenvectors, then

$$\sum_{i=1}^{n} q_i^T \hat{B}_\vartriangle q_i = \operatorname{tr}(\hat{B}_\vartriangle) < \operatorname{tr}(B_\vartriangle) = \sum_{i=1}^{n} q_i^T B_\vartriangle q_i$$

and therefore

$$\exists k \in \{1, \ldots, n\}: \quad q_k^T \hat{B}_\vartriangle q_k < q_k^T B_\vartriangle q_k.$$

Since $B_\vartriangle - \hat{B}_\vartriangle = B_\triangledown - \hat{B}_\triangledown$, this also means that $q_k^T \hat{B}_\triangledown q_k < q_k^T B_\triangledown q_k$, such that

$$q_k^T \hat{B}_\vartriangle q_k < q_k^T B_\vartriangle q_k = \lambda_k(B_\vartriangle) = \lambda_k(B_\triangledown)^{-1} = (q_k^T B_\triangledown q_k)^{-1} < (q_k^T \hat{B}_\triangledown q_k)^{-1}.$$

Moreover, the positive semidefinitenes of

$$\begin{bmatrix} q_k^T \hat{B}_\triangledown^{-1} q_k & 1 \\ 1 & q_k^T \hat{B}_\triangledown q_k \end{bmatrix} = \begin{bmatrix} q_k^T \hat{B}_\triangledown^{-\frac{1}{2}} \\ q_k^T \hat{B}_\triangledown^{\frac{1}{2}} \end{bmatrix} \begin{bmatrix} q_k^T \hat{B}_\triangledown^{-\frac{1}{2}} \\ q_k^T \hat{B}_\triangledown^{\frac{1}{2}} \end{bmatrix}^T \in \mathbb{S}_+^2$$

implies a nonnegative determinant of this matrix, which in turn requires that $(q_k^T \hat{B}_\triangledown^{-1} q_k)(q_k^T \hat{B}_\triangledown q_k) \geqslant 1$. Taken together, we obtain the inequality

$$q_k^T \hat{B}_\vartriangle q_k < (q_k^T \hat{B}_\triangledown q_k)^{-1} \leqslant q_k^T \hat{B}_\triangledown^{-1} q_k,$$

which violates the positive semidefinite condition $\hat{B}_\vartriangle \succeq \hat{B}_\triangledown^{-1}$, thereby contradicts our assumption and finishes the proof.

The efficiency of constraint (10) depends to a significant amount on the scaling of B. For QAP instances in which the spectral norm of $\|B\|$ is much greater than 1, the effect on the corresponding feasible set is hardly noticeable. On the other hand, if $\|B\| \ll 1$, the validity of (8) is purchased by introducing a relatively large redundancy. To counteract this behavior, we utilize a linear homogeneous function $\tau\colon \mathbb{S}^n \to \mathbb{R}$ and replace condition (8) with

$$B_\vartriangle \succeq \tau(B)^2 B_\triangledown^{-1} \succeq 0. \tag{13}$$

By numerical tests, we discovered that the trace norm of a projection of the respective matrix is a suitable base for τ. In the actual implementation, we use the renormalization function τ defined as

$$\tau(B) := \frac{1}{4n} \sum_{i=1}^{n} \sigma_i(PBP), \tag{14}$$

where the orthogonal projection matrix P is defined as $P := I - \frac{1}{n}ee^T$, and $\sigma_i(\cdot)$ denotes the i-th singular value of the corresponding matrix. Among the tested matrix norms and various scalings of these, the choice given in (14) worked best for a large range of problems.

For QAP instances with low-rank parameter matrices B, it is possible to strengthen the semidefinite constraint by replacing the inverse property in (8) with the pseudoinverse relations

$$B_\vartriangle \succeq B_\triangledown^\dagger \succeq 0 \qquad \text{and} \qquad B_\triangledown \succeq B_\vartriangle^\dagger \succeq 0. \tag{15}$$

Any matrix pair $(B_\vartriangle, B_\triangledown)$ that complies with these two conditions necessarily satisfies

$$\mathcal{R}(B_\vartriangle) \supseteq \mathcal{R}(B_\triangledown^\dagger) = \mathcal{R}(B_\triangledown) \supseteq \mathcal{R}(B_\vartriangle^\dagger) = \mathcal{R}(B_\vartriangle),$$

such that $\mathcal{R}(B_\vartriangle) = \mathcal{R}(B_\triangledown)$. This in turn demonstrates the equivalence of (15) and the semidefinite condition

$$\begin{bmatrix} B_\vartriangle & B_\vartriangle B_\vartriangle^\dagger \\ B_\vartriangle B_\vartriangle^\dagger & B_\triangledown \end{bmatrix} \in \mathbb{S}_+^{2n}.$$

In the actual implementation, we take the approach one step further by incorporating the renormalization function τ and weighting the utilization of the inverse interrelation property against the introduced redundancy. In order to achieve these objectives, we apply the following program:

$$\begin{aligned} \inf_{B_\vartriangle, B_\triangledown, G \in \mathbb{S}^n} \quad & \operatorname{tr}(B_\vartriangle) + \operatorname{tr}(B_\triangledown) - \xi \operatorname{tr}(G) \\ \text{s.t.} \quad & \begin{bmatrix} B_\vartriangle & G \\ G & B_\triangledown \end{bmatrix} \in \mathbb{S}_+^{2n}, \\ & B_\vartriangle - B_\triangledown = B, \\ & \|G\| \leqslant \tau(B), \end{aligned} \tag{16}$$

where ξ is a nonnegative real value that serves as a threshold for the introduced redundancy.

The choice of ξ influences the effectiveness of the generalized inverse interrelation. For the extreme $\xi = 0$ the result is equivalent to the pure non-redundant matrix splitting utilized in relaxation (6), hence $(B_\vartriangle, B_\triangledown, G) = (B_+, B_-, \mathit{0}_{(n,n)})$. On the other hand, for $\xi > 2$ the attained splitting corresponds to the normalized version of the original inverse property given in (13). By no means, however, ξ is used as a trade-off between speed and quality of the respective relaxations. The best bounding results are obtained for values in between these extremes. For the numerical examples in the last section, we use $\xi = \frac{3}{2}$ as this value works well for a large range of problems.

The last piece in the puzzle of designing a new matrix splitting based SDP relaxation for the QAP is the construction of the corresponding quadratic semidefinite constraints. For the optimal matrix triple $(B_\vartriangle, B_\triangledown, G)$ to problem (16), we have $G = B_\triangle^{\frac{1}{2}} B_\triangledown^{\frac{1}{2}} = B_\triangledown^{\frac{1}{2}} B_\triangle^{\frac{1}{2}}$. In the following relaxation framework, we implement the relation

$$\begin{bmatrix} XB_\triangle X^T & XGX^T \\ XGX^T & XB_\triangledown X^T \end{bmatrix} \succeq \begin{bmatrix} XB_\triangle^{\frac{1}{2}} \\ XB_\triangledown^{\frac{1}{2}} \end{bmatrix} \begin{bmatrix} B_\triangle^{\frac{1}{2}} X^T & B_\triangledown^{\frac{1}{2}} X^T \end{bmatrix}.$$

via utilization of the respective Schur complement inequality. Finally, we are in the position to present the SDP basis of the inverse interrelated matrix splitting relaxation, here referred to as *B-IIMS*:

$$\inf_{X \in \mathbb{D}^n,\; G, Y_\triangle, Y_\triangledown \in \mathbb{S}^n} \quad \langle A, Y_\triangle - Y_\triangledown \rangle + \langle C, X \rangle \tag{17a}$$

$$\text{s.t.} \quad \begin{bmatrix} I & B_\triangle^{\frac{1}{2}} X^T & B_\triangledown^{\frac{1}{2}} X^T \\ XB_\triangle^{\frac{1}{2}} & Y_\triangle & G \\ XB_\triangledown^{\frac{1}{2}} & G & Y_\triangledown \end{bmatrix} \in \mathbb{S}_+^{3n}, \tag{17b}$$

$$\begin{bmatrix} \left(\tau(B)I - B_\triangle^{\frac{1}{2}} B_\triangledown^{\frac{1}{2}}\right)^\dagger & UX^T \\ XU & \tau(B)I - G \end{bmatrix} \in \mathbb{S}_+^{2n}, \tag{17c}$$

$$\begin{aligned} &\operatorname{diag}(Y_\triangle) = X \operatorname{diag}(B_\triangle), \quad \operatorname{diag}(Y_\triangledown) = X \operatorname{diag}(B_\triangledown), \\ &\operatorname{diag}(G) = X \operatorname{diag}(B_\triangle^{\frac{1}{2}} B_\triangledown^{\frac{1}{2}}), \end{aligned} \tag{17d}$$

$$Y_\triangle e = XB_\triangle e, \quad Y_\triangledown e = XB_\triangledown e, \tag{17e}$$

where U denotes the orthogonal projection matrix to the column space of $\tau(B)I - B_\triangle^{\frac{1}{2}} B_\triangledown^{\frac{1}{2}}$, that is

$$U := \left(\tau(B)I - B_\triangle^{\frac{1}{2}} B_\triangledown^{\frac{1}{2}}\right)^\dagger \left(\tau(B)I - B_\triangle^{\frac{1}{2}} B_\triangledown^{\frac{1}{2}}\right).$$

3 Additional cuts based on symmetric functions

For many QAPs, it is possible to attain a significant improvement of the respective SDP relaxations by applying additional bounds to its optimization variables. In [17] and [20], Mittelmann, Peng and Li introduced new inequality constraints based on symmetric functions [16].

Definition 2. *A function* $\mathrm{f}(v)\colon \mathbb{R}^n \to \mathbb{R}$ *is said to be symmetric if for any permutation matrix* $X \in \Pi^n$*, the relation* $\mathrm{f}(v) = \mathrm{f}(Xv)$ *holds.*

One of these functions, namely the additive function $\mathrm{f}(v) = \langle e, v \rangle$, has already been used for the constraints (6d) and (17e). Other symmetric functions, that are useful for the construction of valid constraints, are the minimum and the maximum function as well as p-norms:

$$\forall v \in \mathbb{R}^n: \quad \min(v) = \min_{1 \leqslant i \leqslant n} v_i, \quad \max(v) = \max_{1 \leqslant i \leqslant n} v_i, \quad \mathcal{L}_p(v) = \left(\sum_{i=1}^n |v_i|^p\right)^{\frac{1}{p}}.$$

If applied to a matrix $M \in \mathbb{M}^{m,n}$, these operators act along the rows of the matrix, i.e.

$$\min(M) = [\,\min(e_1^T M), \ldots, \min(e_m^T M)\,]^T.$$

In [17], [20], [21] and also [11], the minimum and maximum functions are used to obtain linear bounds for several optimization variables.

$$e_i^T X \min(B) \leqslant (Y_+ - Y_-)_{ij} \leqslant e_i^T X \max(B) \qquad \text{for} \quad 1 \leqslant i, j \leqslant n. \tag{18}$$

The same authors used constraints based on p-norm conditions for a further tightening of their relaxation frameworks:

$$\mathcal{L}_p(Y_+ - Y_-) \leqslant X \mathcal{L}_p(B_+ - B_-). \tag{19}$$

In [20], Peng et al. extended this approach by applying the same kind of constraint to each matrix variable Y_+ and Y_- as well as their sum.

3.1 Further improvements

The linear inequalities given in (18) can be presented in the form of so-called sum-matrix inequalities. In accordance to [21], a sum-matrix is defined as:

Definition 3. *A matrix $M \in \mathbb{M}^n$ is called a sum-matrix if M is representable as*

$$M = ve^T + ew^T \tag{20}$$

for some $v, w \in \mathbb{R}^n$. In the symmetric case it is $v = w$.

Let $v_{\min} := \min(B)$ and $v_{\max} := \max(B)$ denote the vectors consisting of the minimal and maximal row elements of B, respectively. Condition (18) may then be rewritten as

$$X v_{\min} e^T \leqslant Y_+ - Y_- \leqslant X v_{\max} e^T.$$

Indeed, by the nonnegativity of X, it is straightforward to show that $v_{\min} e^T \leqslant B \leqslant v_{\max} e^T$ implies

$$X v_{\min} e^T = X v_{\min} e^T X^T \leqslant XBX^T \leqslant X v_{\max} e^T X^T = X v_{\max} e^T$$

and thus yields (18). The last observation motivates a further exploitation of sum-matrix inequalities for the attainment of tighter constraints. Define for instance

$$w_{\min} := \min(B - e v_{\min}^T) \qquad \text{and} \qquad w_{\max} := \max(B - e v_{\max}^T).$$

It obviously is $v_{\min} e^T + e w_{\min}^T \leqslant B \leqslant v_{\max} e^T + e w_{\max}^T$, which in turn gives the inequality constraints

$$X v_{\min} e^T + e w_{\min}^T X^T \leqslant Y_+ - Y_- \leqslant X v_{\max} e^T + e w_{\max}^T X^T.$$

By $w_{\min} \geqslant 0$ and $w_{\max} \leqslant 0$, it is apparent that these bounds are at least as good as the ones in (18).

For the linear inequalities based on the minimum respectively maximum function, Mittelmann and Peng [17] pointed out that - since the diagonal elements of Y_+ and Y_- are already described by the corresponding equality constraints - it is sufficient to account solely the off-diagonal variables. We further observe that, due to symmetry of B, the symmetric parts of the respective sum-matrices satisfy the same bounding conditions, i.e.

$$ve^T + ew^T \leqslant_{\text{off}} B \quad \Longrightarrow \quad \tfrac{1}{2}(v+w)e^T + \tfrac{1}{2}e(v+w)^T \leqslant_{\text{off}} B. \tag{21}$$

Let the gap between a sum-matrix $ve^T + ew^T = (v_i + w_j)$ and an arbitrary real matrix $B = (b_{ij})$ of the same dimension be defined as

$$\delta_{\text{gap}}(B, v, w) := \sum_{\substack{i,j \\ i \neq j}} |b_{ij} - v_i - w_j|. \tag{22}$$

A suitable approach for the attainment of tight sum-matrix inequalities is the minimization of the respective gaps.

By $\delta_{\text{gap}}(B, v, w) = \delta_{\text{gap}}(B, \frac{1}{2}(v+w), \frac{1}{2}(v+w))$ and the implication in (21), it is apparently sufficient to concentrate on the lower respectively upper triangular elements of symmetric sum-matrices. The following linear programming problem can be used to compute lower and upper symmetric sum-matrix bounds for B that accompany minimal gaps:

$$\begin{aligned} \inf_{\mathrm{v}_l, \mathrm{v}_u \in \mathbb{R}^n} \quad & \langle e, \mathrm{v}_u - \mathrm{v}_l \rangle \\ \text{s. t.} \quad & \mathrm{v}_l e^T + e\mathrm{v}_l^T \leqslant_{\text{tri}} B \leqslant_{\text{tri}} \mathrm{v}_u e^T + e\mathrm{v}_u^T. \end{aligned} \tag{23}$$

The solution vectors to this problem are used to implement the following linear inequality conditions

$$X\mathrm{v}_l e^T + e\mathrm{v}_l^T X^T \leqslant_{\text{tri}} Y_+ - Y_- \leqslant_{\text{tri}} X\mathrm{v}_u e^T + e\mathrm{v}_u^T X^T. \tag{24}$$

Suitable approaches for a further tightening of these bounds are the application of multiple varying sum-matrix inequalities and the construction of the same type of bounds for linear combinations of the respective matrix variables.

In a very similar way, it is possible to apply the sum-matrix reformulation technique from above for a tightening of the respective p-norm based constraints. However, numerical tests have shown that the effect of these extensions is relatively small. For this reason, we avoid the necessity of further computations for the determination of suitable sum-matrix updates.

4 Numerical Results

In the last section of this paper, we want to discuss the practical applicability of the presented relaxation strategy on the basis of numerical tests. For this purpose, we compare our own frameworks with one of the best performing low-dimensional SDP relaxations for the QAP, namely *F-SVD* which was introduced in [20].

The actual implementation of the SDP problems is realized via Yalmip [14] in Octave [7]. The used solver is SDPT3 [24]. For the presentation of the respective bounds, we follow the style in [20] and use the relative gap defined as

$$R_{\text{gap}} = 1 - \frac{\text{Lower bound from relaxation}}{\text{Optimal or best known feasible objective value}}.$$

The corresponding computation times are listed in seconds under the 'CPU' columns. Since the discussed relaxation frameworks are not designed for a specific class of QAPs, we chose the instances for our numerical tests arbitrarily from the quadratic assignment problem library [4]. The names in the column 'prob.' consists of three or four letters which indicate the names of their authors or contributors, and a number that gives their dimension. If the authors provided multiple problem instances for the same dimension, the respective instance is indicated by another letter at the end of the name. For more information on the naming scheme and the individual applications, see [4].

Prior to the comparison of the full frameworks with all additional constraints being applied, in Table 1, we compare the pure SDP relaxation bases presented in Section 2.

	B-SVD		*B-IIMS*	
prob.	$\mathrm{R}_{gap}(\%)$	CPU	$\mathrm{R}_{gap}(\%)$	CPU
Esc16b	17,34	2	17,09	3
Had20	5,34	4	3,61	6
Kra32	42,64	13	32,27	36
LiPa40a	4,88	28	3,31	63
Nug30	12,39	11	9,93	22
Scr20	60,02	5	45,35	7
Ste36a	57,54	25	44,97	64
Tai30b	15,82	17	15,34	41
Tai50a	39,03	103	28,37	244
Tho40	14,94	40	13,06	91

Table 1. Selected bounds for comparison of base relaxations

The results presented in Table 1 reveal the significant differences between the considered relaxation approaches. As expected, the new relaxation program *B-IIMS* is more expensive than *B-SVD*. On the other hand, for many problem instances the additional computational costs pay off by resulting in significantly improved lower bounds.

For the attainment of the full relaxation frameworks, we extend the problems (6) and (17) by adding the constraints (24) together with the 2-norm conditions of the form (19) which are also present in *F-SVD*. We denote the full version of problem (6) by *F-SVD2*, since the only difference two the framework *F-SVD* from [20] is the utilization of different inequality constraints. Instead of the $8n^2 - 8n$ minimum and maximum bound inequalities applied in *F-SVD*, here we solely use the $n^2 - n$ constraints from (24). The full version of problem (17) applies the respective adaptations of the same constraints. The integration is realized simply by replacing the term $Y_+ - Y_-$ with $Y_\vartriangle - Y_\triangledown$. We follow the general naming scheme and denote this program by *F-IIMS*.

	F-SVD		*F-SVD2*		*F-IIMS*	
prob.	$\mathrm{R}_{gap}(\%)$	CPU	$\mathrm{R}_{gap}(\%)$	CPU	$\mathrm{R}_{gap}(\%)$	CPU
Esc16b	5,82	3	6,73	3	6,56	4
Had20	2,53	8	2,67	6	2,32	8
Kra32	18,77	34	18,93	24	18,67	36
LiPa40a	0,11	74	0,24	42	0,23	74
Nug30	8,05	26	8,12	18	7,88	33
Scr20	16,18	10	16,24	7	16,01	8
Ste36a	19,06	55	19,35	40	18,55	55
Tai30b	12,69	32	12,88	24	13,50	48
Tai50a	21,43	250	21,58	197	21,49	240
Tho40	12,61	76	12,76	54	12,13	102

Table 2. Selected bounds for comparison of full QAP relaxations

The results in Table 2 demonstrate the efficiency of the constraints in (24) compared to the significantly greater number of linear inequalities used in *F-SVD*. The difference between the bounds computed with *F-SVD* and *F-SVD2* is generally really small whereas the computation times of *F-SVD2* are noticeable shorter. Nevertheless, the results in Table 2 also reveal that the combined effect of the additional linear bounds applied in *F-SVD* is superior to the improvement of a single sum-matrix bound. The sheer number of additional constraints is difficult to beat.

The second observation from the results given in Table 2 is that the presence of the additional cuts diminishes the effect of the incorporation of the artificial inverse interrelation property. Among the tested QAP instances there is even an instance for which the application of the inverse interrelated matrix splitting approach is disadvantageous. Overall, the computational costs as well as the bounding quality of the frameworks *F-SVD* and *F-IIMS* are very similar. The latter relaxation, however, has a greater potential for even stronger bounds, for instance via the utilization of so-called QAP reformulations or the incorporation of a similar number of linear inequalities as used in *F-SVD*. An elaborate investigation of these possibilities is left for subsequent studies.

Acknowledgments

The author thanks the anonymous referees for their helpful remarks that lead to a better structure of the paper.

References

1. Albert, A.: Conditions for positive and nonnegative definiteness in terms of pseudoinverses. SIAM J. Appl. Math. 17(2), 434–440 (1969), http://dx.doi.org/10.1137/0117041
2. Burer, S., Monteiro, R.D.: Local minima and convergence in low-rank semidefinite programming. Math. Programming 103(3), 427–444 (2004), http://dx.doi.org/10.1007/s10107-004-0564-1
3. Burkard, R.E., Dell'Amico, M., Martello, S.: Assignment Problems. SIAM Philadelphia (2012), http://dx.doi.org/10.1137/1.9781611972238
4. Burkard, R.E., Karisch, S.E., Rendl, F.: QAPLIB - a quadratic assignment problem library. J. Global Optim. 10(4), 391–403 (1997), http://dx.doi.org/10.1023/A:1008293323270
5. Çela, E.: The Quadratic Assignment Problem: Theory and Algorithms, Combinatorial Optimization, vol. 1. Springer US (1998), http://dx.doi.org/10.1007/978-1-4757-2787-6
6. Ding, Y., Wolkowicz, H.: A low-dimensional semidefinite relaxation for the quadratic assignment problem. Math. Oper. Res. 34(4), 1008–1022 (2009)
7. Eaton, J.W., Bateman, D., Hauberg, S.: GNU Octave version 3.0.1 manual: a high-level interactive language for numerical computations. CreateSpace Independent Publishing Platform (2009), http://www.gnu.org/software/octave/doc/interpreter, ISBN 1441413006
8. Edwards, C.S.: A branch and bound algorithm for the Koopmans-Beckmann quadratic assignment problem. In: Combinatorial Optimization II, Mathematical Programming, vol. 13, pp. 35–52. Springer US (1980), http://dx.doi.org/10.1007/BFb0120905
9. Gilmore, P.C.: Optimal and suboptimal algorithms for the quadratic assignment problem. SIAM J. Appl. Math. 10(2), 305–313 (1962), http://dx.doi.org/10.1137/0110022
10. de Klerk, E., Sotirov, R.: Exploiting group symmetry in semidefinite programming relaxations of the quadratic assignment problem. Math. Programming 122(2), 225–246 (2010), http://dx.doi.org/10.1007/s10107-008-0246-5
11. de Klerk, E., Sotirov, R., Truetsch, U.: A new semidefinite programming relaxation for the quadratic assignment problem and its computational perspectives. INFORMS J. Comput. 27(2), 378–391 (2015), http://dx.doi.org/10.1287/ijoc.2014.0634
12. Koopmans, T.C., Beckmann, M.: Assignment problems and the location of economic activities. Econometrica 25(1), 53–76 (1957), http://dx.doi.org/10.2307/1907742
13. Lawler, E.L.: The quadratic assignment problem. Manag. Sci. 9(4), 586–599 (1963)
14. Löfberg, J.: Yalmip: A toolbox for modeling and optimization in MATLAB. In: Proceedings of the CACSD Conference (2004), http://users.isy.liu.se/johanl/yalmip
15. Loiola, E.M., de Abreu, N.M.M., Boaventura-Netto, P.O., Hahn, P., Querido, T.: A survey for the quadratic assignment problem. Eur. J. Oper. Res. 176(2), 657–690 (2007), http://dx.doi.org/10.1016/j.ejor.2005.09.032

16. Macdonald, I.G.: Symmetric Functions and Hall Polynomials. The Clarendon Press, Oxford University Press, New York, 2 edn. (1995)
17. Mittelmann, H., Peng, J.: Estimating bounds for quadratic assignment problems associated with Hamming and Manhattan distance matrices based on semidefinite programming. SIAM J. Optim. 20(6), 3408–3426 (2010), http://dx.doi.org/10.1137/090748834
18. Moore, E.H.: On the reciprocal of the general matrix. Bull. Amer. Math. Soc. 26, 394–395 (1920)
19. Pardalos, P.M., Rendl, F., Wolkowicz, H.: The quadratic assignment problem: A survey and recent developments. In: Quadratic Assignment and Related Problems. DIMACS Series in Discrete Mathematics and Theoretical Computer Science, vol. 16, pp. 1–42. American Mathematical Society (AMS) (1994)
20. Peng, J., Mittelmann, H., Li, X.: A new relaxation framework for quadratic assignment problems based on matrix splitting. Math. Prog. Comp. 2(1), 59–77 (2010), http://dx.doi.org/10.1007/s12532-010-0012-6
21. Peng, J., Zhu, T., Luo, H., Toh, K.C.: Semi-definite programming relaxation of quadratic assignment problems based on nonredundant matrix splitting. Comput. Optim. Appl. (2014), http://dx.doi.org/10.1007/s10589-014-9663-y
22. Penrose, R., Todd, J.A.: A generalized inverse for matrices. Math. Proc. Camb. Phil. Soc. 51(03), 406–413 (1955), http://dx.doi.org/10.1017/S0305004100030401
23. Rendl, F., Sotirov, R.: Bounds for the quadratic assignment problem using the bundle method. Math. Programming 109(2–3), 505–524 (2007), http://dx.doi.org/10.1007/s10107-006-0038-8
24. Tütüncü, R.H., Toh, K.C., Todd, M.J.: Solving semidefinite-quadratic-linear programs using SDPt3. Math. Programming 95(2), 189–217 (2003), http://dx.doi.org/10.1007/s10107-002-0347-5
25. Yang, L., Sun, D., Toh, K.C.: SDPnal+: a majorized semismooth Newton-CG augmented Lagrangian method for semidefinite programming with nonnegative constraints. Math. Prog. Comp. (2015), http://dx.doi.org/10.1007/s12532-015-0082-6
26. Zhao, Q., Karisch, S.E., Rendl, F., Wolkowicz, H.: Semidefinite programming relaxations for the quadratic assignment problem. J. Comb. Optim. 2(1), 71–109 (1998), http://dx.doi.org/10.1023/A:1009795911987