Semidefinite approximations for quadratic programs over orthogonal matrices

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Abstract

Finding global optimum of a non-convex quadratic function is in general a very difficult task even when the feasible set is a polyhedron.

We show that when the feasible set of a quadratic problem consists of orthogonal matrices from $\mathbb{R}^{n\times k}$, then we can transform it into a semidefinite program in matrices of order kn which has the same optimal value.

This opens new possibilities to get good lower bounds for several problems from combinatorial optimization, like the *Quadratic Assignment Problem* (QAP) and the *Graph Partitioning Problem* (GPP). In particular we show how to improve significantly the well-known Hoffman-Wielandt eigenvalue lower bound for QAP and the Donath-Hoffman eigenvalue lower bound for GPP by semidefinite programming.

In the last part of the paper we show that the copositive strengthening of the semidefinite lower bounds for QAP and GPP yields the exact values.

Key words: quadratic programming, semidefinite programming, copositive programming, eigenvalue bound, quadratic assignment problem, graph partitioning problem.

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1 Introduction

Non-convex quadratic problems are a common research topic since they appear very often in combinatorial optimization. They are in general very hard, since already the following simple non-convex quadratic problem

$$\min\{x^T Qx : x \in \mathbb{R}^n_+, \sum_i x_i = 1\} \tag{1}$$

is NP-hard to solve. More specifically, when $Q = A + I$ and A is the adjacency matrix of a graph G, then the optimal value of (1) yields the stability number of G (see [12]) which is NP-hard to compute.

In this paper we consider the following general non-convex quadratic program:

$$(QP) \qquad OPT_{QP} = \min\{\mathrm{trace}(X^T AXB) : X \in \mathbb{R}^{n\times k}_+, X^T X = M, Q(X) = q\},$$

where A and B are arbitrary symmetric matrices, M is diagonal matrix and $Q(X) = q$ denotes some additional quadratic constraints. Several well-known NP-hard problems can be restated in the form QP, e.g. the Quadratic assignment problem, the Graph partitioning problem, the Weighted sums of eigenvalues problem etc.

The problems listed above are very tough, and there is no polynomial time algorithm which finds the optimal solution of these problems (unless P=NP). Optimal solutions are often computed with a branch and bound algorithm which has the exponential time complexity. The efficiency of this algorithm strongly depends on the quality of upper and lower bounds for the optimal value of the problem. Upper bounds we get with any heuristic, while computing lower bounds typically consists in relaxing some hard constraint and computing the optimal value of the relaxed problem.

Many researchers studied relaxations which yield spectral lower bounds. Hoffman and Wielandt [10] established an eigenvalue lower bound for the optimal value of QP for the case when the feasible set consists of non-negative square orthonormal matrices. They dropped the sign constraint and computed the optimal value of the relaxed problem which is determined by the eigenvalues of A and B, see Section 2. This is also known as the eigenvalue lower bound for the Quadratic assignment problem.

Donath and Hoffman [8] presented an eigenvalue lower bound for the Graph partitioning problem which is another special case of QP. They again relaxed the original problem which is NP-hard by ignoring the sign constraint and reformulated the resulting problem as an eigenvalue optimization problem.

Helmberg et al. [9] and Rendl and Wolkowicz [19] studied the projected eigenvalue lower bounds for the minimum cut problem and graph partitioning problems.

Anstreicher and Wolkowicz [1] reformulated the Hoffman-Wielandt and the Donath-Hoffman lower bounds as optimal values of semidefinite programs. A similar result was obtained by Povh and Rendl for the eigenvalue lower bound from [9], see [15]. These results are very important because further strengthenings of the eigenvalue lower bounds lead to untractable problems, while the semidefinite reformulation enables adding additional constraints and therefore improving the lower bounds.

Our contribution to the literature on approximation of non-convex quadratic programs consists of the following results:

- In Section 2 we prove a representation theorem which states that the Lagrangian relaxation of the quadratic program over the set of orthogonal matrices which is a semidefinite program is tight, if we add on the primal side a redundant semidefinite constraint. This results generalizes the Anstreicher-Wolkowicz result from [1] and yields much smaller semidefinite programs for the Donath-Hoffman lower bound.

- In Section 3 we present the implications of the representation theorem on computing lower bounds for the Quadratic assignment problem and the Graph partitioning problem. We show in particular that the Donath-Hoffman lower bound arises as the Lagrangian relaxation of the properly relaxed Graph partitioning problem, but there is in general non-zero duality gap in the relaxation. Nevertheless, this procedure opens new possibilities for further strengthening of the Donath-Hoffman lower bound by semidefinite programming.
- We study semidefinite lower bounds for QAP and GPP and propose some new constraints which significantly improve eigenvalue lower bounds and yield semidefinite programs which seem to be the tradeoff between the accuracy and time complexity, see Section 3.
- We show that replacing the semidefinite constraint by completely positive constraint improves the lower bound, and in the case of GPP yields even the exact value. This is the contents of Section 5.

1.1 Notation

We denote the ith standard unit vector by e_i. The vector of all ones is $u_n \in \mathbb{R}^n$ (or u, if the dimension n is obvious). The square matrix of all ones is J_n (or J), the identity matrix is I and $E_{ij} = e_i e_j^T$.

In this paper we consider the following sets of matrices:

- The vector space of real symmetric $n \times n$ matrices: $\mathcal{S}_n = \{X \in \mathbb{R}^{n\times n} : X = X^T\}$,
- the cone of $n \times n$ positive semidefinite matrices: $\mathcal{S}_n^+ = \{X \in \mathcal{S}_n \colon y^T X y \geq 0 \forall y \in \mathbb{R}^n\}$,
- the cone of $n \times n$ copositive matrices: $\mathcal{C}_n = \{X \in \mathcal{S}_n \colon y^T X y \geq 0 \forall y \in \mathbb{R}^n_+\}$,
- the cone of $n \times n$ completely positive matrices: $\mathcal{C}_n^* = \operatorname{conv}\{yy^T : y \in \mathbb{R}^n_+\}$.

We also use $X \succeq 0$ for $X \in \mathcal{S}_n^+$. A linear program over $\mathbb{R}^n_+$ is called a linear program, a linear program over $\mathcal{S}_n^+$ is called a semidefinite program, while a linear program over $\mathcal{C}_n$ or $\mathcal{C}_n^*$ is called a copositive program.

The sign $\otimes$ stands for the Kronecker product. When we consider the matrix $X \in \mathbb{R}^{m\times n}$ as a vector from $\mathbb{R}^{mn}$, we write this vector as $\operatorname{vec}(X)$ or x. By $\langle\cdot,\cdot\rangle$ we denote the standard scalar product, i.e. $\langle u,\, v\rangle = u^T v$ for $u, v \in \mathbb{R}^n$, and for $X, Y \in \mathbb{R}^{m\times n}$ we have $\langle X,\, Y\rangle = \operatorname{trace}(X^T Y)$. For matrix columns and rows we use the Matlab notation: $X(i,:)$ and $X(:,i)$ stand for ith row and column, respectively. If $a \in \mathbb{R}^n$, then $\operatorname{Diag}(a)$ is an $n \times n$ diagonal matrix with a on the main diagonal and $\operatorname{diag}(X)$ is the main diagonal of a square matrix X.

For a matrix $Z \in \mathcal{S}_{kn}$ we often use the following block notation:

$$Z = \begin{bmatrix} Z^{11} & \cdots & Z^{1k} \\ \vdots & \ddots & \vdots \\ Z^{k1} & \cdots & Z^{kk} \end{bmatrix}, \tag{2}$$

where $Z^{ij} \in \mathbb{R}^{n\times n}$.

When P or $P_{subscript}$ is the name of the optimization problem, then OPT_P or $OPT_{subscript}$, respectively, denote their optimal values.

2 Semidefinite programming relaxations for QP

2.1 Representation theorem

Hoffman and Wielandt [10] showed that

$$OPT_{HW} \quad = \quad \min\{\langle X,\, AXB\rangle :\ X \in \mathbb{R}^{n\times n},\ X^TX = I\ \} \quad = \quad \langle \lambda,\, \sigma\rangle_- \tag{3}$$

where λ and σ are the vectors of eigenvalues of A and B, respectively, and $\langle \lambda,\, \sigma\rangle_-$ denotes the scalar product, where we first sort the components of λ increasingly and the components of σ decreasingly. OPT_{HW} is a lower bound for OPT_{QP}, since the problem (3) is obtained from QP by omitting sign constraints and the quadratic constraint $Q(X) = q$.

Anstreicher and Wolkowicz [1] formulated this lower bound as the optimal value of a semidefinite program. They added in problem (3) the redundant constraint $XX^T = I$ and then considered the Lagrangian dual of the problem which is semidefinite program (4). They showed that strong duality holds for this case, hence we have

$$OPT_{HW} \quad = \quad \max\{\mathrm{trace}(S) + \mathrm{trace}(T) \colon S \in \mathcal{S},\, T \in \mathcal{S},\, S \otimes I + I \otimes T \preceq B \otimes A\}. \tag{4}$$

In this section we extend this result to a more general case when the matrices $X \in \mathbb{R}^{n\times k}$ still have orthonormal columns but are not square. In this case we have $X^TX = I_k$, but the other constraint $XX^T = I_n$ is not satisfied, if $k < n$. Therefore we can not repeat the Anstreicher-Wolkowicz procedure. The following lemma shows how the constraint $XX^T = I_n$ should be generalized to close the duality gap.

Lemma 1 *If $X \in \mathbb{R}^{n\times k}$ and $X^TX = I_k$, then $XX^T \preceq I_n$.*

Proof: Let us fix X. We can complete the columns of X into an orthonormal basis $(u_1, u_2, \ldots, u_n)$ of the space $\mathbb{R}^n$, hence for $1 \le i \le k$ we have $u_i = X(:, i)$. Let $u = \sum_{i=1}^n \alpha_i u_i$ be an arbitrary vector from $\mathbb{R}^n$. We have $u^T(I - XX^T)u = \sum_{i=k+1}^n \alpha_i^2 \ge 0$, hence $I - XX^T \succeq 0$. □

Now we can prove the theorem.

Theorem 2 *If $A \in \mathcal{S}_n$ and $B \in \mathcal{S}_k$, then*

$$\begin{aligned} &\min\{\langle X,\, AXB\rangle \colon X \in \mathbb{R}^{n\times k},\, X^TX = I_k\} = \\ &\max\{\mathrm{trace}(S) - \mathrm{trace}(T) \colon S \in \mathcal{S}_k,\, T \in \mathcal{S}_n^+,\, S \otimes I_n - I_k \otimes T \preceq B \otimes A\} \end{aligned} \tag{5}$$

Proof: The proof mostly consists of extensions of the ideas from [1]. Let OPT_1 and OPT_2 be the optimal values of the first and the second problem in (5), resp. Firstly we show that the second problem is the Lagrangian relaxation of the first problem, if we add the seemingly redundant constraint $XX^T \preceq I$. In the sequel we reduce it to a linear program and finally prove that the optimal value of the dual linear program is

$$\sum_i \sigma_i \lambda_{\varphi(i)}$$

where φ is some injection from $\{1, \ldots, k\}$ into $\{1, \ldots, n\}$ and $\lambda,\ \sigma$ are vectors with the eigenvalues of A and B, resp. This is at least OPT_1 [9, Theorem 5] and completes the chain of inequalities.

We introduce the dual variable S for the constraint $X^T X = I_k$ and the dual variable T for the newly added constraint $XX^T \preceq I_n$. Clearly $S \in \mathcal{S}_k$, $T \in \mathcal{S}_n^+$ and we have

$$\begin{aligned} OPT_1 &= \min\{\langle X,\, AXB\rangle \colon X \in \mathbb{R}^{n\times k},\ X^TX = I_k,\ XX^T \preceq I_n\} \\ &= \min_{X\in\mathbb{R}^{n\times k}} \Big\{ \max_{S\in\mathcal{S}_k,\ T\in\mathcal{S}_n^+} \{\langle X,\, AXB\rangle + \langle S,\, I_k - X^TX\rangle - \langle T,\, I_n - XX^T\rangle\}\Big\} \\ &\geq \max_{S\in\mathcal{S}_k,\ T\in\mathcal{S}_n^+} \Big\{\operatorname{trace}(S) - \operatorname{trace}(T) + \min_{x\in\mathbb{R}^{nk}} x^T(B\otimes A - S\otimes I_n + I_k\otimes T)x\Big\} \\ &= \max\{\operatorname{trace}(S) - \operatorname{trace}(T) \colon S\in\mathcal{S}_k,\ T\in\mathcal{S}_n^+,\ S\otimes I_n - I_k\otimes T \preceq B\otimes A\} \\ &= OPT_2. \end{aligned}$$

The first inequality follows from exchanging min and max and the last equality is due to the inner minimization problem which is a quadratic unconstrained problem and is therefore bounded from below if and only if its Hessian $B\otimes A - S\otimes I_n + I_k\otimes T$ is positive semidefinite. We also used the fact that

$$\langle X,\, AXB\rangle = x^T(B\otimes A)x \quad \text{for } x = \operatorname{vec}(X).$$

We show that there is an equality above by transforming the last semidefinite program into a linear program. Since A and B are symmetric, we can find an orthonormal decomposition $A = P\Lambda P^T$ and $B = Q\Sigma Q^T$, where $\Lambda = \operatorname{Diag}(\lambda)$, $\Sigma = \operatorname{Diag}(\sigma)$, vectors λ, σ are as above and P, Q are matrices whose columns are eigenvectors of A and B, respectively. We can write

$$\begin{aligned} OPT_2 &= \max\ \{\operatorname{trace}(S) - \operatorname{trace}(T) \colon S\in\mathcal{S}_k,\ T\in\mathcal{S}_n^+,\ S\otimes I_n - I_k\otimes T \preceq \Sigma\otimes\Lambda\} \\ &= \max\ \{u_k^T s - u_n^T t \colon s\in\mathbb{R}^k,\ t\in\mathbb{R}^n_+,\ s_i - t_j \leq \sigma_i\lambda_j,\ \forall i,j\} \\ &= \min\ \{\textstyle\sum_{i,j}\sigma_i\lambda_j z_{ij} \colon y\in\mathbb{R}^n_+,\ Z\in\mathbb{R}^{k\times n}_+,\ Zu_n = u_k,\ Z^Tu_k + y = u_n\}. \end{aligned}$$

The first equality in the expression above follows from the fact that the cost function depends only on diagonal entries of the matrices S and T, so we may ignore all non-diagonal entries and write $s = \operatorname{diag}(S)$ and $t = \operatorname{diag}(T)$. The last optimization problem is a dual linear program to the last but one problem. We should note that the system matrix in the last linear program is totally unimodular, hence there exists (see [13]) an integer optimal solution

$$(Z^*, y^*) \in \mathbb{R}^{k\times n}_+ \times \mathbb{R}^n_+.$$

The matrix Z^* is therefore a 0-1 matrix and defines an injection $\varphi^* \colon \{1,\ldots,k\} \to \{1,\ldots,n\}$ with $\varphi^*(i) = j \iff z^*_{ij} = 1$. This means that we have proved

$$OPT_2 = \sum_{i=1}^k \sigma_i\lambda_{\varphi^*(i)} \geq \min\ \Big\{\sum_i \sigma_i\lambda_{\varphi(i)} \colon \varphi \text{ injection } : \{1,\ldots,k\}\to\{1,\ldots,n\}\Big\}.$$

The optimal value of the right-hand side problem above is exactly OPT_1 (see e.g. [9, Theorem 5]), and from all relations from the beginning we can conclude that $OPT_1 = OPT_2$. □

Remark 1 *If $k = n$, then (4) and (5) are equivalent. Indeed, if $(S^*, T^*) \in \mathcal{S}_k\times\mathcal{S}_n$ is feasible for (4), then $(\bar S, \bar T)$ defined by $\bar S = S + \lambda_{\max}(T)$ and $\bar T = -T + \lambda_{\max}(T)$ is a feasible solution for (5) with the same objective value. Similarly any feasibly pair (S,T) for (5) gives feasible solution $(S, -T)$ for (4) with the same objective value.*

2.2 SDP relaxations for QP

Suppose that we have in QP only "pure" quadratic constraints, i.e. $Q(X) = q$ contains only equations of type $\langle X, A_i X B_i\rangle = q_i$, where A_i and B_i are arbitrary matrices such that the scalar product is defined. Based on the Theorem 2 we can obtain the following semidefinite lower bound for the optimal value of QP

$$
\begin{array}{rcl}
OPT_{QP} & \geq & \min \;\; \mathrm{trace}(X^T AXB) \\
 & & X \in \mathbb{R}^{n\times k},\; X^T X = M \\
 & & \langle X, A_i X B_i\rangle = q_i, \forall i \\
 & = & \min \;\; \mathrm{trace}(Y^T AYM^{1/2}BM^{1/2}) \\
 & & Y \in \mathbb{R}^{n\times k},\; Y^T Y = I \\
 & & \langle Y, A_i YM^{1/2}B_i M^{1/2}\rangle = q_i, \forall i \\
 & \geq & \max \;\; \mathrm{trace}(S) - \mathrm{trace}(T) + q^T y \\
 & & S \in \mathcal{S}_k,\, T \in \mathcal{S}_n^+, \\
 & & S \otimes I_n - I_k \otimes T + \sum_i y_i\, (M^{1/2}B_i^T M^{1/2}) \otimes A_i \preceq (M^{1/2}BM^{1/2}) \otimes A \\
 & = & \min \;\; \langle M^{1/2}BM^{1/2} \otimes A,\, Z\rangle \\
 & & Z \in \mathcal{S}_{kn}^+,\; W \in \mathcal{S}_n^+ \\
 & & \sum_i Z^{ii} + W = I,\;\; \langle I,\, Z^{ij}\rangle = \delta_{ij}, \\
 & & \langle M^{1/2}B_i^T M^{1/2} \otimes A_i,\; Z\rangle = q_i, \forall i \\
 & = & \min \;\; \langle B \otimes A,\, V\rangle \\
(QP_{SDP}) & & V \in \mathcal{S}_{kn}^+,\; W \in \mathcal{S}_n^+ \\
 & & \sum_i \frac{1}{m_i} V^{ii} + W = I,\;\; \langle I,\, V^{ij}\rangle = m_i\delta_{ij}, \\
 & & \langle B_i^T \otimes A_i,\; V\rangle = q_i, \forall i
\end{array}
$$

The second quadratic problem above is obtained from the first by substitution $Y = XM^{-1/2}$. The first semidefinite program above is the Lagrangian dual of the second quadratic problem. The second semidefinite program is Lagrangian dual of the first semidefinite program. The last semidefinite program is obtained from the second semidefinite program by reverse substitution $V = (M^{1/2} \otimes I)Z(M^{1/2} \otimes I)$.

The first inequality appears since we dropped out the sign constraint in the quadratic problem QP, while the second inequality is due to the fact that the Lagrangian relaxation of non-convex quadratic program might have non-zero gap. This actually happens very often (see also Subsection 3.2 and Example 1). If we do not have quadratic equations $\langle X, A_i X B_i\rangle = q_i$, then the second inequality is equality due to Theorem 2.

Note that the Lagrangian semidefinite duals have zero duality gap, since $S = 0, T = \alpha I$ and $y = 0$ are strictly feasible solution for the first semidefinite program above, if $\alpha > 0$ is sufficiently large (i.e. the matrices T and $(M^{1/2}BM^{1/2}) \otimes A + I_k \otimes T$ are positive definite when $T = \alpha I$ for $\alpha > 0$ sufficiently large).

Remark 2 *If quadratic constraint $Q(X) = q$ contains also linear terms, i.e. is of the form $\langle X, A_i X B_i\rangle + \langle C_i, X\rangle = q_i$, $C_i \neq O$, then we can repeat the procedure by adding zero row and column into matrix variable in the semidefinite program. Constraints $\langle X, A_i X B_i\rangle + \langle C_i, X\rangle = q_i$ would be transformed this way into $\langle \tilde{D}, \tilde{Z}\rangle = q_i$, where*

$$
\tilde{D} = \begin{bmatrix} 0 & \frac{1}{2}\mathrm{vec}(C)^T \\ \frac{1}{2}\mathrm{vec}(C) & B_i^T \otimes A_i \end{bmatrix} \quad \textit{and} \quad \tilde{Z} = \begin{bmatrix} 1 & z^T \\ z & Z \end{bmatrix}.
$$

3 New semidefinite lower bounds for the Quadratic assignment problem and the Graph partitioning problem

In this section we demonstrate how to use the semidefinite representation results from the previous section to obtain better lower bounds for the Quadratic assignment and the Graph partitioning problem. These problems can be naturally expressed as QP hence we can apply the bounding technique from the Subsection 2.2.

3.1 Quadratic assignment problem

The Quadratic Assignment Problem (QAP) can be stated in the following way. Let Π be the set of $n \times n$ permutation matrices (a matrix X is a permutation matrix, if it corresponds to some permutation ϕ, i.e. $x_{ij} \in \{0, 1\}$ and $x_{ij} = 1 \iff \phi(i) = j$). For given real symmetric $n \times n$ matrices A and B we want to find a permutation matrix $X \in \Pi$ which gives

$$\text{(QAP)} \qquad OPT_{QAP} = \min\{\langle X, AXB\rangle : X \in \Pi\}.$$

The QAP is nowadays widely considered as a classical combinatorial optimization problem, but it is also known as a generic model for various real-life problems, see the QAP library [7] for more references on QAP. The QAP is well known to be NP-hard, and even approximating the OPT_{QAP} within a constant factor is an NP-hard problem. The computational effort to solve the QAP is very likely to grow exponentially with the problem size, and problems of size $n \geq 25$ are currently considered as large instances.

The most recent and promising trends of research to find good lower bounds for OPT_{QAP} are based on semidefinite programming. Zhao et al. [20], Sotirov and Rendl [18] and Povh and Rendl [16] lifted the problem from the vector space $\mathbb{R}^{n\times n}$ to $\mathcal{S}^+_{n^2+1}$ or $\mathcal{S}^+_{n^2}$ and formulated several semidefinite programs which give increasingly tight lower bounds for the QAP. They used several methods to solve these semidefinite programs. The computational results show that these lower bounds are among the strongest but also the most expensive to compute (in practice they could solve these programs for $n \leq 35$).

In this subsection we present a new lower bound for the QAP, based on semidefinite programming which is obtained by strengthening the Hoffman-Wielandt eigenvalue lower bound. Indeed, we may express the set of permutation matrices as $\Pi = \{X \in \mathbb{R}^{n\times n}_+ : X^TX = I\}$, yielding the QP form for the QAP:

$$(QAP) \qquad OPT_{QAP} \; = \; \min\{\text{trace}(X^TAXB) : \; X \in \mathbb{R}^{n\times n}_+, \; X^TX = I, \; Q(X) = q\},$$

Note that we do not need any quadratic constraint in $Q(X) = q$ in the last formulation for QAP. Nevertheless, it becomes important when we start relaxing the QAP, hence we add initially quadratic constraint which are redundant for the set of permutation matrices. An example of such constraint is

$$\langle X, JXJ\rangle = n^2 \tag{6}$$

which is equivalent to $u^TXu = n$ and is automatically satisfied for permutation matrices, since they have in each row and each column exactly one non-zero element equal to 1.

From Subsection 2.2 it follows that

$$
(QAP_{SDP}) \qquad \begin{array}{rcl} OPT_{QAP} & \geq & \min \ \langle B \otimes A, Z \rangle \\ & & Z \in \mathcal{S}^+_{n^2}, \ W \ \in \ \mathcal{S}^+_n \\ & & \sum_i Z^{ii} + W \ = \ I, \ \ \langle I, Z^{ij} \rangle \ = \ \delta_{ij}, \\ & & \langle B_i^T \otimes A_i, \ Z \rangle = q_i, \forall i \end{array}
$$

Remark 3 *If (Z, W) are feasible for QAP_{SDP}, then it follows that*

$$
\mathrm{trace}(W) = \mathrm{trace}(I) - \sum_i \mathrm{trace}(Z^{ii}) = n - n = 0.
$$

Matrix W is positive semidefinite with zero trace, hence $W = 0$ and we can eliminate it from QAP_{SDP}.

Semidefinite program QAP_{SDP} is therefore a model which can give rise to several lower bounds for OPT_{QAP}. The tightness of this bound is tuned by the quadratic equations included in $Q(X) = q$. If this constraint contains no equation, then the resulting lower bound is exactly the Hoffman-Wielandt eigenvalue lower bound for OPT_{QAP} denoted by OPT_{HW} (this follows from the fact that QP_{SDP} is in this case exactly the conic dual of (4) with zero duality gap).

If $Q(X) = q$ contains only (6) which becomes on the dual side

$$
\langle J_{n^2}, Z \rangle = n^2, \tag{7}
$$

this gives new lower bound denoted by OPT_{new1} which improves the Hoffman-Wielandt lower bound significantly.

We may add beside the "total sum" constraint (6) the so-called "Gangster" constraint [20]:

$$
x_{ij} x_{ik} = 0, \quad x_{ji} x_{ki} = 0 \ \ \forall i, j, k, \ j \neq k,
$$

which captures the property that each permutation matrix has in each row and in each column exactly one non-zero element. It yields in QAP_{SDP} the following equations:

$$
\langle E_{jk} \otimes E_{ii}, Z \rangle = 0, \quad \langle E_{ii} \otimes E_{jk}, Z \rangle = 0 \ \ \forall i, j, k, \ j \neq k. \tag{8}
$$

We denote this lower bound by OPT_{new2}.

The tightness of several lower bounds is demonstrated in Table 1. The first column contains the name of the problem instance which also tells us the size of the instance. The second column contains the Hoffman-Wielandt eigenvalue lower bound OPT_{HW}, the third column contains the new lower bound OPT_{new1} obtained by adding the "total sum" constraint (7) and the fourth column contains the second lower bound OPT_{new2} obtained by further inclusion of the "Gangster" constraint (8).

The fifth column contains the strongest known semidefinite lower bound OPT_{best} (this is the lower bound, based on the QAP_{R_3} model from [18]) and in the last column we have the optimal value of the QAP instance. Data for the last two columns are taken from [6].

We can see that the single constraint (6) improves the eigenvalue lower bound significantly. We also point out that the resulting semidefinite program is still quite simple (it has $\mathcal{O}(n^2)$ linear constraints) comparing to the program underlaying the best lower bound which contains $\mathcal{O}(n^4)$ linear constraints.

The second lower bound OPT_{new2} is also very tight, but we have to pay a big price for it: it contains $\mathcal{O}(n^3)$ linear constraints. These constraints are mostly orthogonal, therefore we can compute OPT_{new2} by the boundary point method from [17] which performs well on such problems. Indeed, for $n \geq 25$ we computed OPT_{new2} by using this method.

Remark 4 *By inspection we can see that the bounds OPT_{new1} and OPT_{new2} are equivalent to the bounds QAP_{AW+} and QAP_{R_2} from [16] and [18] which were obtained as semidefinite relaxations of the copositive formulation of the Quadratic assignment problem.*

name	OPT_{HW}	OPT_{new1}	OPT_{new2}	OPT_{best}	OPT_{QAP}
tai15a	-414351	325410	349528	377111	388214
tai20a	-714902	576806	619033	671685	703482,00
tai25a	-1050896	959295	1009453	1112862	1167256,00
tai30a	-1505554	1501252	1576943	1706875	1818146,00
tai35a	-2015234	1941527	2029726	*	*
tai40a	-2559063	2481593	2549838	*	*
tai40b	-1659647368	398654801	552755351	*	*

Table 1: The new lower bounds OPT_{new1} and OPT_{new2} improve the eigenvalue lower bound OPT_{HW} significantly and are not very far from OPT_{best}, while the underlaying semidefinite program has much smaller complexity. With '*' we denote the values which are currently unavailable in the literature and we were also incapable to compute them due to the complexity reasons.

3.2 The Graph partitioning problem

The Graph partitioning problem (GPP) is a classical problem from combinatorial optimization. Given a simple undirected graph $G = (V, E)$ with $|V| = n$, a number of partitions $k > 1$ and a vector $m = (m_1, m_2, \ldots, m_k) \in \mathbb{N}^k$ with $1 \leq m_1 \leq m_2 \leq \ldots \leq m_k$, $\sum_i m_i = n$, we are interested in a partition $(S_1, S_2, \ldots, S_k)$ of the vertex set V such that $|S_i| = m_i$ and the total number of cut edges (i.e. edges between different sets) is minimal.

We may represent any partition into k blocks with prescribed sizes by a (partition) matrix $X \in \{0, 1\}^{n\times k}$, where $x_{ij} = 1$ if and only if the ith vertex belongs to the jth set. With this notation the total number of cut edges is exactly $0.5\langle X, AXB\rangle$, where A is the adjacency matrix of the graph (i.e. $a_{ij} = 1$ if (ij) is an edge and $a_{ij} = 0$ otherwise) and $B = J_k - I_k$. If L is Laplacian matrix of a graph, then it holds $0.5\langle X, AXB\rangle = 0.5\langle X, LX\rangle$.

The set of all partition matrices may be described as

$$\{X \in \mathbb{R}_+^{n\times k} \colon X^T X = M,\ \mathrm{Diag}(XX^T) = u_n\}, \tag{9}$$

where $M = \mathrm{Diag}(m)$. We may describe the partition matrices also by other equations, but the equations from (9) are the most convenient for our bounding procedure.

Graph partitioning problem may be therefore formulated as

$$\text{(GPP)} \qquad OPT_{GPP} = \min\{\frac{1}{2}\langle X, LX\rangle :\ X \in \mathbb{R}_+^{n\times k},\ X^T X = M,\ \mathrm{Diag}(XX^T) = u_n\}.$$

We can write constraint $\mathrm{Diag}(XX^T) = u_n$ as $\langle X, E_{ii}X\rangle = 1,\ 1 \leq i \leq n$, hence GPP is a special instance for QP. Procedure from Subsection 2.2 yields the following semidefinite lower bound for OPT_{GPP}:

$$\begin{array}{rcl} OPT_{GPP} & \geq & \min\ \frac{1}{2}\langle I\otimes L, V\rangle \\ & & V \in \mathcal{S}_{kn}^+,\ W \in \mathcal{S}_n^+ \\ (GPP_{SDP}) & & \sum_i \frac{1}{m_i} V^{ii} + W = I,\ \ \langle I, V^{ij}\rangle = m_i\delta_{ij}, \\ & & \langle I\otimes E_{ii},\ V\rangle = 1,\ 1 \leq i \leq n \end{array}$$

We denote the optimal value of the semidefinite program from above by OPT_{DH}, since it is exactly the Donath-Hoffman eigenvalue lower bound [8] for OPT_{GPP}, as follows from the following theorem.

Theorem 3 *Optimal value of GPP_{SDP} is exactly the Donath-Hoffman eigenvalue lower bound for OPT_{GPP}.*

Proof:
Anstreicher and Wolkowicz [1] showed that the OPT_{DH}, defined as

$$OPT_{DH} = \max\left\{\frac{1}{2}\sum_{i=1}^{k} m_{k-i+1}\lambda_i(L+D) \colon D = \mathrm{Diag}(d),\ u^T d = 0\right\} \tag{10}$$

where $\lambda_1(L+D) \le \lambda_2(L+D) \le \cdots \lambda_n(L+D)$ are the eigenvalues of $L+D$, can be represented as the optimal solution of the following semidefinite program

$$\begin{aligned} OPT_{DH} \quad = \quad & \max\ \mathrm{trace}(S) + \mathrm{trace}(T) \\ & \text{s. t.}\ \ \bar{M} \otimes (L + \mathrm{Diag}(v)) - I \otimes S - T \otimes I \succeq 0 \\ & \qquad\ \ u_n^T v = 0,\ v \in \mathbb{R}^n,\ S, T \in \mathcal{S}_n, \end{aligned}$$

where

$$\bar{M} = \frac{1}{2}\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}.$$

This semidefinite program has matrix variable of order $n^2 \times n^2$ and is therefore much larger than GPP_{SDP}. It is obviously strictly feasible, hence its dual semidefinite program has the same optimal solution. Therefore we have

$$\begin{aligned} OPT_{DH} \quad = \quad & \min\ \langle \bar{M} \otimes L,\, Y\rangle \\ & \text{s. t.}\ \ Y \in \mathcal{S}^+_{n^2},\ \ \textstyle\sum_{i=1}^n Y^{ii} = I,\ \ \sum_{i=1}^k m_i \,\mathrm{diag}(Y^{ii}) = u, \\ & \qquad \mathrm{trace}(Y^{ij}) = \delta_{ij},\ 1 \le i \le j \le n. \end{aligned}$$

One can see that OPT_{DH} is determined only by blocks Y^{ij} for $1 \le i, j \le k$, therefore we can write

$$\begin{aligned} OPT_{DH} \quad = \quad & \min\ \tfrac{1}{2}\langle M \otimes L,\, Y\rangle \\ & \text{s. t.}\ \ Y \in \mathcal{S}^+_{kn},\ \ \textstyle\sum_{i=1}^k Y^{ii} \preceq I,\ \ \sum_{i=1}^k m_i \,\mathrm{diag}(Y^{ii}) = u, \\ & \qquad \mathrm{trace}(Y^{ij}) = \delta_{ij},\ 1 \le i \le j \le k, \end{aligned}$$

After introducing $V = (M^{1/2} \otimes I)Y(M^{1/2} \otimes I)$ we obtain exactly the problem GPP_{SDP}. □

We can strengthen the lower bound OPT_{DH} by adding further constraints to GPP which are redundant for the partition matrices, but become important on the dual side. The "total sum" constraint

$$\langle X,\, J_n X J_k\rangle = n^2 \tag{11}$$

is a good candidate. It implies in GPP_{SDP} the constraint $\langle J_{kn},\, V\rangle = n^2$ which is no more redundant, hence we obtain a new lower bound for OPT_{GPP} denoted by OPT_{new1} which is strictly better than OPT_{DH}.

We can improve OPT_{new1} further by exploring the orthogonality of the columns of partition matrices. If X is a partition matrix, it holds

$$x_{ij}x_{ik} = 0 \quad \forall i, j, k,\ j \ne k,$$

and we obtain in GPP_{SDP} the following new equations:

$$\langle E_{jk} \otimes E_{ii},\, Z \rangle = 0 \;\; \forall i, j, k, \;\; j \neq k, \tag{12}$$

which imply new lower bound OPT_{new2} strictly better than OPT_{new1}.

Table 2 demonstrates the quality of these lower bounds on 9 random graphs with 50 nodes, where the probability that there exists an edge between two nodes varies from 0.1 to 0.9 (the probability is included in the name of the instance in the first column). For each instance we took $m = (5, 10, 15, 20)$. The second column contains the number of graph nodes, the third column contains the number of graph edges and the last three columns contain the lower bounds OPT_{DH}, OPT_{new1} and OPT_{new2}.

name	n	$\lvert E\rvert$	OPT_{DH}	OPT_{new1}	OPT_{new2}
g50.01	50	111	17.92236	22.76201	23.55990
g50.02	50	256	81.95602	95.91899	99.93125
g50.03	50	342	124.71776	148.70114	152.18022
g50.04	50	478	204.30261	236.69719	242.42469
g50.05	50	611	287.20402	332.79142	338.11772
g50.06	50	759	378.24995	440.78017	442.77462
g50.07	50	897	470.15719	544.23761	549.70123
g50.08	50	984	530.48562	615.03507	619.51603
g50.09	50	1098	618.86660	719.45628	722.23682

Table 2: Lower bounds for Graph partitioning problem, where $m = (5,\ 10,\ 15,\ 20)$

We can see that these lower bounds are closer to each other comparing to lower bounds for QAP. Table 2 also demonstrates that adding few constraints to a semidefinite formulation of an eigenvalue lower bound does not make the semidefinite problem much harder, but the optimal value is improved significantly. Lower bound OPT_{new1} is obtained by improving the eigenvalue bound OPT_{DH} by only one constraint (11). On the other hand further tightening by (12) which contains $nk(k-1)/2$ equations yields much smaller improvement comparing to the additional effort needed to compute OPT_{new2}.

4 Tightness of the proposed relaxations

In the previous sections we show how to obtain semidefinite lower bounds for OPT_{QP} and how to improve them by adding new constraints. In all cases we are interested in accurate and computationally cheap semidefinite relaxations, but this is not always possible. When computing ε-optimal solution for QP is an NP-hard problem (this is true e.g. for QAP), then there might always happen a non-zero gap between the optimal values of QP and QP_{SDP} (unless P=NP), since finding an ε-optimal solution of semidefinite programs has polynomial time complexity [4].

There are two sources for the gap between the optimal values of QP and QP_{SDP}, as there are two inequalities in the term on page 6. If the sign constraint is redundant, then the first inequality is equality, but this happens very rarely (actually we could not provide an example).

The second reason for the gap is the duality gap in the Lagrangian relaxation of the non-convex quadratic problem. In Theorem 2 we only proved that there is no duality gap, if there is no quadratic constraint in QP beside the orthogonality constraint $X^T X = M$.

As we could see in Section 3, additional (redundant) quadratic constraints become necessary in QP after dropping out the sign constraint, since they decrease both sources of gap.

The following example demonstrates this situation.

Example 1 *Let $G = K_3$ be the complete graph on 3 vertices and $m = (1, 2)$ be the partitioning vectors for the Graph partitioning problem. Obviously we have $OPT_{GPP} = 2$ and any partitioning matrix is optimal. As we proved in Subsection 3.2, the Donath-Hoffman lower bound (10) is obtained as Lagrangian relaxation of the following quadratic problem*

$$\min\{\frac{1}{2}\langle X, LX\rangle : X \in \mathbb{R}^{n\times k},\ X^TX = M,\ \mathrm{Diag}(XX^T) = u_n\}$$

By a short exercise we can see that this quadratic problem has optimal value $3 - \sqrt{2} \approx 1.586$, while $OPT_{DH} = 1.500$. Here we have both gaps non-zero. Further strengthenings of OPT_{DH} by adding (11) and (12) yield $OPT_{\mathrm{new1}} = OPT_{\mathrm{new2}} = 2$.

5 Approximating OPT_{QP} by copositive programming

Several authors have proved recently that some quadratic programs can be restated as linear programs over the cone of copositive or completely positive matrices (in the sequel we call such problems copositive programs). Bomze et al. [3] proved that the standard quadratic programming problem can be rewritten as linear program over the cone of completely positive matrices. De Klerk and Pasechnik [11] reformulated the stability number problem as copositive program. Povh and Rendl [15, 16] proved that the three-partitioning problem and the quadratic assignment problem have a copositive representation. The strongest representation result by the time being belongs to Burer [5] who showed that any quadratic problem in binary and continuous variables can be rewritten as copositive program.

All problems mentioned above are NP-hard problems and rewriting them as copositive programs does not make them tractable, but only opens a new line of possible relaxations based on approximations of the copositive or completely positive cone.

In this section we show that the lower bounds for the quadratic program QP can also be improved by copositive programming.

As we pointed out in Section 4, there are two possible sources for the gap between the optimal values of QP and QP_{SDP}. The first is due to the fact that we eliminated the sign constraint $X \geq 0$ in QP before computing the Lagrangian relaxation of QP. If we keep the sign constraint, then we get in the Lagrangian relaxation the copositive constraint

$$(M^{1/2}BM^{1/2}) \otimes A - S \otimes I_n + I_k \otimes T - \sum_i y_i\, (M^{1/2}B_i^TM^{1/2}) \otimes A_i \in \mathcal{C}_{kn},$$

and in the last semidefinite program QP_{SDP} the constraint $V \in \mathcal{S}_{kn}^+$ rewrites into $V \in \mathcal{C}_{kn}^*$. The resulting copositive program is therefore

$$(QP_{CP}) \qquad \begin{array}{rcl} OPT_{CP} & = & \min\ \langle B\otimes A, V\rangle \\ & & V \in \mathcal{C}_{kn}^*,\ W \in \mathcal{S}_n^+ \\ & & \sum_i \frac{1}{m_i}V^{ii} + W = I,\ \ \langle I, V^{ij}\rangle = m_i\delta_{ij}, \\ & & \langle B_i^T \otimes A_i,\ V\rangle = q_i\ \forall i \end{array}$$

Obviously we have $OPT_{QP} \geq OPT_{CP} \geq OPT_{SDP}$. We wonder when we get the equality $OPT_{QP} = OPT_{CP}$. In the following example we present the case when there is strict inequality.

Example 2 *Suppose $A = J_n, B = J_n - I_n$, $m = u_n$ and we have no constraint of the type $\langle X,\, A_i X B_i\rangle = q_i$. Therefore QP is a trivial Quadratic assignment problem, and for any feasible matrix X (which is a permutation matrix) we have $\langle X, AXB\rangle = n^2 - n$, hence $OPT_{QP} = n^2 - n$. On the other hand the matrices $V = \frac{1}{n} I_{n^2}$ and $W = O_n$ are feasible for the copositive relaxation QP_{CP} with $\langle B \otimes A,\, V\rangle = 0$, hence we have gap $OPT_{QP} - OPT_{CP} = n^2 - n$.*

5.1 Copositive relaxation for Graph partitioning problem is tight

When we consider the Graph partitioning problem (see Subsection 3.2 for the definition), then we can describe the feasible set of GPP by

$$\begin{aligned} \mathrm{FEAS}_{GPP} &= \{X \in \{0,1\}^{n\times k} \colon X^T X = M\} \\ &= \{X \in \mathbb{R}_+^{n\times k} \colon X^T X = M,\ \mathrm{Diag}(XX^T) = u_n, \langle X,\, J_n X J_k\rangle = n^2\}. \end{aligned} \tag{13}$$

Recall that in the second formulation we do not need the constraint $\langle X,\, J_n X J_k\rangle = n^2$, but it becomes important in the copositive relaxation of the problem for the same reason as in the previous sections.

By repeating the procedure from the beginning of the section we obtain the following copositive lower bound for OPT_{GPP}

$$(GPP_{CP}) \qquad \begin{aligned} OPT_{GPP} \ \geq\ & \min\ \tfrac{1}{2}\langle I \otimes L,\, V\rangle \\ & V \in \mathcal{C}^*_{kn},\ W \in \mathcal{S}^+_n \\ & \textstyle\sum_i \frac{1}{m_i} V^{ii} + W = I,\quad \langle I,\, V^{ij}\rangle = m_i \delta_{ij}\ \forall i,j \\ & \langle I \otimes E_{ii},\, V\rangle = 1\ \forall i,\ \langle J_{kn},\, V\rangle = n^2. \end{aligned}$$

Note that the bound OPT_{CP} is actually a strengthening of the OPT_{new1} lower bound from Subsection 3.2, since we replace $V \in \mathcal{S}^+_{kn}$ by $V \in \mathcal{C}^*_{kn}$. A closer look reveals that this lower bound is tight, i.e. $OPT_{GPP} = OPT_{CP}$. We can say more: there is a strong relation between the set of all partition matrices and the feasible set for GPP_{CP}, as follows from the following lemma.

Lemma 4 *The following is equivalent:*

(a) $V \in \mathcal{C}^*_{kn}$ is feasible for GPP_{CP};

(b) $V = \sum_s \lambda_s p_s p_s^T$, where $\lambda_s \geq 0$, $\sum_s \lambda_s = 1$, $p_s = \mathrm{vec}(P_s)$ and P_s is a partition matrix for all s.

Proof: The implication (b)⇒(a) is easy: if P is a partition matrix, then pp^T is completely positive and is feasible for GPP_{CP}. The same is true for any convex combination of such matrices.

The direction (a)⇒(b) is more involved. Let $V \in \mathcal{C}^*_{kn}$ be feasible for GPP_{CP}. By definition we have $V = \sum_s q_s q_s^T$, where $q_s \in \mathbb{R}^{kn}_+$ and $q_s \neq 0\ \forall s$. We can obtain from each vector q_s a matrix Q_s such that $q_s = \mathrm{vec}(Q_s)$. The constraint $\langle I,\, V^{ij}\rangle = m_i\delta_{ij}$ implies that $\sum_s \langle I,\, Q_s(:,i) Q_s(:,j)^T\rangle = m_i\delta_{ij}$ or equivalently $\sum_s Q_s^T Q_s = M$. In particular this means that each Q_s has orthogonal columns.

The matrix

$$\hat{V} = \sum_{i,j} V^{ij} = (u_k \otimes I_n)^T V (u_k \otimes I_n)$$

is positive semidefinite and satisfies $\mathrm{diag}(\hat{V}) = u_n$, $\langle J_n,\, \hat{V}\rangle = n^2$. This implies that $\hat{V} = J_n$ or equivalently $\langle J_k \otimes E_{ij}, V\rangle = 1$ for all i, j. Let us denote by $r_i(Q)$ the sum of i-th row of Q. Therefore we have for each pair $1 \le i < j \le n$:

$$\begin{aligned}
\langle J_k \otimes E_{ii}, V\rangle &= \sum_s r_i(Q_s)^2 = 1,\\
\langle J_k \otimes E_{jj}, V\rangle &= \sum_s r_j(Q_s)^2 = 1,\\
\langle J_k \otimes E_{ij}, V\rangle &= \sum_s r_i(Q_s) r_j(Q_s) = 1.
\end{aligned}$$

The Cauchy-Schwarz inequality for the equality case implies $r_i(Q_s) = \alpha r_j(Q_s)$ and $\alpha = 1$. Since we have $r_i(Q_s) = r_j(Q_s)$ for all $1 \le i \le j \le n$, we can define $P_s = \frac{1}{r_1(Q_s)} Q_s$ and $\lambda_s = r_1^2(Q_s)$ (note that $r_i(Q_s) \ne 0\ \forall i, s$, since $q_s \ne 0\ \forall s$). It follows $V = \sum_s \lambda_s p_s p_s^T$ and $\sum_s \lambda_s = 1$. We already have the factorization of V, stated by the lemma. To finish the proof, we need to show that P_s are partition matrices.

We know by definition that each P_s has non-negative entries, orthogonal columns and $r_i(P_s) = 1\ \forall i$. This implies $P_s \in \{0,1\}^{n\times k}$ and $\sum_{i,j} P_s(i,j) = n$, hence $\sum_i P_s(i,j) = \sum_i P_s(i,j)^2\ \forall j$. It remains to show that $\sum_i P_s(i,j) = m_j\ \forall j$. This will be done in the last part of the proof.

The constraint $\langle I, V^{jj}\rangle = \sum_s \lambda_s \sum_i P_s(i,j)^2 = m_j$ implies:

$$\begin{aligned}
\langle J, V^{jj}\rangle &= \sum_s \lambda_s (\sum_i P_s(i,j))^2 \ge (\sum_s \lambda_s \sum_i P_s(i,j))^2\\
&= (\sum_s \lambda_s \sum_i P_s(i,j)^2)^2 = m_j^2.
\end{aligned}$$

On the other hand, from $\sum_i \frac{1}{m_i} V^{ii} \preceq I$ it follows

$$n \ge \sum_i \frac{1}{m_i} \langle J, V^{ii}\rangle \ge \sum_i \frac{1}{m_i} m_i^2 = n,$$

hence $\langle J, V^{jj}\rangle = m_j^2\ \forall j$.

The matrix $\tilde V = \sum_{i,j} \langle J, V^{ij}\rangle E_{ij} = (I_k \otimes u_n)^T V (I_k \otimes u_n)$ is positive semidefinite with $\tilde V_{ii} = m_i^2$ and $\langle J, \tilde V\rangle = n^2$, hence it must hold $\tilde V_{i,j} = m_i m_j\ \forall i, j$, or equivalently $\langle J, V^{ij}\rangle = m_i m_j$. Using this property we obtain for each pair $1 \le i < j \le k$:

$$\begin{aligned}
\langle J, V^{ii}\rangle &= \sum_s \lambda_s (\sum_t P_s(t,i))^2 = m_i^2,\\
\langle J, V^{jj}\rangle &= \sum_s \lambda_s (\sum_t P_s(t,j))^2 = m_j^2,\\
\langle J, V^{ij}\rangle &= \sum_s \lambda_s (\sum_t P_s(t,i))(\sum_t P_s(t,j)) = m_i m_j.
\end{aligned}$$

The Cauchy-Schwarz inequality again implies $\sum_t P_s(t,i) = \frac{m_i}{m_j} \sum_t P_s(t,j)\ \forall s$, hence, since the sum of all entries in each P_s is n, we obtain $\sum_t P_s(t,i) = m_i,\ 1 \le i \le k$. $\square$

Note that we can write GPP also in the form

$$\begin{aligned}
OPT_{GPP} &= \Big\{ \min\ \frac{1}{2} \langle I \otimes L, V\rangle \colon V = pp^T,\ P \ldots \text{partition matrix} \Big\}\\
&= \Big\{ \min\ \frac{1}{2} \langle I \otimes L, V\rangle \colon V = \sum_s \lambda_s p_s p_s^T,\ \lambda_s \ge 0,\ \sum_s \lambda_s = 1,\ P_s \ldots \text{partition matrices} \Big\}.
\end{aligned}$$

Lemma 4 implies that any feasible solution for GP_{CP} is feasible for the later formulation of GPP and vice versa, hence the following theorem follows immediately.

Theorem 5 *For the Graph partitioning problem we have* $OPT_{GPP} = OPT_{CP}$.

We also have the following corollary.

Corollary 6 *If we replace constraint* $V \in \mathcal{S}^+_{n^2}$ *by the completely positive constraint* $V \in \mathcal{C}^*_{n^2}$ *in the semidefinite program underlaying the* QAP_{new1} *lower bound, we obtain the exact value* OPT_{QAP}.

Proof: Note that QAP is a special instance of GPP obtained by taking $m = u_n$. Let us denote the copositive program obtained by the copositive strengthening of the semidefinite program underlaying the QAP_{new1} lower bound by QAP_{CP}. The only difference between QAP_{CP} and GPP_{CP} is that in QAP_{CP} is missing the constraint $\langle I \otimes E_{ii}, V\rangle = 1$. But this constraint is redundant here, since we know that $\sum_i V^{ii} = I$ (see Remark 3) and that all off-diagonal blocks V^{ij} $\forall\, i \neq j$, have zeros on the main diagonal. $\square$

Results from Theorem 5.1 and Corollary 6 are not surprising, since similar results were obtained by Povh and Rendl [16, 15] also for the 3-partitioning problem and for the Quadratic assignment problem.

6 Conclusions

Computing good lower bounds for hard problems from combinatorial optimization is very important, especially if we plan to solve the problem by Branch and Bound method. In the paper we present how to improve by semidefinite programming the eigenvalue lower bounds for some problems, where the feasible set consists of orthogonal matrices.

We rewrite the quadratic problem over the set of (non-quadratic) orthogonal matrices as a semidefinite program. This result is a generalization of the result from Anstreicher and Wolkowicz [1], and opens new possibilities for approximating some hard quadratic problems, where the feasible set consists of orthogonal matrices subject to some additional constraints (like the Quadratic assignment problem (QAP), the Graph partitioning problem (GPP), the Weighted sums of eigenvalues problem etc.). We offer a generic semidefinite program which gives tighter lower bounds for these problems, comparing to the eigenvalue lower bounds. The semidefinite bound can be further improved towards the optimum of the original problem by adding linear constraints which correspond to some valid constraint in the original problem. We also suggested few such constraints for QAP and GPP and they indeed improved the bounds significantly. We give some preliminary computational results which show the potential of this approach.

In the last section we demonstrate the power of copositive programming. If we replace the semidefinite constraint in the generic semidefinite program by completely positive constraint, we obtain better lower bounds. In the case of Graph partitioning problem the resulting copositive program even delivers the exact value.

We also try to address the question whether we can extend Theorem 2 to a larger class of quadratic problems at least to quadratic programs over the orthogonal matrices which satisfy some additional quadratic or linear constraints? While Beck [2] provided a weak but positive answer to the first question we show that the Graph partitioning problem certainly does not belong to any of these classes (see Example 1).

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