B-469 Simplified Copositive and Lagrangian Relaxations for Linearly Constrained Quadratic Optimization Problems in Continuous and Binary Variables

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Abstract. For a quadratic optimization problem (QOP) with linear equality constraints in continuous nonnegative variables and binary variables, we propose three relaxations in simplified forms with a parameter λ: Lagrangian, completely positive, and copositive relaxations. These relaxations are obtained by reducing the QOP to an equivalent QOP with a single quadratic equality constraint in nonnegative variables, and applying the Lagrangian relaxation to the resulting QOP. As a result, an unconstrained QOP with a Lagrangian multiplier λ in nonnegative variables is obtained. The other two relaxations are a primal-dual pair of a completely positive programming (CPP) relaxation in a variable matrix with the upper-left element set to 1 and a copositive programming (CP) relaxation in a single variable. The CPP relaxation is derived from the unconstrained QOP with the parameter λ, based on the recent result by Arima, Kim and Kojima. The three relaxations with a same parameter value $\lambda > 0$ work as relaxations of the original QOP. The optimal values $\zeta(\lambda)$ of the three relaxations coincide, and monotonically converge to the optimal value of the original QOP as λ tends to infinity under a moderate assumption. The parameter λ serves as a penalty parameter when it is chosen to be positive. Thus, the standard theory on the penalty function method can be applied to establish the convergence.

Key words. Nonconvex quadratic optimization, 0-1 mixed integer program, Lagrangian relaxation, copositve programming relaxation, completely positive programming relaxation.

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1 Introduction

We consider a class of linearly constrained quadratic optimization problems (QOPs) in continuous nonnegative and binary variables. The standard 0-1 mixed integer linear optimization problem is included in this class as a special case. This class of QOPs has long been studied for various solution methods, including semidefinite programming (SDP) relaxation.

Recently, completely positive programming (CPP) relaxation for this class of QOPs was proposed by Burer [3]. The class was extended to a more general class of QOPs by Eichfelder and Povh [6, 7] and by Arima, Kim and Kojima [1]. Theoretically strong results were presented in their papers [3, 6, 7, 1] showing that the exact optimal values of QOPs in their classes coincide with the optimal values of their CPP relaxation problems.

A general CPP problem is characterized as linear optimization problems over closed convex cones as a general SDP problem. It is well-known, however, that solving a general CPP problem, or even a simple CPP problem derived as the CPP relaxation problem of the QOP over the simplex [2] is much more difficult than solving a general SDP problem. Efficient numerical methods for solving CPPs have not been developed whereas the primal-dual interior-point methods have been effective for solving SDPs. In fact, the fundamental problem of determining whether a given variable matrix is completely positive (or copositive) still remains a very challenging problem.

If developing efficient numerical methods for CPP relaxations from QOPs in the classes is an important goal to achieve in the future, a first step toward that goal may be representing the QOPs in a simplified form. We say that the QOPs are in a simplified form if the numbers of constrains and variables are reduced. Then, CPP relaxations derived from the simplified QOPs have a reduced number of constraints and variables, alleviating some of difficulties of handling a large number of constrains and variables. This will decrease the difficulty of solving CPP relaxations.

For this purpose, three types of "extremely simple" relaxations are proposed for a class of linearly constrained QOPs in continuous and nonnegative variables and binary variables, the class studied in Burer [3]. The first relaxation is an unconstrained QOP in nonnegative variables. The other two relaxations are a primal-dual pair of an unconstrained CPP problem in a variable matrix whose upper-left element is fixed to 1 and a copositive programming (CP) problem in a single variable. We may regard that such a CPP is one of the simplest CPPs, except trivial ones over the completely positive cone with no constraint, and that such a CP problem is one of the simplest CPs, except trivial ones with no variable. If the problem of determining whether a given variable matrix is completely positive is resolved in the future [15], the proposed relaxations can be used for designing efficient numerical methods for solving the class of QOPs.

A technique to reduce a linearly constrained QOP in continuous nonnegative variables and binary variables to a QOP with a single quadratic equality constraint in nonnegative variables was introduced by Arima, Kim and Kojima in [1]. The resulting QOP was relaxed to a CPP problem with a single linear equality constraint in a variable matrix with upper-left element fixed to 1. They showed that the optimal value of the CPP relaxation problem coincides with the optimal value of the original QOP. Taking the dual of the CPP problem leads to a CP problem in two variables. As will be shown in the subsequent section, the dual CP has no optimal solution in general. This is the second motivation of this paper.

The first proposed relaxation is obtained by applying the Lagrangian relaxation to the QOP with a single quadratic equality constraint in nonnegative variables, which has been reduced from the given QOPs using the technique in [1]. The application of the Lagrangian relaxation results in an unconstrained QOP with the Lagrangian multiplier parameter λ in nonnegative variables. For any fixed λ, the optimal value of this unconstrained QOP in nonnegative variables, denoted by $\zeta(\lambda)$, bounds the optimal value of the original linearly constrained QOP in continuous nonnegative variables and binary variables, denoted by ζ^*, from below. If the Lagrangian multiplier parameter λ is chosen to be positive, λ works as a penalty parameter. Thus, the standard theory on the penalty function method [8] can be utilized to prove that the optimal value $\zeta(\lambda)$ of the unconstrained QOP with the parameter value $\lambda > 0$ monotonically converges to ζ^* as λ tends to ∞ under a moderate assumption. In addition, the unconstrained QOP may play an important role for developing numerical methods. More precisely, if the feasible region of the original QOP can be scaled into the unit box $[0,1]^n$, then the box constraints can be added to the unconstrained QOP. Many global optimization technique developed for this type of QOPs can be used. See, for example, [4, 5].

The application of CPP relaxation in [1] to the QOP with the parameter $\lambda > 0$ provides a primal-dual pair of an unconstrained CPP problem with the parameter $\lambda > 0$ in a variable matrix with the upper-left element fixed to 1 and a CP problem with the parameter λ in a single variable. We show under the same moderate assumption that the primal-dual pair of problems with the parameter value $\lambda > 0$ both have optimal solutions with no duality gap, and share the optimal value $\zeta(\lambda)$ with the QOP for the parameter value $\lambda > 0$.

After introducing notation and symbols in Section 2, we state our main results, Theorems 3.1 and 3.3 in Section 3. We give a proof of Theorem 3.1 in Section 4, and some remarks in Section 5.

2 Notation and symbols

We use the following notation and symbols throughout the paper.

$$
\begin{array}{rcl}
\mathbb{R}^n & = & \text{the space of } n\text{-dimensional column vectors}, \\
\mathbb{R}^n_+ & = & \text{the nonnegative orthant of } \mathbb{R}^n, \\
\mathbb{S}^n & = & \text{the space of } n \times n \text{ symmetric matrices}, \\
\mathbb{S}^n_+ & = & \text{the cone of } n \times n \text{ symmetric positive semidefinite matrices}, \\
\mathbb{C} & = & \left\{ \boldsymbol{A} \in \mathbb{S}^n : \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} \geq 0 \text{ for all } \boldsymbol{x} \in \mathbb{R}^n_+ \right\} \text{ (the copositive cone)}, \\
\mathbb{C}^* & = & \left\{ \sum_{i=1}^{r} \boldsymbol{x}_j \boldsymbol{x}_j^T : \boldsymbol{x}_j \in \mathbb{R}^n_+ \ (j = 1, 2, \ldots, r) \text{ for some } r \geq 1 \right\} \\
& & \text{(the completely positive cone)}, \\
\boldsymbol{Y} \bullet \boldsymbol{Z} & = & \text{trace of } \boldsymbol{Y}\boldsymbol{Z} \text{ for every } \boldsymbol{Y},\ \boldsymbol{Z} \in \mathbb{S}^n \text{ (the inner product)}, \\
\text{cl conv } G & = & \text{the closure of the convex hull of } G \subset \mathbb{S}^n.
\end{array}
$$

3 Main results

3.1 Linearly constrained QOPs in continuous and binary variables

Let $\boldsymbol{A}$ be a $q \times m$ matrix, $\boldsymbol{b} \in \mathbb{R}^q$, $\boldsymbol{c} \in \mathbb{R}^m$ and $r \leq m$ a positive integer. We consider a QOP of the form

$$
\begin{array}{ll}
\text{minimize} & \boldsymbol{u}^T \boldsymbol{Q}_0 \boldsymbol{u} + 2\boldsymbol{c}^T \boldsymbol{u} \\
\text{subject to} & \boldsymbol{u} \in \mathbb{R}^m_+,\ \boldsymbol{A}\boldsymbol{u} + \boldsymbol{b} = \boldsymbol{0},\ u_i(1 - u_i) = 0 \ (i = 1, 2, \ldots, r).
\end{array} \tag{1}
$$

Burer [3] studied this type of QOP, and proposed a completely positive cone programming (CPP) relaxation whose objective value is the same as the QOP (1). When $\boldsymbol{Q}_0 = \boldsymbol{O}$ is taken, the problem becomes a standard 0-1 mixed integer linear optimization problem. We assume throughout the paper that QOP (1) has an optimal solution $\boldsymbol{u}^*$ with the optimal value ζ^*.

We first convert the QOP (1) into a QOP with a single equality constraint according to the discussions in Section 5.1 and 5.2 of [1]. Note that the constraint $u_i(1-u_i) = 0$ implies $0 \leq u_i \leq 1$ $(i = 1, 2, \ldots, r)$, thus, we may assume without loss of generality that $q \geq r$, $m \geq 2r$, and that the equalities $u_i + u_{i+r} - 1 = 0$ $(i = 1, 2, \ldots, r)$ are included in the equality $\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b} = \boldsymbol{0}$. More precisely, we assume that $\boldsymbol{A}$ and $\boldsymbol{b}$ are of the forms

$$\boldsymbol{A} = \begin{pmatrix} \boldsymbol{A}_{11} & \boldsymbol{A}_{12} & \boldsymbol{A}_{13} \\ \boldsymbol{I} & \boldsymbol{I} & \boldsymbol{O} \end{pmatrix}, \ \boldsymbol{b} = \begin{pmatrix} \boldsymbol{b}_1 \\ -\boldsymbol{e} \end{pmatrix}, \tag{2}$$

where $\boldsymbol{I}$ denotes an $r \times r$ matrix and $\boldsymbol{e}$ the r-dimensional column vector of ones. If the 0-1 constraint $u_i(1-u_i) = 0$ is replaced by the complementarity constraint $u_i u_{i+r} = 0$ $(i = 1, 2, \ldots, r)$ and the linear equality constraint $\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b} = \boldsymbol{0}$ by a quadratic equality constraint $(\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b})^T(\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b}) = 0$, QOP (1) is rewritten by

$$\begin{array}{ll} \text{minimize} & \boldsymbol{u}^T \boldsymbol{Q}_0 \boldsymbol{u} + 2\boldsymbol{c}^T \boldsymbol{u} \\ \text{subject to} & \boldsymbol{u} \in \mathbb{R}^m_+, \ (\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b})^T(\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b}) = 0, \ u_i u_{i+r} = 0 \ (i = 1, 2, \ldots, r). \end{array} \tag{3}$$

Notice that the left hand sides of all quadratic equality constraints $(\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b})^T(\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b}) = 0$ and $u_i u_{i+r} = 0$ $(i = 1, 2, \ldots, r)$ are nonnegative for every $\boldsymbol{u} \in \mathbb{R}^m_+$. Thus, we can unify the constraints into a single equality constraint to reduce the QOP (3) to

$$\text{minimize} \quad \boldsymbol{u}^T \boldsymbol{Q}_0 \boldsymbol{u} + 2\boldsymbol{c}^T \boldsymbol{u} \quad \text{subject to} \quad \boldsymbol{u} \in \mathbb{R}^m_+, \ g(\boldsymbol{u}) = 0, \tag{4}$$

where $g(\boldsymbol{u}) = (\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b})^T(\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b}) + \sum_{i=1}^{r} u_i u_{i+r}$.

In the main results presented in Theorems 3.1 and 3.3, one of the following conditions will be imposed on (4).

(a) The feasible region of QOP (4) is bounded.

(b) $\boldsymbol{Q}_0$ is copositive-plus and the set of optimal solutions of QOP (4) is bounded. Here $\boldsymbol{A} \in \mathbb{C}$ is called copositive-plus if $\boldsymbol{u} \geq \boldsymbol{0}$ and $\boldsymbol{u}^T \boldsymbol{A} \boldsymbol{u} = 0$ imply $\boldsymbol{A}\boldsymbol{u} = \boldsymbol{0}$.

3.2 A parametric unconstrained QOP over the nonnegative orthant

We now introduce a Lagrangian relaxation of QOP (4) by defining a Lagrangian function $f : \mathbb{R}^m_+ \times \mathbb{R} \to \mathbb{R}$ by $f(\boldsymbol{u}, \lambda) = \boldsymbol{u}^T \boldsymbol{Q}_0 \boldsymbol{u} + 2\boldsymbol{c}^T \boldsymbol{u} + g(\boldsymbol{u})\lambda$,

$$\text{minimize} \quad f(\boldsymbol{u}, \lambda) \quad \text{subject to} \quad \boldsymbol{u} \in \mathbb{R}^m_+. \tag{5}$$

Notice that (5) is an unconstrained QOP over the nonnegative orthant with the Lagrangian multiplier parameter $\lambda \in \mathbb{R}$ for the equality constraint of QOP (4).

Let us choose a positive number for λ so that $g(\cdot)\lambda : \mathbb{R}^m_+ \to \mathbb{R}$ serves as a penalty function for QOP (4). In fact, we see that

$$\begin{array}{lcll} g(\boldsymbol{u}) & \geq & 0 & \text{for every } \boldsymbol{u} \in \mathbb{R}^m_+, \\ g(\boldsymbol{u}) & = & 0 & \text{if and only if } \boldsymbol{u} \in \mathbb{R}^m_+ \text{ satisfies the equality constraint of (4)}, \\ g(\boldsymbol{u})\lambda & \to & \infty \text{ as } 0 \leq \lambda \to \infty & \text{otherwise.} \end{array}$$

For each $\lambda > 0$, define a level set $L(\lambda) = \left\{ \boldsymbol{u} \in \mathbb{R}^m_+ : \zeta^* \geq f(\boldsymbol{u}, \lambda) \right\}$ and the optimal objective value $\zeta(\lambda) = \inf \left\{ f(\boldsymbol{u}, \lambda) : \boldsymbol{u} \in \mathbb{R}^m_+ \right\}$ of QOP (5). Then, for $0 < \lambda < \mu$,

$$\begin{array}{l} L(\lambda) \supset L(\mu) \supset \text{the set of optimal solutions of (4)}, \\ \zeta(\lambda) = \inf \left\{ f(\boldsymbol{u}, \lambda) : \boldsymbol{u} \in L(\lambda) \right\} \leq \zeta(\mu) \leq \zeta^*. \end{array} \tag{6}$$

Hence, if $L(\bar{\lambda})$ is bounded for some $\bar{\lambda} > 0$ and $\lambda \geq \bar{\lambda}$, then QOP (5) has an optimal solution with the finite objective value $\zeta(\lambda)$, and all optimal solutions of QOP (5) are contained in the bounded set $L(\bar{\lambda})$. The next theorem ensures that QOP (5) with the parameter $\lambda > 0$ serves as sequential unconstrained QOPs over $\mathbb{R}^m_+$ for solving QOP (4) under condition (a) or (b).

Theorem 3.1.

(i) If condition (a) is satisfied, then $L(\lambda)$ is bounded for every sufficiently large $\lambda > 0$.

(ii) If condition (b) is satisfied, then $L(\lambda)$ is bounded for any $\lambda > 0$.

(iii) Assume that $L(\bar{\lambda})$ is bounded for some $\bar{\lambda} > 0$. Let $\left\{ \lambda^k \geq \bar{\lambda} : k = 1, 2, \ldots, \right\}$ be a sequence diverging monotonically to ∞ as $k \to \infty$, and $\left\{ \boldsymbol{u}^k \in \mathbb{R}^m_+ : k = 1, 2, \ldots, \right\}$ a sequence of optimal solutions of QOP (5) with $\lambda = \lambda^k$. Then, any accumulation point of the sequence $\left\{ \boldsymbol{u}^k \in \mathbb{R}^m_+ \right\}$ is an optimal solution of QOP (4), and $\zeta(\lambda^k)$ converges monotonically to ζ^* as $k \to \infty$.

Although some of the assertions in Theorem 3.1 can be proved easily by applying the standard arguments on the penalty function method (for example, see [8]), we present complete proofs of all assertions for completeness in Section 4.

It would be desirable if any optimal solution of the problem (5) were an optimal solution of (4) for every sufficiently large λ. However, this is not true in general, as shown in the following illustrative example:

$$\text{minimize} \quad 2u_1 \quad \text{subject to } u_1 \geq 0, \ u_1 - 1 = 0, \tag{7}$$

which has the unique optimal solution $u_1^* = 1$ with the optimal value $\zeta^* = 2$. In this case, the Lagrangian relaxation problem is described as

$$\text{minimize } 2u_1 + (u_1 - 1)^2 \lambda \quad \text{subject to} \quad u_1 \geq 0.$$

For every $\lambda > 1$, this problem has the unique minimizer $u_1^* = 1 - 1/\lambda$ with the optimal value $\zeta(\lambda) = 2 - 1/\lambda$.

3.3 Completely positive cone programming and copositive cone programming relaxations of QOP (5) with the parameter $\lambda > 0$

We now relate the Lagrangian relaxation (5) of QOP (4) to the CPP relaxation of QOP (4), which was discussed in Sections 5.1 and 5.2 of [1]. Let

$$\begin{array}{rcl} n & = & 1 + m, \ \boldsymbol{x} = \begin{pmatrix} u_0 \\ \boldsymbol{u} \end{pmatrix} \in \mathbb{R}^n, \ \boldsymbol{Q} = \begin{pmatrix} 0 & \boldsymbol{c}^T \\ \boldsymbol{c} & \boldsymbol{Q}_0 \end{pmatrix} \in \mathbb{S}^n, \\ \boldsymbol{C}_i & = & \text{the } m \times m \text{ matrix with the } (i, i+r)\text{th component } 1/2 \text{ and } 0 \text{ elsewhere} \\ & & (i = 1, 2, \ldots, r), \\ \boldsymbol{H}_0 & = & \begin{pmatrix} 1 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{O} \end{pmatrix} \in \mathbb{S}^n, \ \boldsymbol{H}_1 = \begin{pmatrix} \boldsymbol{b}^T\boldsymbol{b} & \boldsymbol{b}^T\boldsymbol{A} \\ \boldsymbol{A}^T\boldsymbol{b} & \boldsymbol{A}^T\boldsymbol{A} \end{pmatrix} + \sum_{i=1}^{r} \begin{pmatrix} 0 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{C}_i + \boldsymbol{C}_i^T \end{pmatrix}. \end{array}$$

Then,

$$\begin{aligned}
\boldsymbol{Q} \bullet \boldsymbol{x}\boldsymbol{x}^T &= \boldsymbol{Q} \bullet \begin{pmatrix} u_0 \\ \boldsymbol{u} \end{pmatrix} \begin{pmatrix} u_0 \\ \boldsymbol{u} \end{pmatrix}^T = \boldsymbol{u}^T \boldsymbol{Q}_0 \boldsymbol{u} + 2\boldsymbol{c}^T u_0 \boldsymbol{u}, \\
\boldsymbol{H}_0 \bullet \boldsymbol{x}\boldsymbol{x}^T &= \boldsymbol{H}_0 \bullet \begin{pmatrix} u_0 \\ \boldsymbol{u} \end{pmatrix} \begin{pmatrix} u_0 \\ \boldsymbol{u} \end{pmatrix}^T = u_0^2, \\
\boldsymbol{H}_1 \bullet \boldsymbol{x}\boldsymbol{x}^T &= \boldsymbol{H}_1 \bullet \begin{pmatrix} u_0 \\ \boldsymbol{u} \end{pmatrix} \begin{pmatrix} u_0 \\ \boldsymbol{u} \end{pmatrix}^T = (\boldsymbol{b}u_0 + \boldsymbol{A}\boldsymbol{u})^T (\boldsymbol{b}u_0 + \boldsymbol{A}\boldsymbol{u}) + \sum_{i=1}^{r} u_i u_{i+r}
\end{aligned}$$

for every $\boldsymbol{x} = \begin{pmatrix} u_0 \\ \boldsymbol{u} \end{pmatrix} \in \mathbb{R}^n$. It should be noted that $\boldsymbol{H}_0, \ \boldsymbol{H}_1 \in \mathbb{C}$. Using these identities, we rewrite QOP(4) as

$$\text{minimize} \quad \boldsymbol{Q} \bullet \boldsymbol{X} \quad \text{subject to} \quad \boldsymbol{X} \in \widetilde{G}_1, \tag{8}$$

and QOP (5) as

$$\text{minimize} \quad (\boldsymbol{Q} + \boldsymbol{H}_1 \lambda) \bullet \boldsymbol{X} \quad \text{subject to } \boldsymbol{X} \in \widetilde{G}_0. \tag{9}$$

Here,

$$\begin{aligned}
\widetilde{G}_0 &= \left\{ \boldsymbol{x}\boldsymbol{x}^T \in \mathbb{S}^n : \boldsymbol{x} \in \mathbb{R}^n_+, \ \boldsymbol{H}_0 \bullet \boldsymbol{x}\boldsymbol{x}^T = 1 \right\} = \left\{ \boldsymbol{x}\boldsymbol{x}^T \in \mathbb{S}^n : \boldsymbol{x} \in \mathbb{R}^n_+, \ x_1^2 = 1 \right\}, \\
\widetilde{G}_1 &= \left\{ \boldsymbol{x}\boldsymbol{x}^T \in \widetilde{G}_0 : \boldsymbol{H}_1 \bullet \boldsymbol{x}\boldsymbol{x}^T = 0 \right\} \\
&= \left\{ \boldsymbol{x}\boldsymbol{x}^T \in \mathbb{S}^n : \boldsymbol{x} \in \mathbb{R}^n_+, \ \boldsymbol{H}_0 \bullet \boldsymbol{x}\boldsymbol{x}^T = 1, \ \boldsymbol{H}_1 \bullet \boldsymbol{x}\boldsymbol{x}^T = 0 \right\}.
\end{aligned}$$

It was shown in [1] that the constraint sets cl conv $\widetilde{G}_0$ and cl conv $\widetilde{G}_1$ coincide with their CPP relaxations $\widehat{G}_0$ and $\widehat{G}_1$, respectively, where

$$\begin{aligned}
\widehat{G}_0 &= \left\{ \boldsymbol{X} \in \mathbb{C}^* : \boldsymbol{H}_0 \bullet \boldsymbol{X} = 1 \right\} = \left\{ \boldsymbol{X} \in \mathbb{C}^* : X_{11} = 1 \right\}, \\
\widehat{G}_1 &= \left\{ \boldsymbol{X} \in \widehat{G}_0 : \boldsymbol{H}_1 \bullet \boldsymbol{X} = 0 \right\} = \left\{ \boldsymbol{X} \in \mathbb{C}^* : \boldsymbol{H}_0 \bullet \boldsymbol{X} = 1, \ \boldsymbol{H}_1 \bullet \boldsymbol{X} = 0 \right\}.
\end{aligned}$$

See Theorem 3.5 of [1]. Since the objective functions of the problems (8) and (9) are linear with respect to $\boldsymbol{X} \in \mathbb{S}^n$, (8) has the same optimal objective value as

$$\text{minimize} \quad \boldsymbol{Q} \bullet \boldsymbol{X} \quad \text{subject to} \quad \boldsymbol{X} \in \widehat{G}_1 \ (= \text{cl conv } \widetilde{G}_1), \tag{10}$$

and (9) has the same optimal objective value as

$$\text{minimize} \quad (\boldsymbol{Q} + \boldsymbol{H}_1 \lambda) \bullet \boldsymbol{X} \quad \text{subject to } \boldsymbol{X} \in \widehat{G}_0 \ (= \text{cl conv } \widetilde{G}_0). \tag{11}$$

We note that CPP (10) and QOP (4) have the equivalent optimal value ζ^*, and that both CPP (11) and QOP (5) have the optimal value $\zeta(\lambda) \leq \zeta^*$.

As dual problems of (10) and (11), we have

$$\text{maximize} \quad y_0 \quad \text{subject to} \quad \boldsymbol{Q} - \boldsymbol{H}_0 y_0 + \boldsymbol{H}_1 y_1 \in \mathbb{C}, \tag{12}$$

and

$$\text{maximize} \quad y_0 \quad \text{subject to} \quad \boldsymbol{Q} - \boldsymbol{H}_0 y_0 + \boldsymbol{H}_1 \lambda \in \mathbb{C}, \tag{13}$$

respectively. Either (12) or (13) forms a simple copositive cone programming (CP). The difference is that y_1 is a variable in (12) whereas $\lambda > 0$ is a parameter to be fixed in advance in (13). As a result, (13) involves just one variable. Obviously, CPP (11) has an interior feasible solution. By the standard duality theorem (see, for examples, Theorem 4.2.1 of [14]), CP (13) and CPP (11) have an equivalent optimal value. It is already observed that CPP (11) and QOP (5) share the common optimal value $\zeta(\lambda)$. Thus, Theorem 3.1 leads to the following theorem. It shows that, under condition (a) or (b), (11) and (13) serve as a parametric CPP relaxation and a parametric CP relaxation, respectively, and these parametric CP and CPP relaxations bound the optimal value ζ^* of QOP (4) from below by $\zeta(\lambda)$ converging monotonically to ζ^* as $\lambda \to \infty$.

Theorem 3.2. *Assume that condition (a) or (b) holds.*

(iv) CPP (11) and QOP (5) have the equivalent optimal value $\zeta(\lambda) \leq \zeta^*$, which converges monotonically to ζ^* as $\lambda \to \infty$.

(v) CP (13) and QOP (5) have the equivalent optimal value $\zeta(\lambda) \leq \zeta^*$, which converges monotonically to ζ^* as $\lambda \to \infty$.

Now, we discuss whether the dual (12) of CPP (10) has an optimal solution with the same optimal objective value ζ^* of CPP (10).

Theorem 3.3.

(vi) rank $\boldsymbol{X} \leq n -$ rank $\boldsymbol{A}$ if $\boldsymbol{X} \in \widehat{G}_1$.

(vii) Assume that condition (a) or (b) is satisfied. Then, the strong duality equality between CPP (10) and CP (12)

$$\zeta^* \quad = \quad \min\left\{\boldsymbol{Q} \bullet \boldsymbol{X} : \boldsymbol{X} \in \widehat{G}_1\right\} \quad = \quad \sup\left\{y_0 : \boldsymbol{Q} - \boldsymbol{H}_0 y_0 + \boldsymbol{H}_1 y_1 \in \mathbb{C}\right\} \qquad (14)$$

holds.

Since $\mathbb{C}^* \subset \mathbb{S}^n_+$ and any $\boldsymbol{X} \in \mathbb{S}^n$ with rank $\boldsymbol{X} < n$ lies on the boundary of $\mathbb{S}^n_+$, *(vi)* of Theorem 3.3 implies that CPP (10) does not have an interior feasible solution. Hence, the standard duality theorem can not be applied to the primal dual pair of (10) and (12). Thus, the assertion *(vii)* is important.

Proof of *(vi)*: Suppose that $\boldsymbol{x}\boldsymbol{x}^T \in \widetilde{G}_1$. Then,

$$\boldsymbol{x} \in \mathbb{R}^n_+,\ 0 = \boldsymbol{H}_1 \bullet \boldsymbol{x}\boldsymbol{x}^T = \left(\begin{pmatrix} \boldsymbol{b}^T\boldsymbol{b} & \boldsymbol{b}^T\boldsymbol{A} \\ \boldsymbol{A}^T\boldsymbol{b} & \boldsymbol{A}^T\boldsymbol{A} \end{pmatrix} + \sum_{i=1}^r \begin{pmatrix} 0 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{C}_i + \boldsymbol{C}_i^T \end{pmatrix} \right) \bullet \boldsymbol{x}\boldsymbol{x}^T,$$

$$\begin{pmatrix} \boldsymbol{b}^T\boldsymbol{b} & \boldsymbol{b}^T\boldsymbol{A} \\ \boldsymbol{A}^T\boldsymbol{b} & \boldsymbol{A}^T\boldsymbol{A} \end{pmatrix} \bullet \boldsymbol{x}\boldsymbol{x}^T \geq 0,\ \left(\sum_{i=1}^r \begin{pmatrix} 0 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{C}_i + \boldsymbol{C}_i^T \end{pmatrix} \right) \bullet \boldsymbol{x}\boldsymbol{x}^T \geq 0.$$

It follows that

$$0 \quad = \quad \boldsymbol{x}^T \begin{pmatrix} \boldsymbol{b}^T\boldsymbol{b} & \boldsymbol{b}^T\boldsymbol{A} \\ \boldsymbol{A}^T\boldsymbol{b} & \boldsymbol{A}^T\boldsymbol{A} \end{pmatrix} \boldsymbol{x} = \boldsymbol{x}^T \begin{pmatrix} \boldsymbol{b}^T \\ \boldsymbol{A}^T \end{pmatrix} \begin{pmatrix} \boldsymbol{b} & \boldsymbol{A} \end{pmatrix} \boldsymbol{x}.$$

Thus, $(\boldsymbol{b}\ \boldsymbol{A})\boldsymbol{x}\boldsymbol{x}^T = \boldsymbol{O}$ holds for every $\boldsymbol{x}\boldsymbol{x}^T \in \widetilde{G}_1$. Consequently, we have that $(\boldsymbol{b}\ \boldsymbol{A})\boldsymbol{X} = \boldsymbol{O}$ for every $\boldsymbol{X} \in \text{cl conv}\ \widetilde{G}_1 = \widehat{G}_1$, which implies that rank $\boldsymbol{X} \leq n - \text{rank}\ (\boldsymbol{b}\ \boldsymbol{A}) = n - \text{rank}\ \boldsymbol{A}$. ▮

Proof of *(vii)***:** By assertion *(ii)* of Theorem 3.2, we know that

$$\zeta^* = \lim_{0<\lambda\to\infty} \zeta(\lambda) = \sup_{\lambda>0} \max\{y_0 : \boldsymbol{Q} - \boldsymbol{H}_0 y_0 + \boldsymbol{H}_1\lambda \in \mathbb{C}\}.$$

This implies the desired result. ▮

In general, (12) does not have an optimal solution with the optimal objective value ζ^*. To verify this, assume on the contrary that (12) has an optimal solution (y_0^*, y_1^*) with the optimal value $y_0^* = \zeta^*$. Since $\boldsymbol{H}_1 \in \mathbb{C}$, (y_0^*, y_1) remains an optimal solution with the optimal value $y_0^* = \zeta^*$ for every $y_1 \geq y_1^*$. Thus, (13) attains the optimal value ζ^* for every $\lambda > \max\{0, y_1^*\}$. By the weak duality relation, (11) (hence (5)) attains the optimal value ζ^* of QOP (4) for every $\lambda > \max\{0, y_1^*\}$. This contradicts what we have observed in the simple example (7). Furthermore, if we reformulate the simple problem (7) as (8), the constraint of (12) becomes

$$\begin{pmatrix} -y_0 + y_1 & 1 - y_1 \\ 1 - y_1 & y_1 \end{pmatrix} \in \mathbb{C}. \tag{15}$$

We can verify numerically that if $y_0 = \zeta^* = 2$, then, for any finite $y_1 \in \mathbb{R}$, the matrix on the left side has a negative eigenvalue λ with a eigenvector $\boldsymbol{v} > \boldsymbol{0}$. Thus,

$$\boldsymbol{v}^T \begin{pmatrix} -2 + y_1 & 1 - y_1 \\ 1 - y_1 & y_1 \end{pmatrix} \boldsymbol{v} = \lambda \boldsymbol{v}^T\boldsymbol{v} < 0.$$

As a result, the matrix on the left side of (15) with $y_0 = \zeta^* = 2$ can not be in $\mathbb{C}$ for any $y_1 \in \mathbb{R}$. This is a direct proof for the assertion that (12) does not have an optimal solution with the optimal value $y_0^* = \zeta^*$. If $y_0 < \zeta^* = 2$, then the matrix on the left side of (15) becomes positive definite for every sufficiently large $y_1 > 0$. Thus, the strong duality equality (14) holds.

Remark 3.4. Assume that QOP (1) satisfies condition (a) and we know a positive constant α such that $\boldsymbol{e}^T\boldsymbol{u} \leq \alpha$ for any feasible solution $\boldsymbol{u}$ of QOP (1) and the m-dimensional vector of ones $\boldsymbol{e}$. Then, QOP (1) can be transformed into a QOP in a strictly positive quadratic form, $\boldsymbol{u}^T\boldsymbol{Q}_0\boldsymbol{u}$ with all $[\boldsymbol{Q}_0]_{ij} > 0$, to be minimized over a bounded feasible region. Thus, the resulting QOP satisfies condition (b). We show this under the assumption that the last component u_m of $\boldsymbol{u} \in \mathbb{R}^m$ serves as a slack variable for the inequality constraint that bounds the sum of the other components u_j $(j = 1, 2, \ldots, m-1)$ by α, and that the last row of the equality constraint $\boldsymbol{A}\boldsymbol{u} + \boldsymbol{b} = \boldsymbol{0}$ is of the form $\boldsymbol{e}^T\boldsymbol{u} - \alpha = 0$. Then, for any $\beta \in \mathbb{R}$ and every feasible solution $\boldsymbol{u}$ of (1),

$$\boldsymbol{u}^T\left(\boldsymbol{Q}_0 + \frac{\boldsymbol{c}\boldsymbol{e}^T}{\alpha} + \frac{\boldsymbol{e}\boldsymbol{c}^T}{\alpha} + \beta\boldsymbol{e}\boldsymbol{e}^T\right)\boldsymbol{u} = \boldsymbol{u}^T\boldsymbol{Q}_0\boldsymbol{u} + 2\boldsymbol{c}^T\boldsymbol{u} + \beta\alpha^2.$$

Thus, the objective function $\boldsymbol{u}^T\boldsymbol{Q}_0\boldsymbol{u} + 2\boldsymbol{c}^T\boldsymbol{u}$ can be replaced by $\boldsymbol{u}^T\left(\boldsymbol{Q}_0 + \frac{\boldsymbol{c}\boldsymbol{e}^T}{\alpha} + \frac{\boldsymbol{e}\boldsymbol{c}^T}{\alpha} + \beta\boldsymbol{e}\boldsymbol{e}^T\right)\boldsymbol{u}$. Taking $\beta > 0$ sufficiently large, we have a QOP in a strictly positive quadratic form. Therefore, in the relaxation problems (10), (11), (12) and (13), we can assume that $\boldsymbol{Q}$ is of the form $\begin{pmatrix} 0 & \boldsymbol{0}^T \\ \boldsymbol{0} & \boldsymbol{Q}_0 \end{pmatrix}$ with all $[\boldsymbol{Q}_0]_{ij} > 0$. This conversion can be used for developing numerical methods for the QOP (1) with a bounded feasible region in the future. However, it may not be numerically efficient because the coefficient matrix $\boldsymbol{Q}_0$ of the resulting QOP becomes fully dense.

4 Proof of Theorem 3.1

A sequence $\left\{(\boldsymbol{u}^k, \lambda^k) \in \mathbb{R}^{m+1} : k = 1, 2, \ldots, \right\}$ is used in the proofs of assertions *(i), (ii)* and *(iii)* below such that

$$\boldsymbol{u}^k \geq 0, \ \lambda^k > 0, \tag{16}$$
$$\zeta^* \geq f(\boldsymbol{u}^k, \lambda^k) = (\boldsymbol{u}^k)^T \boldsymbol{Q}_0 \boldsymbol{u}^k + 2\boldsymbol{c}^k \boldsymbol{u}^k + g(\boldsymbol{u}^k)\lambda^k. \tag{17}$$

We note that such a sequence always satisfies

$$(\boldsymbol{A}\boldsymbol{u}^k + \boldsymbol{b})^T (\boldsymbol{A}\boldsymbol{u}^k + \boldsymbol{b}) \geq 0, \ \sum_{i=1}^r u_i^k u_{i+r}^k \geq 0, \tag{18}$$
$$\zeta^* \geq (\boldsymbol{u}^k)^T \boldsymbol{Q}_0 \boldsymbol{u}^k + 2\boldsymbol{c}^k \boldsymbol{u}^k. \tag{19}$$

4.1 Proof of assertion *(i)*

Assume on the contrary that $L(\lambda)$ is unbounded for any $\lambda > 0$. Then, $\lambda^k \to \infty$ and $\|\boldsymbol{u}^k\| \to \infty$ as $k \to \infty$ for some sequence $\left\{(\lambda^k, \boldsymbol{u}^k) : k = 1, 2, \ldots, \right\}$ satisfying (16) through (19). We may assume without loss of generality that $\boldsymbol{u}^k / \|\boldsymbol{u}^k\|$ converges to some nonzero $\boldsymbol{d} \geq \boldsymbol{0}$.

We divide the inequality (17) by $\lambda^k \|\boldsymbol{u}^k\|^2$ and the inequalities in (18) by $\|\boldsymbol{u}^k\|^2$, respectively, and take the limit on the resulting inequalities as $k \to \infty$. Then, we observe that $\boldsymbol{d} \geq \boldsymbol{0}$ satisfies

$$0 \geq (\boldsymbol{A}\boldsymbol{d})^T (\boldsymbol{A}\boldsymbol{d}) + \sum_{i=1}^r d_i^k d_{i+r}^k, \ (\boldsymbol{A}\boldsymbol{d})^T (\boldsymbol{A}\boldsymbol{d}) \geq 0, \ \sum_{i=1}^r d_i^k d_{i+r}^k \geq 0. \tag{20}$$

It follows that $\boldsymbol{A}\boldsymbol{d} = \boldsymbol{0}$ and $d_i = 0$ $(i = 1, 2, \ldots, 2r)$ (recall that $\boldsymbol{A}$ is of the form (2)). Hence, $\boldsymbol{u}^* + \nu \boldsymbol{d}$ remains a feasible solution of (4) for every $\nu \geq 0$. This can not happen if condition (a) is satisfied.

4.2 Proof of assertion *(ii)*

Let us fix $\lambda > 0$ arbitrarily. Assume that $\{\boldsymbol{u} \geq \boldsymbol{0} : \zeta^* \geq f(\boldsymbol{u}, \lambda)\}$ is unbounded. We can take a sequence $\{\boldsymbol{u}^k : k = 1, 2, \ldots, \}$ satisfying (16) through (19) with λ_k fixed to λ and $\|\boldsymbol{u}^k\| \to \infty$ as $k \to \infty$. We may assume that $\boldsymbol{u}^k / \|\boldsymbol{u}^k\|$ converges to some nonzero $\boldsymbol{d} \geq \boldsymbol{0}$. Since $\boldsymbol{Q}_0$ is assumed to be copositive-plus, it follows from (17) that

$$\zeta^* \geq 2\boldsymbol{c}^k \boldsymbol{u}^k + \left((\boldsymbol{A}\boldsymbol{u}^k + \boldsymbol{b})^T (\boldsymbol{A}\boldsymbol{u}^k + \boldsymbol{b}) + \sum_{i=1}^r u_i^k u_{i+r}^k \right) \lambda, \tag{21}$$

and from (19) that $\zeta^* \geq 2\boldsymbol{c}\boldsymbol{u}^k$. We first divide the inequality (21) by $\lambda \|\boldsymbol{u}^k\|^2$, the inequalities in (18) by $\|\boldsymbol{u}^k\|^2$, and the inequalities (19) by $\|\boldsymbol{u}^k\|^2$, respectively. Next, take the limit on the resulting inequalities and the inequality $\zeta^* / \|\boldsymbol{u}^k\| \geq 2\boldsymbol{c}^T \boldsymbol{u}^k / \|\boldsymbol{u}^k\|$ as $k \to \infty$. Then, we obtain (20), which implies $\boldsymbol{A}\boldsymbol{d} = \boldsymbol{0}$ and $d_i = 0$ $(i = 1, 2, \ldots, 2r)$, and $0 \geq 2\boldsymbol{c}^T \boldsymbol{d}$. In addition, $0 \geq \boldsymbol{d}^T \boldsymbol{Q}_0 \boldsymbol{d}$, which implies $\boldsymbol{d}^T \boldsymbol{Q}_0 \boldsymbol{d} =$ and $\boldsymbol{Q}_0 \boldsymbol{d} = \boldsymbol{0}$ (recall that $\boldsymbol{Q}_0$ is copositive-plus). Therefore, $\boldsymbol{u}^* + \nu \boldsymbol{d}$ remains a feasible solution of QOP (4) for every $\nu \geq 0$ and that $\zeta^* \geq (\boldsymbol{u}^* + \nu \boldsymbol{d})^T \boldsymbol{Q}_0 (\boldsymbol{u}^* + \nu \boldsymbol{d}) + 2\boldsymbol{c}^T (\boldsymbol{u}^* + \nu \boldsymbol{d})$ for every $\nu \geq 0$. This contradicts condition (b).

4.3 Proof of assertion *(iii)*

We observe that the sequence $\left\{(\boldsymbol{u}^k, \lambda^k)\right\}$ satisfies (16) through (19) with $f(\boldsymbol{u}^k, \lambda^k) = \zeta(\lambda^k)$. Let $\{\boldsymbol{u}^{k_j} : j = 1, 2, \ldots, \}$ be a subsequence that converges to $\bar{\boldsymbol{u}} \geq \boldsymbol{0}$. From (17),

$$\frac{\zeta^*}{\lambda^{k_j}} \geq \frac{(\boldsymbol{u}^{k_j})^T \boldsymbol{Q}_0 \boldsymbol{u}^{k_j} + 2\boldsymbol{c}^k \boldsymbol{u}^{k_j}}{\lambda^{k_j}} + g(\boldsymbol{u}^{k_j}),\ g(\boldsymbol{u}^{k_j}) \geq 0,\ \zeta^* \geq \zeta(\lambda^{k_j}) \geq (\boldsymbol{u}^{k_j})^T \boldsymbol{Q}_0 \boldsymbol{u}^{k_j} + 2\boldsymbol{c}^k \boldsymbol{u}^{k_j}$$

$(j = 1, 2, \ldots,)$ hold. Taking the limit as $j \to \infty$ in the inequality above, we have $g(\bar{\boldsymbol{u}}) = 0$ and $\zeta^* \geq \lim_{j\to\infty} \zeta(\lambda^{k_j}) \geq (\bar{\boldsymbol{u}})^T \boldsymbol{Q}_0 \bar{\boldsymbol{u}} + 2\boldsymbol{c}^T \bar{\boldsymbol{u}}$. Thus, $\bar{\boldsymbol{u}}$ is an optimal solution of (4) and $\lim_{j\to\infty} \zeta(\lambda^{k_j}) = \zeta^*$. By (6), we also know that $\zeta(\lambda) \leq \zeta(\mu) \leq \zeta^*$ if $\lambda \leq \mu$. Consequently, the sequence $\left\{\zeta(\lambda^k)\right\}$ itself converges monotonically to ζ^* as $k \to \infty$.

5 Concluding remarks

We have proposed the three relaxations, the unconstrained QOP (5) in nonnegative variables, the CPP problem (11) and the CP problem (13). Computing an optimal solution of any of the proposed relaxations numerically is difficult. As mentioned in Section 1, to develop a numerical method for the second and third relaxations, the problem of checking whether a given matrix lies in the completely positive cone and the copositive cone needs to be resolved, respectively, which was shown in [12] as a co-NP-complete problem.

One practical method to overcome this difficulty is to relax the completely positive cone $\mathbb{C}^*$ by the so-called doubly nonnegative cone $\mathbb{S}^n_+ \bigcap \mathbb{N}$ in (11), where $\mathbb{N}$ denotes the cone of $n \times n$ symmetric matrices with nonnegative components. This idea of replacing $\mathbb{C}^*$ by $\mathbb{S}^n_+ \bigcap \mathbb{N}$ in CPP problems has been used in [9, 16]. Even in their cases, the resulting SDPs can not be solved efficiently when the size of variable matrix $\boldsymbol{X}$ is large because of the $(n-1)n/2$ inequality constraints $X_{ij} \geq 0$ $(1 \leq i < j \leq n)$. In particular, the inequality constraints make it difficult to exploit sparsity in the SDPs, which is an effective tool to solve large scale SDPs efficiently.

If we replace $\mathbb{C}^*$ by $\mathbb{S}^n_+ \bigcap \mathbb{N}$ in (11), we have the following problem rewritten as an SDP, which serves as a relaxation of (11).

$$\text{minimize} \quad (\boldsymbol{Q} + \boldsymbol{H}_1\lambda) \bullet \boldsymbol{X} \quad \text{subject to } X_{11} = 1, X_{ij} \geq 0\ (1 \leq i < j \leq n),\ \boldsymbol{X} \in \mathbb{S}^n_+. \tag{22}$$

Note that the number of inequalities is increased. As a result, sparsity can not be exploited efficiently, although it involves only a single equality constraint $X_{11} = 1$. To exploit sparsity in (22), we need to reduce the number of inequality constraints. For example, we can take $K = \{(i,j) : 1 \leq i < j \leq n,\ [\boldsymbol{Q} + \boldsymbol{H}_1\lambda]_{ij} \neq 0\}$, expecting that K satisfies a structured sparsity in practice, and replace the inequality constraints by $X_{ij} \geq 0$ $((i,j) \in K)$. Further studies and numerical experiments along this direction are important subjects of future research. We refer to [10, 11, 13] for exploiting sparsity in SDPs.

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