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Notoriously hard (mixed-)binary QPs: empirical evidence on new completely positive approaches

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Abstract

By now, many copositive reformulations of mixed-binary QPs have been discussed, triggered by Burer's seminal characterization from 2009. In conic optimization, it is very common to use approximation hierarchies based on positive-semidefinite (psd) matrices where the order increases with the level of the approximation. Our purpose is to keep the psd matrix orders relatively small to avoid memory size problems in interior point solvers. Based upon on a recent discussion on various variants of completely positive reformulations and their relaxations (Bomze et al. in Math Program 166(1–2):159–184, 2017), we here present a small study of the notoriously hard multidimensional quadratic knapsack problem and quadratic assignment problem. Our observations add some empirical evidence on performance differences among the above mentioned variants. We also propose an alternative approach using penalization of various classes of (aggregated) constraints, along with some theoretical convergence analysis. This approach is in some sense similar in spirit to the alternating projection method proposed in Burer (Math Program Comput 2:1–19, 2010) which completely avoids SDPs, but for which no convergence proof is available yet.

Keywords Copositivity · Completely positive · Quadratic optimization · Reformulations · Nonlinear optimization · Nonconvex optimization · Penalization method · Quadratic assignment problem · Mul tidimensional knapsack problem

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1 Introduction

1.1 Motivation and structure of the paper

Several co(mpletely) positive (CP) reformulations have been widely studied in the literature since the pioneering work of Burer (2009). It is well known that copositive problems are NP-hard problems (Murty and Kabadi 1987). Therefore, various relaxations are proposed where the co(mpletely) positive cones are replaced by tractable approximations. In a recent work (Bomze et al. 2017), we studied various CP reformulations and their relaxations. Based upon this, we study in this paper two notoriously hard optimization problems, namely the multidimensional knapsack problem and quadratic assignment problem. In addition to the comparison of different CP reformulations, we propose an alternative approach based on the penalization of various classes of aggregated constraints together with some theoretical convergence analysis. The following subsections present the notations and the CP reformulations. Our penalization approach is discussed in Sect. 2. Purely binary quadratic problems are studied in Sect. 3. Numerical results are given in Sect. 4. Section 5, finally, discusses future work and concludes the paper.

1.2 Basic concepts, notation and terminology

We abbreviate by $[m\colon n] = \{m, m+1, \dots, n\}$ the integer range between two integers m, n with $m \leq n$. By bold-faced lower-case letters we denote vectors in n-dimensional Euclidean space $\mathbb{R}^n$ (e.g., the zero vector o), by upper case boldface letters matrices (e.g., the zero matrix O), and by $^\top$ transposition. The nonnegative orthant is denoted by $\mathbb{R}^n_+ = \{\mathsf{x} \in \mathbb{R}^n \colon x_i \geq 0 \text{ for all } i \in [1\colon n]\}$. I_n is the $n \times n$ identity matrix with columns e_i, $i \in [1\colon n]$, while $\mathsf{e} = \sum_{i=1}^n \mathsf{e}_i = [1, \dots, 1]^\top \in \mathbb{R}^n$. We denote by $\mathbb{R}^{d\times p}$ the set of all $d \times p$ matrices, $\mathbb{R}^{d\times p}_+$ the subset of those with no negative entries, and

$$\mathcal{S}^d = \left\{\mathsf{X} \in \mathbb{R}^{d\times d} \colon \mathsf{X} = \mathsf{X}^\top\right\}.$$

The Frobenius inner product is denoted by $\langle \mathsf{S}, \mathsf{X}\rangle = \operatorname{trace}(\mathsf{SX})$, where $\{\mathsf{S}, \mathsf{X}\} \subset \mathcal{S}^d$. With respect to any duality, we consider the dual cone

$$\mathcal{A}^* = \{\mathsf{b} \colon \langle \mathsf{a}, \mathsf{b}\rangle \geq 0 \text{ for all } \mathsf{a} \in \mathcal{A}\}$$

of a given cone $\mathcal{A}$.

For a given symmetric matrix $\mathsf{H} = \mathsf{H}^\top$, we denote the fact that H is positive-semidefinite by $\mathsf{H} \succeq \mathsf{O}$. Sometimes we write instead "H is psd.", and introduce the cone of all psd matrices of a given order d by

$$\mathcal{S}^d_+ = \left\{\mathsf{X} \in \mathcal{S}^d \colon \mathsf{X} \succeq \mathsf{O}\right\}.$$

Furthermore, $\mathcal{N}^d = \left\{\mathsf{X} \in \mathcal{S}^d \colon X_{ij} \geq 0 \text{ for all } i, j\right\}$, while $\mathcal{COP}^d$ denotes the cone of all symmetric $d \times d$ copositive matrices:

$$\mathcal{COP}^d = \left\{\mathsf{M} \in \mathcal{S}^d \colon \mathsf{x}^\top \mathsf{M}\mathsf{x} \geq 0 \text{ for all } \mathsf{x} \in \mathbb{R}^d_+\right\}.$$

and $\mathcal{CP}^d$ the cone of all completely positive matrices of order d:

$$\mathcal{CP}^d = \left\{\mathsf{X} \in \mathcal{S}^d \colon \mathsf{X} = \sum_{i=1}^{p(d)} \mathsf{f}_i \mathsf{f}_i^\top \text{ for some } \mathsf{f}_i \in \mathbb{R}^d_+\right\}.$$

where $p(d)$ is an upper bound on the necessary number of summands for X, the so-called *cp-rank* of X. One can always use $p(d) = \max\left\{\binom{d+1}{2} - 4, d\right\}$ which is tight when d is large (Bomze et al. 2015; Shaked-Monderer et al. 2015).

1.3 Variants of CP reformulations

In this paper we consider the following mixed-binary quadratic optimization problem:

$$\begin{array}{lll} \min & \mathsf{x}^\top \mathsf{Q}\mathsf{x} + 2\mathsf{c}^\top \mathsf{x} & \\ \text{s.t.} & \mathsf{a}_i^\top \mathsf{x} = b_i & \text{for } i \in [1\colon m] \\ & \mathsf{x} \in \mathbb{R}^n_+ & \\ & x_j \in \{0, 1\} & \text{for } j \in B, \end{array} \tag{P}$$

where $B \subseteq [1\colon n]$, $\mathsf{Q} \in \mathcal{S}^n$, $\mathsf{b} \in \mathbb{R}^m$, and $\{\mathsf{c}, \mathsf{a}_1, \ldots, \mathsf{a}_m\} \subset \mathbb{R}^n$, with $\mathsf{a}_1, \ldots, \mathsf{a}_m$ being linearly independent.

We define the polyhedron $\mathcal{Z} = \{\mathsf{x} \in \mathbb{R}^n_+ \colon \mathsf{a}_i^\top \mathsf{x} = b_i,\ i \in [1\colon m]\}$, noting that the feasible set of (P) is contained in $\mathcal{Z}$.

As Burer (2009), we also assume that the following key assumption holds for this problem:

$$\mathsf{v} \in \mathcal{Z} \quad \Longrightarrow \quad v_j \leq 1 \text{ for all } j \in B. \tag{1}$$

Adding slack variables can always make this assumption hold.

Burer (2009) showed that under the key assumption (1), problem (P) has the same optimal value as problem (CPP) below. Unfortunately, optimizing over the completely positive cone is a very difficult problem (in fact an NP-hard problem Bomze et al. 2000, 2012; Dickinson and Gijben 2014; Murty and Kabadi 1987). So we need to consider approximations of this, and these may vary in performance even when the original alternative reformulations are equivalent. We start with the by now classical reformulation by Burer (2009):

$$\begin{array}{lll} \min & \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} & \\ \text{s.t.} & \mathsf{a}_i^\top \mathsf{x} = b_i & \text{for } i \in [1\colon m] \\ & \langle \mathsf{a}_i \mathsf{a}_i^\top, \mathsf{X}\rangle = b_i^2 & \text{for } i \in [1\colon m] \\ & X_{jj} = x_j & \text{for } j \in B \\ & \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{CP}^{n+1}. & \end{array} \tag{CPP}$$

A natural relaxation of problem (CPP) would be the following:

$$\begin{array}{lll} \min & \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} & \\ \text{s.t.} & \mathsf{a}_i^\top \mathsf{x} = b_i & \text{for } i \in [1\colon m] \\ & \langle \mathsf{a}_i \mathsf{a}_i^\top, \mathsf{X}\rangle = b_i^2 & \text{for } i \in [1\colon m] \\ & X_{jj} = x_j & \text{for all } j \in B \\ & \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}. & \end{array} \tag{2}$$

From the computational point of view, this problem remains difficult to solve due to the large positive semidefinite constraints. Moreover, we never have an interior point for the problem. Indeed, for any feasible (x, X) and any i we have

$$\begin{pmatrix} -b_i \\ \mathsf{a}_i \end{pmatrix}^\top \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \begin{pmatrix} -b_i \\ \mathsf{a}_i \end{pmatrix} = \mathsf{a}_i^\top \mathsf{X} \mathsf{a}_i - 2b_i\, \mathsf{a}_i^\top \mathsf{x} + b_i^2 = 0,$$

which implies that $\begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix}$ is on the boundary of the positive semidefinite cone.

In this paper, we study three equivalent alternatives to (CPP) put forward in Bomze et al. (2017). Here, equivalent means that these alternatives have the same feasible sets and the same objective function. These alternatives may avoid above-mentioned drawbacks.

To this end, let $\{\mathsf{a}_{m+1}, \ldots, \mathsf{a}_n\} \subset \mathbb{R}^n$ be linearly independent vectors with $\mathsf{a}_i^\top \mathsf{a}_{m+j} = 0$ for all $i \in [1\colon m]$, all $j \in [1\colon n-m]$. This then implies that

$$\left\{\mathsf{x} \in \mathbb{R}^n \colon \mathsf{a}_i^\top \mathsf{x} = 0 \text{ for } i \in [1\colon m]\right\} = \left\{\sum_{i=1}^{n-m} y_i \mathsf{a}_{m+i} \colon \mathsf{y} \in \mathbb{R}^{n-m}\right\} \quad \text{and that} \tag{3}$$

$$\left\{\mathsf{x} \in \mathbb{R}^n \colon \mathsf{a}_i^\top \mathsf{x} = b_i \text{ for } i \in [1\colon m]\right\} = \left\{\mathsf{x}_0 + \sum_{i=1}^{n-m} y_i \mathsf{a}_{m+i} \colon \mathsf{y} \in \mathbb{R}^{n-m}\right\}. \tag{4}$$

Next, let $\mathsf{x}_0 \in \operatorname{int} \mathbb{R}_+^n \cap \mathcal{Z}$ (without loss of generality we may and do assume such an x_0 exists, cf. Bomze et al. 2017) and define a matrix

$$\mathsf{R} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \mathsf{x}_0 & \mathsf{a}_{m+1} & \mathsf{a}_{m+2} & \cdots & \mathsf{a}_n \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+1-m)}.$$

We then have

$$\left\{\begin{pmatrix}\zeta\\ \mathsf{z}\end{pmatrix} \in \mathbb{R}^{n+1} : \mathsf{a}_i^\top \mathsf{z} = b_i \zeta \text{ for } i\in[1\colon m]\right\} = \left\{\mathsf{R}\mathsf{y} : \mathsf{y} \in \mathbb{R}^{n+1-m}\right\}. \tag{5}$$

Note that R has full column rank thanks to the linear independence of $\mathsf{a}_{m+1}, \ldots, \mathsf{a}_n$, and thus for any $\mathsf{Y} \in \mathcal{S}^{n+1-m}$ we have (Bomze et al. 2017)

$$\mathsf{R}\mathsf{Y}\mathsf{R}^\top \in \mathcal{S}_+^{n+1} \iff \mathsf{Y} \in \mathcal{S}_+^{n+1-m}, \tag{6}$$

$$\mathsf{R}\mathsf{Y}\mathsf{R}^\top = 0 \iff \mathsf{Y} = 0. \tag{7}$$

The first alternative reformulation of (2) reduces the size of the psd matrices:

$$\begin{aligned}
\min \quad & \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} \\
\text{s.t.} \quad & X_{jj} = x_j \quad \text{for all } j \in B \\
& \mathsf{R}\mathsf{Y}\mathsf{R}^\top = \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \\
& \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \in \mathcal{N}^{n+1},\ \mathsf{Y} \in \mathcal{S}_+^{n+1-m}.
\end{aligned} \tag{8}$$

Still, presence of binary constraints prohibits strict feasibility (and sometimes even sheer feasibility). Furthermore, computationally (8) still has the problem that if $|B|$ is large then we have a large number of linear constraints. This can be solved by aggregating. To the best of our knowledge, the first such aggregated reformulation was put forward by (Arima et al. 2014):

$$\begin{aligned}
\min \quad & \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} \\
\text{s.t.} \quad & \sum_{i=1}^{m} \left(\mathsf{a}_i^\top \mathsf{X}\mathsf{a}_i - 2b_i\, \mathsf{a}_i^\top \mathsf{x} + b_i^2 x_0\right) = 0 \\
& \sum_{j\in B} (X_{jj} - x_j) = 0 \\
& \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \in \mathcal{CP}^{n+1}
\end{aligned} \tag{9}$$

along with its doubly-nonnegative (DNN) relaxation,

$$\begin{aligned}
\min \quad & \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} \\
\text{s.t.} \quad & \sum_{i=1}^{m} \left(\mathsf{a}_i^\top \mathsf{X}\mathsf{a}_i - 2b_i\, \mathsf{a}_i^\top \mathsf{x} + b_i^2\right) = 0 \\
& \sum_{j\in B} (X_{jj} - x_j) = 0 \\
& \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \in \mathcal{N}^{n+1} \cap \mathcal{S}_+^{n+1},
\end{aligned} \tag{10}$$

again with a large-order psd constraint. Inspired by Burer (2010) and Dickinson (2013), another reformulation of (2) was recently put forward in Bomze et al. (2017) which combines both above approaches (and performance advantages):

$$
\begin{array}{ll}
\min & \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} \\
\text{s.t.} & \sum_{j\in B} (X_{jj} - x_j) = 0 \\
& \mathsf{RYR}^\top = \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \\
& \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{CP}^{n+1},\ \mathsf{Y} \in \mathcal{S}^{n+1-m},
\end{array}
\tag{11}
$$

along with its relaxation

$$
\begin{array}{ll}
\min & \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} \\
\text{s.t.} & \sum_{j\in B} (X_{jj} - x_j) = 0 \\
& \mathsf{RYR}^\top = \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \\
& \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{N}^{n+1},\ \mathsf{Y} \in \mathcal{S}_+^{n+1-m}.
\end{array}
\tag{12}
$$

For the general case (i.e., also in absence of binary variables where we would have a Slater point $\mathsf{Y} = \varepsilon\mathsf{I} + (1-\varepsilon)\mathsf{e}_0\mathsf{e}_0^\top$), a comparison to previous approaches is provided in Bomze et al. (2017), along with a thorough discussion of (strong) conic duality of all these variants and their relaxations.

In Bomze et al. (2017), the equivalence of problems (CPP), (9) and (11) and similar results for the relaxation (12) have been shown. For convenient notation, we introduce the following four linear subspaces of $\mathcal{S}^{n+1}$:

$$
\begin{aligned}
\mathcal{L}_1 &= \left\{ \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}^{n+1} \colon \exists \mathsf{Y} \in \mathcal{S}^{n+1-m} \text{ s.t. } \mathsf{RYR}^\top = \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\} = \mathsf{R}\mathcal{S}^{n+1-m}\mathsf{R}^\top, \\
\mathcal{L}_2 &= \left\{ \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}^{n+1} \colon \begin{array}{ll} \mathsf{a}_i^\top \mathsf{x} = b_i x_0 & \text{for } i \in [1\colon m], \\ \mathsf{a}_i^\top \mathsf{X} = b_i \mathsf{x}^\top & \text{for } i \in [1\colon m] \end{array} \right\}, \\
\mathcal{L}_3 &= \left\{ \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}^{n+1} \colon \begin{array}{ll} \mathsf{a}_i^\top \mathsf{x} = b_i x_0 & \text{for } i \in [1\colon m], \\ \mathsf{a}_i^\top \mathsf{X}\mathsf{a}_i = b_i^2 x_0 & \text{for } i \in [1\colon m] \end{array} \right\}, \\
\mathcal{L}_4 &= \left\{ \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}^{n+1} \colon \sum_{i=1}^m \left(\mathsf{a}_i^\top \mathsf{X}\mathsf{a}_i - 2b_i\, \mathsf{a}_i^\top \mathsf{x} + b_i^2 x_0 \right) = 0 \right\}.
\end{aligned}
$$

Note that from the definition of R, we have $(\mathsf{RYR}^\top)_{00} = (\mathsf{Y})_{00}$, and thus for $\mathcal{L}_1$, an additional constraint of $x_0 = 1$ is equivalent to fixing $(\mathsf{Y})_{00} = 1$.

As shown in Bomze et al. (2017, Theorem 1), the intersection of each $\mathcal{L}_i$ with the positive-semidefinite cone results in the same cone:

$$
\begin{aligned}
&\mathcal{L}_1 = \mathcal{L}_2 \subseteq \mathcal{L}_3 \subseteq \mathcal{L}_4, \\
&\mathcal{L}_1 \cap \mathcal{S}_+^{n+1} = \mathcal{L}_2 \cap \mathcal{S}_+^{n+1} = \mathcal{L}_3 \cap \mathcal{S}_+^{n+1} = \mathcal{L}_4 \cap \mathcal{S}_+^{n+1} = \mathsf{R}\mathcal{S}_+^{n+1-m}\mathsf{R}^\top.
\end{aligned}
$$

In spite of these equalities, we still consider these as separate sets, even when intersected with the positive-semidefinite cone. The difference in description is especially important when considering optimization problems and their duals, along with their relaxations, for algorithmic and implementation reasons.

Again, we follow the approach in Bomze et al. (2017) in aggregating the binary constraints of (P). We consider the following cones:

$$\mathcal{B}_1 = \left\{ \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}^{n+1} \colon X_{jj} = x_j \quad \text{for } j \in B \right\},$$

$$\mathcal{B}_2 = \left\{ \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}^{n+1} \colon \sum_{j \in B} (X_{jj} - x_j) = 0 \right\}.$$

Then we have Bomze et al. (2017, Proposition 1)

$$\begin{aligned} &\mathcal{B}_{k_1} \cap \mathcal{L}_{l_1} \cap \mathcal{CP}^{n+1} = \mathcal{B}_{k_2} \cap \mathcal{L}_{l_2} \cap \mathcal{CP}^{n+1} && \text{for all } k_1, k_2 \in [1\colon 2], l_1, l_2 \in [1\colon 4] \text{ and} \\ &\mathcal{B}_{k_1} \cap \mathcal{L}_{l_1} \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1} = \mathcal{B}_{k_2} \cap \mathcal{L}_{l_2} \cap \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1} && \text{for all } k_1, k_2 \in [1\colon 2], l_1, l_2 \in [1\colon 4]. \end{aligned}$$

Burer (2009) showed that the problems (P) and (CPP) have the same optimal values. So problem (CPP) can rewritten as

$$\min \left\{ \langle \mathsf{Q}, \mathsf{X} \rangle + 2\mathsf{c}^\top \mathsf{x} \colon \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{B}_1 \cap \mathcal{L}_3 \cap \mathcal{CP}^{n+1} \right\},$$

or as

$$\min \left\{ \langle \mathsf{Q}, \mathsf{X} \rangle + 2\mathsf{c}^\top \mathsf{x} \colon \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{B}_2 \cap \mathcal{L}_4 \cap \mathcal{CP}^{n+1} \right\}$$

or as

$$\min \left\{ \langle \mathsf{Q}, \mathsf{X} \rangle + 2\mathsf{c}^\top \mathsf{x} \colon \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{B}_2 \cap \mathcal{L}_1 \cap \mathcal{CP}^{n+1} \right\},$$

which can be expressed explicitly as problems (9) and (11) respectively.

1.4 Duality

In this subsection we consider the dual problems to the completely positive and positive semidefinite problems considered in the paper so far. In particular we will consider when the optimal solutions in the primal and dual problems are attained and when we have strong duality, i.e. the primal and dual problems have the same optimal value. In order to do this we first need the following result on strong duality for a certain class of conic optimisation problems.

Lemma 1 *For a proper cone $\mathcal{K} \subseteq \mathbb{R}^n$ and $\mathsf{a}_1, \ldots, \mathsf{a}_m \in \mathcal{K}^*$ and $\mathsf{c} \in \mathbb{R}^n$ and $b \in \mathbb{R}^m$, consider the following pair of dual problems:*

$$\begin{array}{lll} \min_{\mathsf{x}} & \langle \mathsf{c}, \mathsf{x} \rangle & \\ \text{s.t.} & \langle \mathsf{a}_i, \mathsf{x} \rangle = b_i & \textit{for } i \in [1\colon m] \\ & \mathsf{x} \in \mathcal{K}, & \end{array} \tag{13}$$

$$\begin{array}{ll} \max_{\mathsf{y}} & \mathsf{b}^\top \mathsf{y} \\ \text{s.t.} & \mathsf{c} - \sum_{i=1}^{m} \mathsf{a}_i y_i \in \mathcal{K}^*. \end{array} \tag{14}$$

Considering the solid convex cone $\mathcal{A} = \mathcal{K}^* + \operatorname{span}\{\mathsf{a}_i : i \in [1\colon m]\}$, we have:

1. *If $\mathsf{c} \in \operatorname{int} \mathcal{A}$: Then (14) is strictly feasible, i.e., there exists $\mathsf{y} \in \mathbb{R}^m$ such that $\mathsf{c} - \sum_{i=1}^{m} \mathsf{a}_i y_i \in \operatorname{int} \mathcal{K}^*$, and thus there is strong duality.*
2. *If $\mathsf{c} \notin \operatorname{cl} \mathcal{A}$: Then (14) is strongly infeasible, i.e., there exists $\mathsf{x} \in \mathcal{K}$ and $\varepsilon > 0$ such that $\left\langle \mathsf{c} - \sum_{i=1}^{m} \mathsf{a}_i y_i, \mathsf{x} \right\rangle \leq -\varepsilon$ for all $\mathsf{y} \in \mathbb{R}^m$. The primal problem (13) is either unbounded (in which case we have strong duality) or infeasible (in which case we have an infinite duality gap).*
3. *If $\mathsf{c} \in \operatorname{bd} \mathcal{A}$: Then (14) is either weakly feasible, i.e., it is feasible but does not have a strictly feasible point or weakly infeasible, i.e., it is infeasible but not strongly infeasible.*

Proof Before going into the main part of this proof, we will first consider some preliminary results that we will require.

We begin by noting that $\mathcal{A}^* = \{\mathsf{x} \in \mathcal{K} \colon \langle \mathsf{a}_i, \mathsf{x} \rangle = 0 \text{ for all } i \in [1\colon m]\}$.

In this proof we will consider the following optimization problem for a nonegative parameter u and a fixed $\mathsf{d} \in \operatorname{int} \mathcal{K}^*$:

$$\nu_u = \min_{\mathsf{x}} \left\{ \left\langle \mathsf{c} + u \sum_{i=1}^{m} \mathsf{a}_i, \mathsf{x} \right\rangle : \mathsf{x} \in \mathcal{K},\ \langle \mathsf{d}, \mathsf{x} \rangle = 1 \right\}.$$

This is a continuous minimization problem over a compact set. We let $\mathsf{x}_u \in \mathcal{K}$ be an optimal solution of ν_u and we let $\mathsf{x}_\infty \in \mathcal{K}$ be a limiting point as $u \to \infty$.

Moreover letting $\mathsf{x}^* \in \mathcal{K}$ be an optimal solution of $\min_{\mathsf{x}} \{\langle \mathsf{c}, \mathsf{x} \rangle : \mathsf{x} \in \mathcal{K},\ \langle \mathsf{d}, \mathsf{x} \rangle = 1\}$, we have

$$\nu_u \geq \left\langle \mathsf{c}, \mathsf{x}^* \right\rangle + u \sum_{i=1}^{m} \underbrace{\langle \mathsf{a}_i, \mathsf{x}_u \rangle}_{\geq 0}.$$

Therefore, if $\nu_u \leq 0$ for all u, then $\langle \mathsf{a}_i, \mathsf{x}_\infty \rangle = 0$ for all $i \in [1\colon m]$, and thus $\mathsf{x}_\infty \in \mathcal{A}^* \backslash \{\mathsf{o}\}$. Noting that $\sum_{i=1}^{m} \mathsf{a}_i \in \mathcal{K}^*$, we have that ν_u is monotonically increasing in u. Therefore if $\nu_u \leq 0$ for all u then $\nu_\infty = \lim_{u \to \infty} \nu_u$ is well defined and we have $\nu_\infty = \lim_{u \to \infty} \left\langle \mathsf{c} + u \sum_{i=1}^{m} \mathsf{a}_i, \mathsf{x}_u \right\rangle \geq \lim_{u \to \infty} \langle \mathsf{c}, \mathsf{x}_u \rangle = \langle \mathsf{c}, \mathsf{x}_\infty \rangle$.

We now prove each part of this lemma separately:

1. We will show that in this case, for u large enough, the matrix $\mathsf{c} + u \sum_{i=1}^{m} \mathsf{a}_i$ is in $\operatorname{int} \mathcal{K}$. Suppose for the sake of contradiction that this is not the case. Then $\nu_u \leq 0$ for all u. Therefore $\mathsf{x}_\infty \in \mathcal{A}^* \backslash \{\mathsf{o}\}$ and thus $0 < \langle \mathsf{c}, \mathsf{x}_\infty \rangle \leq \nu_\infty \leq 0$, which is a contradiction.
2. There exists $\varepsilon > 0$ and $\mathsf{z} \in \mathcal{A}^* \subseteq \mathcal{K}$ such that $\langle \mathsf{c}, \mathsf{z} \rangle = -\varepsilon$. For all $\mathsf{y} \in \mathbb{R}^m$ we then have

$$\left\langle \mathsf{c} - \sum_{i=1}^{m} \mathsf{a}_i y_i , \mathsf{z} \right\rangle = \langle \mathsf{c}, \mathsf{z} \rangle = -\varepsilon.$$

This proves strong infeasibility.

If the primal problem (13) has a feasible point x, then for all $\mu \geq 0$ the points $(\mathsf{x} + \mu \mathsf{z})$ are feasible, and considering $\mu \to \infty$, we get that the primal problem is unbounded.

3. We have $\langle \mathsf{c}, \mathsf{x} \rangle \geq 0$ for all $\mathsf{x} \in \mathcal{A}^*$ and there exists $\widehat{\mathsf{x}} \in \mathcal{A}^* \setminus \{\mathsf{o}\}$ such that $\langle \mathsf{c}, \widehat{\mathsf{x}} \rangle = 0$. For all $\mathsf{y} \in \mathbb{R}^m$ we have

$$\left\langle \mathsf{c} - \sum_{i=1}^{m} \mathsf{a}_i y_i , \widehat{\mathsf{x}} \right\rangle = \langle \mathsf{c}, \widehat{\mathsf{x}} \rangle = 0.$$

Therefore there is no strictly feasible point.
Now suppose for the sake of contradiction that (14) is strongly infeasible. Then there exists $\varepsilon > 0$ such that $\nu_u \leq -\varepsilon$ for all u. This implies that $\mathsf{x}_\infty \in \mathcal{A}^*$ and thus $0 \leq \langle \mathsf{c}, \mathsf{x}_\infty \rangle \leq -\varepsilon < 0$, which is a contradiction. □

This lemma can be trivially extended for problems which can be converted into the form given in the lemma through linear transformations on the a_i's. This occurs in the following theorem. In fact a more general condition, instead of $\mathsf{a}_1, \ldots, \mathsf{a}_m \in \mathcal{K}^*$, is that $\operatorname{span}\{\mathsf{a}_i : i \in [1:m]\} = \operatorname{span}(\mathcal{K}^* \cap \operatorname{span}\{\mathsf{a}_i : i \in [1:m]\})$, however the condition in the lemma is somewhat simpler to understand.

We are now ready to present the main results of this subsection. In order to do this we let $C \subseteq [1:n] \setminus B$ be the indices of unbounded variables in (P), we let $\widetilde{\mathsf{Q}}$ be the principal submatrix of Q corresponding to C, we let $\widetilde{\mathsf{a}}_i$ be the subvector of a_i corresponding to C and define the polyhedral cone

$$\mathcal{R} = \left\{ \mathsf{z} \in \mathbb{R}_+^{|C|} : \widetilde{\mathsf{a}}_i^\top \mathsf{z} = 0 \text{ for all } i \in [1:m] \right\}. \tag{15}$$

Theorem 1 *Let*

$$\mathcal{COP}_{\mathcal{R}} = \left\{ \mathsf{Y} \in \mathcal{S}^{|C|} : \mathsf{z}^\top \mathsf{Y} \mathsf{z} \geq 0 \textit{ for all } \mathsf{z} \in \mathcal{R} \right\}$$

denote the set of all $\mathcal{R}$-copositive matrices. This is a closed convex solid cone. For all $k \in [1:2]$, $l \in [1:4]$, considering the dual problem to $\min\{\langle \mathsf{Q}, \mathsf{X} \rangle + 2\mathsf{c}^\top \mathsf{x} : (1, \mathsf{x}, \mathsf{X}) \in \mathcal{B}_k \cap \mathcal{CP} \cap \mathcal{L}_l\}$ *we have:*

1. *If $C = \emptyset$ or $\widetilde{\mathsf{Q}} \in \operatorname{int} \mathcal{COP}_{\mathcal{R}}$, then the dual problem has a strictly feasible point, and thus there is strong duality.*
2. *If $\widetilde{\mathsf{Q}} \notin \mathcal{COP}_{\mathcal{R}}$, then the dual problem is strongly infeasible. The primal problem is either unbounded (in which case we have strong duality) or infeasible (in which case we have an infinite duality gap).*

3. *If* $\widetilde{\mathsf{Q}} \in \operatorname{bd}\mathcal{COP}_{\mathcal{R}}$*, then the dual problem is either weakly infeasible or weakly feasible.*

Proof We will consider the proof for $k = 2$, $l = 4$. The proof for the other cases follows likewise.

The primal problem is equivalent to the following:

$$\begin{aligned}
\min_{\mathsf{x}} \quad & \left\langle \begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix}, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle \\
\text{s.t.} \quad & \left\langle \begin{pmatrix} 1 & \mathsf{o}^\top \\ \mathsf{o} & \mathsf{O} \end{pmatrix}, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = 1, \\
& \left\langle \sum_{i=1}^m \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix} \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix}^\top, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = 0 \\
& \left\langle \sum_{j\in B} \begin{pmatrix} 1 & -\mathsf{e}_i^\top \\ -\mathsf{e}_i & 2\mathsf{e}_j\mathsf{e}_j^\top \end{pmatrix}, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = |B| \\
& \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{CP}^{n+1}.
\end{aligned}$$

This problem can thus be seen to abide by the requirements of Lemma 1. Using the notation from this lemma, we then have

$$\begin{aligned}
\mathcal{A}^* &= \left\{ \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{CP}^{n+1} \colon \begin{array}{c} \left\langle \begin{pmatrix} 1 & \mathsf{o}^\top \\ \mathsf{o} & \mathsf{O} \end{pmatrix}, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = 0 \\ \left\langle \sum_{i=1}^m \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix} \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix}^\top, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = 0 \\ \left\langle \sum_{j\in B} \begin{pmatrix} 1 & -\mathsf{e}_i^\top \\ -\mathsf{e}_i & 2\mathsf{e}_j\mathsf{e}_j^\top \end{pmatrix}, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = 0 \end{array} \right\} \\
&= \operatorname{conv}\left\{ \begin{pmatrix} 0 \\ \mathsf{x} \end{pmatrix} \begin{pmatrix} 0 \\ \mathsf{x} \end{pmatrix}^\top : \mathsf{x} \in \mathbb{R}^n_+, \quad x_j = 0 \text{ for } j \in B, \quad \mathsf{a}_i^\top \mathsf{x} = 0 \text{ for } i \in [1\colon m] \right\}
\end{aligned}$$

We thus have that

$$\begin{aligned}
& \begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} \in \operatorname{cl}\mathcal{A} \\
\Leftrightarrow & \begin{pmatrix} 0 \\ \mathsf{x} \end{pmatrix}^\top \begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} \begin{pmatrix} 0 \\ \mathsf{x} \end{pmatrix} \geq 0 \text{ for all } \mathsf{x} \in \mathbb{R}^n_+ \qquad x_j = 0 \text{ for } j \in B, \quad \mathsf{a}_i^\top \mathsf{x} = 0 \text{ for } i \in [1\colon m] \\
\Leftrightarrow & \widetilde{\mathsf{Q}} \in \mathcal{COP}_{\mathcal{R}}.
\end{aligned}$$

Similarly for $\begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} \in \operatorname{int}\mathcal{A}$ and $\begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} \in \operatorname{bd}\mathcal{A}$. $\square$

Remark 1 Consider the case when $B = \emptyset$ and the optimal solution to problem (P) is attained. We consider the completely positive formulation $\min\{\langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} \colon (1, \mathsf{x}, \mathsf{X}) \in \mathcal{CP} \cap \mathcal{L}_4\}$ and its dual

$$\begin{aligned} \max_{u,v} \quad & u \\ \text{s.t.} \quad & \begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} - u \begin{pmatrix} 1 & \mathsf{o}^\top \\ \mathsf{o} & \mathsf{O} \end{pmatrix} - v \sum_{i=1}^m \begin{pmatrix} -b_i \\ \mathsf{a}_i \end{pmatrix} \begin{pmatrix} -b_i \\ \mathsf{a}_i \end{pmatrix}^\top \in \mathcal{COP}^{n+1}. \end{aligned}$$

Let $\widehat{\mathsf{x}}$ be an optimal solution of (P) with corresponding optimal value κ. Further suppose that $\widehat{\mathsf{x}}$ is not a first order local minimizer of $f(\mathsf{x}) = \mathsf{x}^\top \mathsf{Q}\mathsf{x} + 2\mathsf{c}^\top \mathsf{x}$ over $\mathbb{R}^n_+$, i.e. the linear constraints play a significant role at the optimal solution. This assumption is equivalent to the existence of a $\mathsf{y} \in \mathbb{R}^n$ such that $\widehat{\mathsf{x}} + \mathsf{y} \in \mathbb{R}^n_+$ and $(\mathsf{Q}\widehat{\mathsf{x}} + \mathsf{c})^\top \mathsf{y} < 0$. For all feasible (u, v) of the dual problem and all $\varepsilon \in (0, 1]$ we have

$$\begin{aligned} 0 &\le \begin{pmatrix} 1 \\ \widehat{\mathsf{x}} + \varepsilon \mathsf{y} \end{pmatrix}^\top \left[\begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} - u \begin{pmatrix} 1 & \mathsf{o}^\top \\ \mathsf{o} & \mathsf{O} \end{pmatrix} - v \sum_{i=1}^m \begin{pmatrix} -b_i \\ \mathsf{a}_i \end{pmatrix} \begin{pmatrix} -b_i \\ \mathsf{a}_i \end{pmatrix}^\top \right] \begin{pmatrix} 1 \\ \widehat{\mathsf{x}} + \varepsilon \mathsf{y} \end{pmatrix} \\ &= \kappa - u + 2\varepsilon \underbrace{(\mathsf{Q}\widehat{\mathsf{x}} + \mathsf{c})^\top \mathsf{y}}_{<0} + \varepsilon^2 \mathsf{y}^\top \left(\mathsf{Q} - v \sum_{i=1}^m \mathsf{a}_i \mathsf{a}_i^\top \right) \mathsf{y}. \end{aligned}$$

Considering ε small enough, we thus have $u < \kappa$. Therefore, if in such a case there is no duality gap then the optimal solution set of the dual problem is empty. The difficulty is that the linear constraints appear in a concise way in the problem, rather than being used to reduce the size of the problem.

Theorem 2 *Let*

$$\mathcal{Q} = \mathcal{N}^{|C|} + \mathcal{S}_+^{|C|} + \operatorname{span}\left\{ \mathsf{e}_j \widetilde{\mathsf{a}}_i^\top + \widetilde{\mathsf{a}}_i \mathsf{e}_j^\top : i \in [1\colon m],\ j \in [1\colon |C|] \right\}. \tag{16}$$

This is a convex solid cone, although it is an open question whether it is closed. For all $k \in [1\colon 2]$, $l \in [1\colon 4]$, *considering the dual problem to* $\min\{\langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} \colon (1, \mathsf{x}, \mathsf{X}) \in \mathcal{B}_k \cap \mathcal{N} \cap \mathcal{L}_l\}$ *we have:*

1. *If* $C = \emptyset$ *or* $\widetilde{\mathsf{Q}} \in \operatorname{int} \mathcal{Q}$, *then the dual problem has a strictly feasible point, and thus there is strong duality.*
2. *If* $\widetilde{\mathsf{Q}} \notin \operatorname{cl} \mathcal{Q}$, *then the dual problem is strongly infeasible. The primal problem is either unbounded (in which case we have strong duality) or infeasible (in which case we have an infinite duality gap).*
3. *If* $\widetilde{\mathsf{Q}} \in \operatorname{bd} \mathcal{Q}$, *then the dual problem is either weakly infeasible or weakly feasible.*

Proof This can be proven by reworking the proof from Theorem 1, however this time we have

$$
\mathcal{A}^* = \left\{ \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1} \colon \begin{array}{r} \left\langle \begin{pmatrix} 1 & \mathsf{o}^\top \\ \mathsf{o} & \mathsf{O} \end{pmatrix}, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = 0 \\ \left\langle \sum_{i=1}^m \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix} \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix}^\top, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = 0 \\ \left\langle \sum_{j \in B} \begin{pmatrix} 1 & -\mathsf{e}_i^\top \\ -\mathsf{e}_i & 2\mathsf{e}_j \mathsf{e}_j^\top \end{pmatrix}, \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle = 0 \end{array} \right\}
$$

$$
= \left\{ \begin{pmatrix} 0 & \mathsf{o}^\top \\ \mathsf{o} & \mathsf{X} \end{pmatrix} \in \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1} \colon \begin{array}{l} \mathsf{X}\mathsf{a}_i = \mathsf{o} \text{ for all } i \in [1\colon m] \\ X_{jj} = 0 \text{ for all} \end{array} \right\}
$$

We note that as the variables in $[1\colon n] \backslash C$ are bounded below, we have the following, where the equality comes from the fact that the first optimization problem has a feasible point x_0:

$$
\begin{aligned}
\infty > \max_{\mathsf{x}} & \left\{ \left\langle \sum_{i \notin C} \mathsf{e}_i, \mathsf{x} \right\rangle : \mathsf{x} \in \mathbb{R}_+^n, \quad \mathsf{a}_i^\top \mathsf{x} = b_i \text{ for all } i \in [1\colon m] \right\} \\
= \min_{\mathsf{y}} & \left\{ \mathsf{y}^\top \mathsf{b} \colon \sum_{i=1}^m y_i \mathsf{a}_i - \sum_{i \notin C} \mathsf{e}_i \in \mathbb{R}_+^n \right\}
\end{aligned}
$$

Therefore there exists $\mathsf{z} \in \operatorname{span}\{\mathsf{a}_i \colon i \in [1\colon m]\} \cap \mathbb{R}_+^n$ such that $z_i > 0$ for all $i \notin C$, and thus we have that

$$
\begin{aligned}
\mathsf{X} \in \mathcal{S}_+^n \cap \mathcal{N}^n, \quad \mathsf{X}\mathsf{a}_i = \mathsf{o} \text{ for all } i \in [1\colon m] \quad & \Rightarrow \quad \mathsf{X} \in \mathcal{S}_+^n \cap \mathcal{N}^n, \quad \mathsf{X}\mathsf{z} = \mathsf{o} \\
& \Rightarrow \quad X_{ij} = 0 \text{ for all } i \in [1\colon n], \;\; j \notin C.
\end{aligned}
$$

Therefore

$$
\begin{aligned}
& \begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} \in \operatorname{cl} \mathcal{A} \\
\Leftrightarrow & \left\langle \begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix}, \begin{pmatrix} 0 & \mathsf{o}^\top \\ \mathsf{o} & \mathsf{X} \end{pmatrix} \right\rangle \geq 0 \quad \text{for all } \mathsf{X} \in \mathcal{S}_+^n \cap \mathcal{N}^n : \quad \begin{array}{l} X_{ij} = 0 \text{ for } i \in [1\colon n], \;\; j \notin C, \\ \mathsf{X}\mathsf{a}_i = \mathsf{o} \text{ for } i \in [1\colon m] \end{array} \\
\Leftrightarrow & \ \widetilde{\mathsf{Q}} \in \mathcal{Q}.
\end{aligned}
$$

Similarly for $\begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} \in \operatorname{int} \mathcal{A}$ and $\begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} \in \operatorname{bd} \mathcal{A}$. □

Lemma 2 *Letting* $\widetilde{\mathsf{B}} = [\widetilde{\mathsf{a}}_{m+1} \ \ldots \ \widetilde{\mathsf{a}}_n]$ *and using the notation from the previous two theorems, we have*

$$
\begin{aligned}
\mathcal{COP}_{\mathcal{R}} &= \mathrm{cl}\left(\mathcal{COP}^{|C|} + \mathrm{span}\{\widetilde{\mathsf{a}}_i\widetilde{\mathsf{a}}_i^\top : i\in[1\colon m]\}\right)\\
&= \mathrm{cl}\left(\mathcal{COP}^{|C|} + \mathrm{span}\{\widetilde{\mathsf{a}}_i\mathsf{e}_j^\top + \mathsf{e}_j\widetilde{\mathsf{a}}_i^\top : i\in[1\colon m],\ \ j\in[1\colon |C|]\}\right),\\
\mathrm{cl}\,\mathcal{Q} &= \mathrm{cl}\left(\mathcal{N}^{|C|} + \mathcal{S}_+^{|C|} + \mathrm{span}\{\widetilde{\mathsf{a}}_i\widetilde{\mathsf{a}}_i^\top : i\in[1\colon m]\}\right)\\
&= \mathrm{cl}\left(\mathcal{N}^{|C|} + \left\{\mathsf{Y}\in\mathcal{S}^{|C|} \colon \widetilde{\mathsf{B}}^\top\mathsf{Y}\widetilde{\mathsf{B}}\in\mathcal{S}_+^{n-m}\right\}\right)\\
\mathcal{S}_+^{|C|} + \mathcal{N}^{|C|} &\subseteq \mathcal{Q}\subseteq\mathcal{COP}_{\mathcal{R}},\\
\mathcal{COP}^{|C|} &\subseteq \mathcal{COP}_{\mathcal{R}}.
\end{aligned}
$$

Proof The techniques from Bomze et al. (2017, Theorem 1), along with basic results on dual cones, give us the following, from which we get the results in this lemma:

$$
\begin{aligned}
(\mathcal{COP}_{\mathcal{R}})^* &= \mathrm{conv}\left\{\mathsf{z}\mathsf{z}^\top \colon \mathsf{z}\in\mathbb{R}_+^n,\ \widetilde{\mathsf{a}}_i^\top\mathsf{z} = 0 \text{ for } i\in[1\colon m]\right\}\\
&= \left\{\mathsf{Z}\in\mathcal{CP}^{|C|}\colon \left\langle \mathsf{Z}, \widetilde{\mathsf{a}}_i\widetilde{\mathsf{a}}_i^\top\right\rangle = 0 \text{ for } i\in[1\colon m]\right\}\\
&= \left\{\mathsf{Z}\in\mathcal{CP}^{|C|}\colon \mathsf{Z}\widetilde{\mathsf{a}}_i = \mathsf{o} \text{ for } i\in[1\colon m]\right\} \quad \text{and}\\
\mathcal{Q}^* &= \mathcal{N}^{|C|}\cap\left\{\mathsf{Z}\in\mathcal{S}_+^{|C|}\colon \mathsf{Z}\widetilde{\mathsf{a}}_i = \mathsf{o} \text{ for } i\in[1\colon m]\right\}\\
&= \mathcal{N}^{|C|}\cap\left\{\mathsf{Z}\in\mathcal{S}_+^{|C|}\colon \left\langle \mathsf{Z}, \widetilde{\mathsf{a}}_i\widetilde{\mathsf{a}}_i^\top\right\rangle = 0 \text{ for } i\in[1\colon m]\right\}\\
&= \mathcal{N}^{|C|}\cap\left\{\mathsf{Z}\in\mathcal{S}^{|C|}\colon \exists\mathsf{W}\in\mathcal{S}_+^{n-m} \text{ s.t. } \widetilde{\mathsf{B}}\mathsf{W}\widetilde{\mathsf{B}}^\top = \mathsf{Z}\right\}.
\end{aligned}
$$

□

In the next section, we present our penalization method.

2 Penalizing constraints

We recall from Bomze et al. (2017, (25), (26)) that the dual of the CPP reformulation and its DNN relaxation can be written as

$$
\begin{aligned}
\max\nolimits_y \quad & y\\
\text{s.t.} \quad & \begin{pmatrix} -y & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q}\end{pmatrix} \in \mathcal{B}_k^\perp + \mathcal{L}_l^\perp + \mathcal{COP}^{n+1},
\end{aligned}
\tag{17}
$$

and

$$
\begin{aligned}
\max\nolimits_y \quad & y\\
\text{s.t.} \quad & \begin{pmatrix} -y & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q}\end{pmatrix} \in \mathcal{B}_k^\perp + \mathcal{L}_l^\perp + \mathcal{S}_+^{n+1} + \mathcal{N}^{n+1},
\end{aligned}
\tag{18}
$$

where $k\in[1:2]$, $l\in[1:4]$, and

$$\mathcal{L}_1^\perp = \left\{\begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \in \mathcal{S}^{n+1} : \mathsf{B}^T \begin{pmatrix} x_0 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \mathsf{B} = \mathsf{O}\right\},$$

$$\mathcal{L}_2^\perp = \operatorname{span}\left\{\begin{pmatrix} 2b_i & -\mathsf{a}_i^\top \\ -\mathsf{a}_i & \mathsf{O}\end{pmatrix} : i\in[1:m]\right\} + \operatorname{span}\left\{\begin{pmatrix} 0 & -b_i\mathsf{e}_j^\top \\ -b_i\mathsf{e}_j & \mathsf{a}_i\mathsf{e}_j^\top + \mathsf{e}_j\mathsf{a}_i^\top\end{pmatrix} : i\in[1:m],\ j\in[1:n]\right\},$$

$$\mathcal{L}_3^\perp = \operatorname{span}\left\{\begin{pmatrix} 2b_i & -\mathsf{a}_i^\top \\ -\mathsf{a}_i & \mathsf{O}\end{pmatrix} : i\in[1:m]\right\} + \operatorname{span}\left\{\begin{pmatrix} b_i^2 & \mathsf{o}^\top \\ \mathsf{o} & -\mathsf{a}_i\mathsf{a}_i^\top\end{pmatrix} : i\in[1:m]\right\},$$

$$\mathcal{L}_4^\perp = \operatorname{span}\left\{\sum_{i=1}^m \begin{pmatrix} b_i^2 & -b_i\mathsf{a}_i^\top \\ -b_i\mathsf{a}_i & \mathsf{a}_i\mathsf{a}_i^\top\end{pmatrix}\right\},$$

$$\mathcal{B}_1^\perp = \operatorname{span}\left\{\begin{pmatrix} 0 & -\mathsf{e}_j^\top \\ -\mathsf{e}_j & 2\mathsf{e}_j\mathsf{e}_j^\top\end{pmatrix} : j\in\mathcal{B}\right\}, \quad \text{and} \quad \mathcal{B}_2^\perp = \operatorname{span}\left\{\sum_{j\in\mathcal{B}} \begin{pmatrix} 0 & -\mathsf{e}_j^\top \\ -\mathsf{e}_j & 2\mathsf{e}_j\mathsf{e}_j^\top\end{pmatrix}\right\}.$$

The proof of Bomze et al. (2017, Proposition 1) uses the following facts: first $\sum_{i=1}^m \left(\mathsf{a}_i^\top \mathsf{X}\mathsf{a}_i - 2b_i\,\mathsf{a}_i^\top\mathsf{x} + b_i^2\right) \geq 0$ for any $\begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \in \mathcal{S}_+^{n+1}$. And second, if $\begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \in \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}$ such that $\sum_{i=1}^m \left(\mathsf{a}_i^\top \mathsf{X}\mathsf{a}_i - 2b_i\,\mathsf{a}_i^\top\mathsf{x} + b_i^2\right) = 0$, then $\sum_{j\in B}(x_j - X_{jj}) \geq 0$, see Bomze et al. (2017, Lemma 2). This suggests that we can move either one of these constraints into the objective function with a penalty. We investigate such penalization methods in this section.

2.1 Penalizing linear constraints

For $\lambda \geq 0$ we consider the following penalized problem and its dual

$$\begin{aligned} L(\lambda) = \min\ & \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top\mathsf{x} + \lambda\sum_{i=1}^m \left(\mathsf{a}_i^\top \mathsf{X}\mathsf{a}_i - 2b_i\,\mathsf{a}_i^\top\mathsf{x} + b_i^2\right) \\ \text{s.t.}\ & \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix} \in \mathcal{CP}^{n+1} \cap \mathcal{B}_2, \end{aligned} \tag{CPP(λ)}$$

$$\begin{aligned} L^*(\lambda) = \max\ & y \\ \text{s.t.}\ & \begin{pmatrix} -y + \lambda\sum_{i=1}^m b_i^2 & \mathsf{c}^\top - \lambda\sum_{i=1}^m b_i\mathsf{a}_i^\top \\ \mathsf{c} - \lambda\sum_{i=1}^m b_i\mathsf{a}_i & \mathsf{Q} + \lambda\sum_{i=1}^m \mathsf{a}_i\mathsf{a}_i^\top\end{pmatrix} \in \mathcal{COP}^{n+1} + \mathcal{B}_2^\perp, \end{aligned} \tag{CPP*(λ)}$$

We now present the following theorem connecting (CPP(λ))–(CPP), where we use the notation from Theorem 1.

Theorem 3 *We have the following results on problem* (CPP(λ)):

1. *We have that* $L(\lambda)$ *is a monotonically increasing function in* λ *and* $L(\lambda) \leq \mathrm{opt}\,$(CPP) *for all* λ.
2. (CPP(λ)) *has a strictly feasible point and thus* $L(\lambda) = L^*(\lambda)$ *for all* λ.
3. $\lim_{\lambda\to\infty} L^*(\lambda)$ *is equal to the optimal value of the dual problem* (17) *to the primal problem* (9) *with* $k = 2$, $l = 4$.
4. *If* $\mathcal{Z}$ *is bounded or* $\widetilde{\mathsf{Q}} \in \mathrm{int}\,\mathcal{COP}_{\mathcal{R}}$ *then* $\lim_{\lambda\to\infty} L(\lambda) = \mathrm{opt}\,$(CPP) *and there exists* $\Lambda \in \mathbb{R}$ *such that*

   (a) *For* $\lambda \geq \Lambda$ *problem* (CPP*(λ)) *is strictly feasible.*
   (b) *For* $\lambda \geq \Lambda$ *the optimal solutions to the primal and dual problems are attained.*
   (c) *Suppose that* $(\mathsf{x}_\lambda, \mathsf{X}_\lambda)$ *is an optimal solution to* (CPP(λ)). *If* (CPP) *is feasible then there is a compact set* $Y \subseteq \mathbb{R}^n \times \mathcal{S}^n$ *such that for all* $\lambda \geq \Lambda$ *we have* $(\mathsf{x}_\lambda, \mathsf{X}_\lambda) \in Y$ *and every limit point of* $(\mathsf{x}_\lambda, \mathsf{X}_\lambda)$ *as* $\lambda \to \infty$ *is an optimal solution to* (CPP).

5. *If* $\mathcal{Z}$ *is unbounded and* $\widetilde{\mathsf{Q}} \notin \mathcal{COP}_{\mathcal{R}}$, *then problem* (CPP*($\lambda$)) *is strongly infeasible for all* λ *and* $L(\lambda) = L^*(\lambda) = -\infty$ *for all* λ. *We then have* $L(\lambda) = \mathrm{opt}\,$(CPP) *if and only if* (CPP) *is feasible.*

Proof We will prove each part in turn:

1. This is immediate, as (CPP(λ))-feasibility implies $\sum_{i=1}^m \left(\mathsf{a}_i^\top \mathsf{X} \mathsf{a}_i - 2b_i\, \mathsf{a}_i^\top \mathsf{x} + b_i^2\right) \geq 0$ and (CPP)-feasibility implies $\sum_{i=1}^m \left(\mathsf{a}_i^\top \mathsf{X} \mathsf{a}_i - 2b_i\, \mathsf{a}_i^\top \mathsf{x} + b_i^2\right) = 0$.
2. From the results in Dickinson (2010) we see that

$$\frac{1}{n+1}\begin{pmatrix} n+1 & 2\mathsf{e}^\top \\ 2\mathsf{e} & \mathsf{e}\mathsf{e}^\top + \mathsf{I}\end{pmatrix} = \frac{1}{n+1}\begin{pmatrix}1\\ \mathsf{e}\end{pmatrix}\begin{pmatrix}1\\ \mathsf{e}\end{pmatrix}^\top + \frac{1}{n+1}\sum_{i=1}^n \begin{pmatrix}1\\ \mathsf{e}_i\end{pmatrix}\begin{pmatrix}1\\ \mathsf{e}_i\end{pmatrix}^\top \in \mathrm{int}\,\mathcal{CP}^{n+1},$$

   Therefore $\mathsf{x} = \frac{2}{n+1}\mathsf{e}$, $\mathsf{X} = \frac{1}{n+1}(\mathsf{e}\mathsf{e}^\top + \mathsf{I})$ is a strictly feasible point of (CPP(λ)).
3. It is trivial to see that if a point is infeasible for (17) with $k = 2$, $l = 4$, then it is infeasible in (CPP*(λ)) for all λ. Alternatively if in (17) with $k = 2$, $l = 4$ we have a feasible point then for λ large enough this point is also feasible in (CPP*(λ)).
4. From Theorem 1 we have that in this case the optimal value of (17) is equal to opt (CPP).

4a. From considering Theorem 1 with $B = \emptyset$, we see that there exist $\Lambda, \omega \in \mathbb{R}$ such that

$$\mathsf{Y}_\lambda = \begin{pmatrix}\omega & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q}\end{pmatrix} + \lambda \sum_{i=1}^m \begin{pmatrix} b_i \\ -\mathsf{a}_i\end{pmatrix}\begin{pmatrix} b_i \\ -\mathsf{a}_i\end{pmatrix}^\top \in \mathrm{int}\,\mathcal{COP}^{n+1} \qquad \text{for all } \lambda \geq \Lambda.$$

This provides a strictly feasible point to problem (CPP*(λ)).

4b. This follows from the fact that both the primal and dual problems have strictly feasible points.

4c. If we can prove the compactness of the optimal solutions then the rest will follow from Bazaraa and Shetty (1979, Thm.9.2.2).
Recall from Theorem 1 that in the case we are considering, problem (17) has a strictly feasible point. As we assume (CPP) is feasible, this implies that problem (9) is feasible, and thus has a finite optimal value. Let ν equal this optimal value and let (x, X) be an arbitrary optimal solution of (CPP(λ)) for an arbitrary $\lambda \geq \Lambda$. We have

$$\nu + \omega \geq \langle \mathsf{Q}, \mathsf{X} \rangle + 2\mathsf{c}^\top \mathsf{x} + \lambda \sum_{i=1}^{m} \left(\mathsf{a}_i^\top \mathsf{X} \mathsf{a}_i - 2b_i \, \mathsf{a}_i^\top \mathsf{x} + b_i^2 \right) + \omega \geq \left\langle \mathsf{Y}_\Lambda, \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \right\rangle.$$

As $\mathsf{Y}_\Lambda \in \operatorname{int} \mathcal{COP}^{n+1}$ is fixed, this restricts $\begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix}$ to lie in a compact set.

5. From Theorem 1 we have that in this case problem (17) is strongly infeasible, and it is trivial to see that this implies that problem ($\mathrm{CPP}^*(\lambda)$) is also strongly infeasible. As the primal problem (CPP(λ)) is feasible, this implies that $L(\lambda) = -\infty$. □

These arguments hold likewise for the doubly nonnegative approximations with "$\mathcal{COP}_\mathcal{R}$" replaced by "$\mathcal{Q}$", using the last results in Sect. 1.4.

2.2 Penalizing binary constraints

The basic idea of this subsection is that the linear constraints can be considered as 'helpful' as they reduce the size of the problem. Instead it is the binary constraints which are the unpleasant constraints.

For $\lambda \geq 0$, we consider the following penalized problem and its dual

$$\begin{aligned} K(\lambda) = \min \ & \langle \mathsf{Q}, \mathsf{X} \rangle + 2\mathsf{c}^\top \mathsf{x} + 2\lambda \sum_{j \in B} (x_j - X_{jj}) \\ \text{s.t.} \ & \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{CP}^{n+1} \cap \mathcal{L}_1, \end{aligned} \tag{19}$$

$$\begin{aligned} K^*(\lambda) = \max \ & y \\ \text{s.t.} \ & \begin{pmatrix} -y & \mathsf{c}^\top + \lambda \sum_{j \in B} \mathsf{e}_j^\top \\ \mathsf{c} + \lambda \sum_{j \in B} \mathsf{e}_j & \mathsf{Q} - 2\lambda \sum_{j \in B} \mathsf{e}_j \mathsf{e}_j^\top \end{pmatrix} \in \mathcal{COP}^{n+1} + \mathcal{L}_1^\perp. \end{aligned} \tag{20}$$

Theorem 4 *We have the following results on problem* (19):

1. *We have that $K(\lambda)$ is a monotonically increasing function in λ and $K(\lambda) \leq$* opt (CPP) *for all λ.*
2. *Problem* (19) *has a feasible point, however there is no strictly feasible point when $m \neq 0$.*
3. *We have that* $\lim_{\lambda \to \infty} K^*(\lambda)$ *is equal to the optimal value of* (17) *for $k = 2, l = 1$.*
4. *If $\mathcal{Z}$ is bounded or $\mathsf{Q} \in \operatorname{int} \mathcal{COP}_\mathcal{R}$ then:*

(a) *We have* $\lim_{\lambda\to\infty} K(\lambda) = \mathrm{opt}\,(\text{CPP})$.
(b) *Problem* (20) *is strictly feasible for all* $\lambda \geq 0$.
(c) *We have* $K(\lambda) = K^*(\lambda)$ *and the optimal solution of problem* (19) *is attained.*
(d) *Suppose that* $(\mathsf{x}_\lambda, \mathsf{X}_\lambda)$ *is an optimal solution to* (19). *If* (CPP) *is feasible then there is a compact set* $Y \subseteq \mathbb{R}^n \times \mathcal{S}^n$ *such that for all* $\lambda \geq 0$ *we have* $(\mathsf{x}_\lambda, \mathsf{X}_\lambda) \in Y$, *and every limit point of* $(\mathsf{x}_\lambda, \mathsf{X}_\lambda)$ *as* $\lambda \to \infty$ *is an optimal solution to* (CPP).

5. *If* $\mathcal{Z}$ *is unbounded and* $\widetilde{\mathsf{Q}} \notin \mathcal{COP}_{\mathcal{R}}$, *then problem* (20) *is strongly infeasible for all* λ *and* $K(\lambda) = -\infty$ *for all* λ. *We then have* $K(\lambda) = \mathrm{opt}\,(\text{CPP})$ *if and only if* (P) ([or (CPP)]) *is feasible.*

Proof Multiple parts of this proof rely on the observation from the proof of Bomze et al. (2017, Lemma 4) that there exists $\mathsf{u} \in \mathbb{R}^n_+$ and $\mathsf{U} \in \mathcal{N}^n$ and $\theta_{ij} \in \mathbb{R}$ for $i \in [1{:}m]$, $j \in [1{:}n]$ such that

$$\sum_{j\in\mathcal{B}} \begin{pmatrix} 0 & -\mathsf{e}_j^\top \\ -\mathsf{e}_j & 2\mathsf{e}_j\mathsf{e}_j^\top \end{pmatrix} = \begin{pmatrix} 0 & \mathsf{u}^\top \\ \mathsf{u} & \mathsf{U} \end{pmatrix} + \sum_{i=1}^m \sum_{j=1}^n \theta_{ij} \begin{pmatrix} 0 & -b_i\mathsf{e}_j^\top \\ -b_i\mathsf{e}_j & \mathsf{a}_i\mathsf{e}_j^\top + \mathsf{e}_j\mathsf{a}_i^\top \end{pmatrix}$$
$$\in \mathcal{N} + \mathcal{L}_2^\perp \subseteq \mathcal{CP}^* + \mathcal{L}_1^\perp.$$

This means that if at a feasible point of (20) we increase λ then the feasible set of (20) will remain feasible [and similarly for (17) with $k = 2, l = 1$].

We will now prove each part in turn (although not in order):

1. This is trivial to see.
2. For x_0 as given in Sect. 1.3, we have that $\mathsf{x} = \mathsf{x}_0$, $\mathsf{X} = \mathsf{x}_0\mathsf{x}_0^\top$ is a feasible point of (19). However, from the discussion in Bomze et al. (2017, Section 2.3), we see that (19) does not have a strictly feasible point when $m \neq 0$.
3. It is trivial to see that if a point is infeasible for (17) with $k = 2, l = 1$, then it is infeasible in (20) for all λ. Alternatively if in (17) for $k = 2, l = 1$ we have a feasible point then for λ large enough this point is also feasible in (20).

4b. As in the proof of Theorem 3 part 4a, there exist $\Lambda, \omega \in \mathbb{R}$ such that

$$\mathsf{Y}_\Lambda = \begin{pmatrix} \omega & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} + \Lambda \sum_{i=1}^m \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix} \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix}^\top \in \operatorname{int} \mathcal{COP}^{n+1}.$$

Therefore, for all $\lambda \geq 0$ we have

$$\begin{pmatrix} \omega & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q} \end{pmatrix} + \lambda \begin{pmatrix} 0 & \mathsf{e}_j^\top \\ \mathsf{e}_j & -2\mathsf{e}_j\mathsf{e}_j^\top \end{pmatrix} + \Lambda \sum_{i=1}^m \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix} \begin{pmatrix} b_i \\ -\mathsf{a}_i \end{pmatrix}^\top$$
$$- \lambda \sum_{i=1}^m \sum_{j\in B} \theta_{ij} \begin{pmatrix} 0 & -b_i\mathsf{e}_j^\top \\ -b_i\mathsf{e}_j & \mathsf{a}_i\mathsf{e}_j^\top + \mathsf{e}_j\mathsf{a}_i^\top \end{pmatrix}$$
$$= \mathsf{Y}_\Lambda + \lambda \begin{pmatrix} 0 & \mathsf{u}^\top \\ \mathsf{u} & \mathsf{U} \end{pmatrix} \in \operatorname{int} \mathcal{COP}^{n+1}.$$

This then gives us a strictly feasible point of (20).

4c. This follows from the fact that problem (20) is strictly feasible and problem (19) is feasible.

4a. From Theorem 1 we have that in this case the optimal value of (17) is equal to opt (CPP). The proof of this part is concluded by considering parts 3 and 4c.

4d. If we can prove the compactness of the optimal solutions then the rest will follow from Bazaraa and Shetty (1979, Thm.9.2.2).

Recall from Theorem 1 we have that in the case we are considering, problem (17) has a strictly feasible point. As we assume (CPP) is feasible, this implies that it has a finite optimal value. Let ν equal this optimal value and let (x, X) be an arbitrary optimal solution of (19) for an arbitrary $\lambda \geq 0$. We have

$$\begin{aligned}\nu + \omega &\geq \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} + 2\lambda \sum_{j\in B}(x_j - X_{jj}) + \omega \geq \langle \mathsf{Q}, \mathsf{X}\rangle + 2\mathsf{c}^\top \mathsf{x} + \omega \\ &= \left\langle \mathsf{Y}_\Lambda, \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix}\right\rangle.\end{aligned}$$

As $Y_\Lambda \in \operatorname{int} \mathcal{COP}^{n+1}$ is fixed, this restricts $\begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X}\end{pmatrix}$ to lie in a compact set.

5. From Theorem 1 we have that (17) is strongly infeasible, and it is trivial to see that this implies that problem (20) is also strongly infeasible. As the primal problem (19) is feasible, this implies that $K(\lambda) = -\infty$. □

The doubly nonnegative approximation for (19) is equivalent to:

$$\begin{array}{ll} \min_{\mathsf{Y}} & \left\langle \mathsf{Y}, \mathsf{B}^\top \left[\begin{pmatrix} 0 & \mathsf{c}^\top \\ \mathsf{c} & \mathsf{Q}\end{pmatrix} + \lambda \sum_{j\in B} \begin{pmatrix} 0 & \mathsf{e}_j^\top \\ \mathsf{e}_j & -2\mathsf{e}_j\mathsf{e}_j^\top\end{pmatrix}\right] \mathsf{B} \right\rangle \\ \text{s.t.} & \mathsf{Y} \in \mathcal{S}_+^{n+1-m} \\ & Y_{00} = 1 \\ & \mathsf{BYB}^\top \in \mathcal{N}^{n+1}. \end{array} \tag{21}$$

This is a positive semidefinite optimization problem with one linear equality constraint, $\frac{1}{2}n(n-1)$ linear inequality constraints and one positive semidefiniteness constraint of order $n+1-m$.

Similar as before, almost all of the results and proofs from Theorem 4, hold likewise for this approximation, replacing $\mathcal{COP}_{\mathcal{R}}$ with $\mathcal{Q}$. The only exception is statement of Theorem 4(2): recall that we assume that x_0 is strictly positive, so there exists $\varepsilon > 0$ such that $\mathsf{Y} = \mathsf{e}_0\mathsf{e}_0^\top + \varepsilon \sum_{i=1}^{n-m} \mathsf{e}_i\mathsf{e}_i^\top$ is a strictly feasible point of the approximation (21).

3 Purely binary quadratic problems

We recall the general form of a purely binary quadratic problem (i.e., $B = [1{:}n]$), which includes the notoriously hard multidimensional quadratic knapsack problem.

Observe that we can get rid of the linear term in the objective easily since $x_i^2 = x_i$ holds for all i. We consider a maximization problem with linear inequality constraints, and no continuous variables.

$$\begin{array}{ll} \max & \mathsf{x}^\top \mathsf{Qx} \\ \text{s.t.} & \widetilde{\mathsf{a}}_i^\top \mathsf{x} \le b_i \quad \text{for } i \in [1:m] \\ & \mathsf{x} \in \{0,1\}^n . \end{array} \tag{22}$$

Without loss of generality we shall assume that if $\mathsf{x} \in \mathbb{R}^n_+$ such that $\widetilde{\mathsf{a}}_i^\top \mathsf{x} \le b_i$ for all $i \in [1:m]$ then $x_j \le 1$ for all $j \in [1:n]$.

Theorem 5 *The purely binary quadratic problem* (22) *is equivalent to the copositive reformulation*

$$\begin{array}{ll} \max & \langle \mathsf{Q}, \mathsf{X} \rangle \\ \text{s.t.} & \sum\limits_{j=1}^n (X_{jj} - x_j) = 0 \\ & \mathsf{B} \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \mathsf{B}^\top = \begin{pmatrix} 1 & \mathsf{x}^\top & \mathsf{v}^\top \\ \mathsf{x} & \mathsf{X} & \mathsf{U}^\top \\ \mathsf{v} & \mathsf{U} & \mathsf{V} \end{pmatrix} \in \mathcal{CP}^{n+m+1} . \\ & \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}^{n+1} . \end{array} \tag{23}$$

where

$$\mathsf{A} = \left(\widetilde{\mathsf{a}}_1, \cdots, \widetilde{\mathsf{a}}_m \right) \in \mathbb{R}^{n \times m}, \quad \textit{and} \quad \mathsf{B} = \begin{pmatrix} 1 & \mathsf{o}^\top \\ \mathsf{o} & \mathsf{I}_n \\ \mathsf{b} & -\mathsf{A}^\top \end{pmatrix} \in \mathbb{R}^{(n+1+m)\times(n+1)} .$$

Problem (23) *can then be relaxed to the problem*

$$\begin{array}{ll} \max & \langle \mathsf{Q}, \mathsf{X} \rangle \\ \text{s.t.} & \sum\limits_{j=1}^n (X_{jj} - x_j) = 0 \\ & \mathsf{B} \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \mathsf{B}^\top = \begin{pmatrix} 1 & \mathsf{x}^\top & \mathsf{v}^\top \\ \mathsf{x} & \mathsf{X} & \mathsf{U}^\top \\ \mathsf{v} & \mathsf{U} & \mathsf{V} \end{pmatrix} \in \mathcal{N}^{n+m+1} \\ & \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}^{n+1}_+ . \end{array} \tag{24}$$

Proof By adding slack variables $v_i \ge 0$, problem (22) is equivalent to

$$\begin{array}{ll} \max & \mathsf{x}^\top \mathsf{Qx} \\ \text{s.t.} & \widetilde{\mathsf{a}}_i^\top \mathsf{x} + v_i = b_i \quad \text{for } i \in [1:m] \\ & \mathsf{x} \in \{0,1\}^n \\ & \mathsf{v} \in \mathbb{R}^m_+ . \end{array} \tag{25}$$

The key assumption (1) then holds for this problem. Now it is easy to see that problem (22) has the same optimal value as (23), and (24) is clearly its straightforward DNN relaxation. □

The relaxation-linearization technique (RLT) (Burer 2015; Sherali and Adams 1990) is a very popular approach to solve hard problems. The next result shows that our approach is closely connected:

Theorem 6 *Problem (22) is equivalent to*

$$\begin{array}{ll} \max & \langle \mathsf{Q}, \mathsf{x}\mathsf{x}^\top \rangle \\ \text{s.t.} & \widetilde{\mathsf{a}}_i^\top \mathsf{x} \le b_i \quad \textit{for } i \in [1\colon m] \\ & \widetilde{\mathsf{a}}_i^\top \mathsf{x}\mathsf{x}^\top \le b_i \mathsf{x}^\top \quad \textit{for } i \in [1\colon m] \\ & b_i \widetilde{\mathsf{a}}_k^\top \mathsf{x} + b_k \widetilde{\mathsf{a}}_i^\top \mathsf{x} - b_i b_k - \widetilde{\mathsf{a}}_i^\top \mathsf{x}\mathsf{x}^\top \widetilde{\mathsf{a}}_k \le 0 \quad \textit{for } i \le k \in [1\colon m] \\ & \sum_{j=1}^n (x_j^2 - x_j) = 0 \\ & \begin{pmatrix} 1 \\ \mathsf{x} \end{pmatrix} \begin{pmatrix} 1 \\ \mathsf{x} \end{pmatrix}^\top \in \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}. \end{array} \tag{26}$$

Relaxing the rank-one constraint, we arrive at the RLT-style relaxation

$$\begin{array}{ll} \max & \langle \mathsf{Q}, \mathsf{X} \rangle \\ \text{s.t.} & \widetilde{\mathsf{a}}_i^\top \mathsf{x} \le b_i \quad \textit{for } i \in [1\colon m] \\ & \widetilde{\mathsf{a}}_i^\top \mathsf{X} \le b_i \mathsf{x}^\top \quad \textit{for } i \in [1\colon m] \\ & b_i \widetilde{\mathsf{a}}_k^\top \mathsf{x} + b_k \widetilde{\mathsf{a}}_i^\top \mathsf{x} - b_i b_k - \widetilde{\mathsf{a}}_i^\top \mathsf{X} \widetilde{\mathsf{a}}_k \le 0 \quad \textit{for } i \le k \in [1\colon m] \\ & \sum_{j=1}^n (X_{jj} - x_j) = 0 \\ & \begin{pmatrix} 1 & \mathsf{x}^\top \\ \mathsf{x} & \mathsf{X} \end{pmatrix} \in \mathcal{S}_+^{n+1} \cap \mathcal{N}^{n+1}. \end{array} \tag{27}$$

Proof The equivalence of (26) and (22) follows by writing out the nonnegative constraints explicitly, and observing that

$$b_i \widetilde{\mathsf{a}}_k^\top \mathsf{x} + b_k \widetilde{\mathsf{a}}_i^\top \mathsf{x} - b_i b_k - \widetilde{\mathsf{a}}_i^\top \mathsf{x}\mathsf{x}^\top \widetilde{\mathsf{a}}_k = -(b_i - \widetilde{\mathsf{a}}_i^\top \mathsf{x})(b_k - \widetilde{\mathsf{a}}_k^\top \mathsf{x}),$$

while the relaxation (27) works exactly as in the classical RLT approach.

4 Numerical study

In this section, we compare the performances of the different proposed DNN relaxations together with the penalizing relaxations on multidimensional quadratic knapsack problems and quadratic assignment problems. All algorithms are implemented in MATLAB using the modeling language CVX (Grant and Boyd 2013, 2008) and the corresponding SDP instances are solved using SeDuMi (Sturm 1999) with default parameters on a machine with an Intel Core i7 2.8 GHz processor and 16.0 GB RAM. Note that before choosing SeDuMi, we compared several SDP solvers. According to our intensive numerical tests, we noticed that SeDuMi is the most stable solver from a numerical point of view.

4.1 Multidimensional quadratic knapsack problems

In the literature, the special case of (22) where $\mathsf{a}_i \in \mathbb{R}^n_+$ for all $i \in [1\!:\!m]$ is frequently called a *multidimensional quadratic knapsack problem*. In this section, these multidimensional quadratic knapsack problems are considered to evaluate numerically the performance of the different proposed approaches. We perform our tests on eight different instance sizes characterized by the following parameters: number of items $n \in \{10, 20, 30, 40, 50, 60, 70, 80\}$, and number of capacity constraints $m \in \{5, 10\}$, while the constraint structure a_i and b_i are taken from the literature (Beasley 2010). The (homogeneous) objective function is randomly generated: the elements of Q are uniformly sampled from the interval [100, 400].

The numerical results of six different relaxations are reported in Table 1. The optimal value was determined by CPLEX,[1] and used to calculate the gap. The following columns show optimal values of the respective relaxations as well as their corresponding CPU time. We can observe in Table 1 that the best results in terms of the solution quality are given by the reduced relaxations where the gap to the optimal solutions is on average less that 5%. The worst relaxation is the one where we merge both linear and binary constraints as the gap to the optimal solution averages 15.78%. From the point of view of the computation time, the reduced relaxations show the best performance, and solve instances up to $n = 80$, $m = 5$. In parallel, merging both linear and binary constraints presents the highest CPU time. Notice that only the reduced relaxations solve the largest instances within a reasonable CPU time. The combination of the reduced variant and merging constraints is slightly more efficient than the variant without merging in terms of CPU time whilst both relaxations have the same objective values. The comparison between the three first relaxations and the reduced one shows that the objective values of these three relaxations are similar; the average gap is less than 1.5%. The worst performance is given by the variant where both linear and binary constraints are merged as the average gap is 10.38%. All our instances are solved using interior point methods implemented in SeDuMi. One of the reasons of the degraded performances of the variant with both merging might be found in the behaviour of interior point methods. It is well known that merging the constraints provides better performances when the subgradient based methods are used (Kiwiel 1983).

Table 2 shows our numerical results for solving the same instances as in Table 1 by the penalization method where the parameter λ takes three values 100, 1000, and 100,000. Similar as the previous results, non merging variants outperform merging ones. Due to inherent numerical instability problems of the penalized methods, the solutions provided by SeDuMi are inaccurate which makes any rigorous comparisons difficult. However, for the instances solved to optimality without numerical perturba-

[1] IBM ILOG, CPLEX Optimizer. http://www.ibm.com/software/integration/optimization/cplex/.

Table 1 Numerical result for the multidimensional knapsack problem using CP reformulations

Orig prob		No merging		Merging linear		Merging binary		Merging both		Reduced no merging		Reduced merging	
(n, m)	Opt val	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU
Prime problem													
(10, 10)	13,840	14,876	0.9	–(– Inf)	1.3	14,877	0.8	16,156*	1.3	14,852	0.5	14,852	0.2
(20, 10)	46,922	48,451	10.1	48,792*	20.8	48,453	10.9	50,572*	28.0	48,435	1.4	48,435	1.4
(30, 5)	48,110	50,890	54	51,186*	120	50,890	59	56,723*	135	50,854	10	50,854	10
(40,5)	105,154	110,296	333	110,809* (150)	721	110,298	351	132,268* (150)	767	110,222	70	110,222	68
(50, 5)	206,590	213,470	2741	215,141*	3413	213,475	2477	228,663*	2682	213,330	558	213,330	502
(60, 5)	176,100	181,041	5425	– (150)	8779	181,043	5386	– (150)	8894	180,953	769	180,953	748
(70, 5)	318,644	–	–	–	–	–	–	–	–	322,884	2484	322,884	2431
(80, 5)	–	–	–	–	–	–	–	–	–	341,745	5248	341,745	5395

"–" means that the problem can not be solved within three hours while "*" means that the problem is not solved accurately. "150" means the algorithm reaches the maximum number of iterations set by `SeDuMi`.

Table 2 Numerical result for the penalization method

Orig prob		$\lambda = 100$				$\lambda = 1000$				$\lambda = 100{,}000$			
		No merging		Merging		No merging		Merging		No merging		Merging	
(n, m)	Opt val	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU
(10, 10)	13,840	15,471	1.2	17,618	1.0	-inf	1.3	17,635*	0.8	15,358*	1.0	18,746*	0.9
(20, 10)	46,922	48,818*	23	57,333	14	48,800*	22	55,930	14	48,745*	17	56,325*	14
(30, 5)	48,110	51,176	125	57,567	80	51,176*	123	54,596	86	51,114	88	52,441	68
(40, 5)	105,154	110,813*	734	131,571	531	110,717	740	126,463	522	110,521*	739	163,701	413
(50, 5)	206,590	215,141	2594	228,641	2245	215,127*	2573	227,731*	1904	214,798*	1566	246,691	1572
(60, 5)	176,100	–	–	225,519*	9880	–	–	2,222,196*	9596	180,953	769	147,063*	8390

"–" means that the problem is unbounded while "*" means that the problem is not solved accurately tions, we notice that the CPU time decreases when λ increases for the non merging reformulations.

4.2 Quadratic assignment problems

We next consider a general quadratic assignment problem as follows:

$$\begin{array}{lll} \min & \langle \mathsf{X}, \mathsf{A}\mathsf{X}\mathsf{B}^\top \rangle & \\ \text{s.t.} & \mathsf{e}^\top \mathsf{X}\mathsf{e}_i = \mathsf{e}_i^\top \mathsf{X}\mathsf{e} = 1 & \text{for } i \in [1\colon n] \\ & X_{ij} \in \{0, 1\} & \text{for } i \in [1\colon n],\ j \in [1\colon n], \end{array} \tag{P}$$

where $\mathsf{A}, \mathsf{B} \in \mathbb{R}^{n\times n}$ are given.

We performed our tests on 5 different instance sizes: $n \in \{6, 8, 10, 11, 12\}$ while A and B are taken from `QAPLIB` (Burkard et al. 1997). The numerical results of six different relaxations as well as their corresponding dual problems are reported in Table 3. The optimal value was determined by `CPLEX` and used to calculate the gap. The following columns show optimal values of the respective relaxation as well as their corresponding CPU time.

Table 3 compares our different relaxations on relatively small instances of QAP problems with up to 12 variables. Larger instances cannot be solved by `SeDuMi` due to both numerical instability and the high computation time. Unlike the multidimensional knapsack problems, our reformulations and their respective relaxations close the gap for all the instances except the variant where both linear and binary constraints are merged. We solve both the dual and the primal formulations for all the variants in order to check the numerical stability of our different relaxations. We notice that the dual, living up to its reputation, shows a better stability than the primal as all the instances are solved to optimality except one whilst the primal did not succeed in solving many instances for merging both linear and binary constraints variant. This shows that the dual formulations are more robust from a numerical point of view. Moreover, our different relaxations are promising for solving hard combinatorial optimization problems like QAP for larger instances once new efficient solvers are available.

5 Conclusion and outlook

In this paper, we present new results of variants of CP reformulations and their relaxations for solving hard combinatorial optimization problems. We study a new penalization method in order to reduce the size of the SDP relaxations. Our numerical results show that the multidimensional knapsack problems can be solved using SDP relaxations with good quality solutions. As for QAP problems, we closed the gaps for almost all the considered instances. Our penalization method gives comparable results with CP reformulations despite the numerical instability of the used solvers. Finally, our reduction based variant is the most efficient and promising for solving large size instances. Further research work will focus mainly on using softwares based on sub-

Table 3 Numerical result for the QAP problems

	Orig prob	No merging		Merging linear		Merging binary		Merging Both		Reduced no merging		Reduced merging	
n	Opt val	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU	Opt val	CPU
Prime problem													
6	8468	8468	0.7	8468	0.8	8468	0.8	8445*	1.7	8468	0.9	8468	0.8
8	7638	7638	20	7638	22	7638	20	7634	66	7638	63	7638	35
10	9636	9636	407	9636	531	9636	467	9631	1486	9636	986	9636	943
11	8860	8860	1276	8860	2467	8860	1513	8853*	5025	8860	4175	8860	3621
12	9552	9552	4820	9552	10,283	9552	5598	9543*	20,553 (150 iter)	9552	12,520 (7 h)	9552	11,730 (6.5 h)
Dual problem													
6	8468	8468	0.6	8468	0.8	8468	0.8	8456*	1.7	8468	2.5	8468	2.4
8	7638	7638	18	7638	20	7638	21	7636	55	7638	129	7638	134
10	9636	9636	354	9636	543	9636	442	9631	1134	9636	3455	9636	3470
11	8860	8860	1340	8860	2573	8860	1569	8852	4543	8860	12,813	8860	14,418
12	9552	9552	4172	9552	10,373	9552	5577	9548	19793	9552	43,022	9552	43,623

"*" means that the problem is not solved accurately gradient methods instead of interior point methods, and also extend our approaches to other combinatorial optimization problems.

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