Quadratic Optimization:
Copositive Modelling, Algorithms and Aspects of Duality

Dissertation

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Abstract

Quadratic optimization problems (QP) have a wide area of application such as combinatorial problems including the max clique problem. Motzkin and Straus [25] showed the equivalence between the max clique problem and the standard quadratic problem. Also mathematical statistics is another field of application of (QP): Many economic models are based on (QP), e.g. the quadratic knapsack problem.

In [5] Bomze et al. reformulated the standard quadratic problem $(StQP)$ into a copositive problem. Subsequently, algorithms to solve this copositive problem were established by Bomze and de Klerk in [6] and Dür and Bundfuss in [9]. While the implementation of those algorithms showed some promising numerical results, they were only able to solve the copositive reformulation of $(StQP)$. In [11] Burer presented a completely positive reformulation for quadratic optimization problems (QP) even with binary constraints. Unfortunately he did not present a method to solve such a completely positive problem nor did he gave a copositive reformulation, for which one could have modify the algorithms mentioned above to solve these problems.

This thesis will establish a new finite algorithm to solve a standard quadratic optimization problem. Furthermore in this thesis copositve representations for quadratic optimization problems restricted by inequalities as well as quadratic optimization problems restricted by equalities will be presented. For the first approach a completely positive reformulation of the (QP) was developed. The copositive reformulation could be obtained by considering the dual problem of the completely positive problem. A more direct approach was made by considering the Lagrangian dual of an equivalent quadratic optimization problem restricted by a semidefinit quadratic constraint. In this context conditions for strong duality are proposed.

Zusammenfassung

Quadratische Optimierungsprobleme (QP) haben ein breites Anwendungsgebiet, wie beispielsweise kombinatorische Probleme einschließlich des maximalen Cliquenroblems. Motzkin und Straus [25] zeigten die Äquivalenz zwischen dem maximalen Cliquenproblem und dem standard quadratischen Problem. Auch mathematische Statistik ist ein weiteres Anwendungsgebiet von (QP), sowie eine Vielzahl von ökonomischen Modellen basieren auf (QP), z.B. das quadratische Rucksackproblem.

In [5] Bomze et al. haben das standard quadratische Optimierungsproblem ($StQP$) in ein Copositive-Problem umformuliert. Im Folgenden wurden Algorithmen zur Lösung dieses copositiviten Problems von Bomze und de Klerk in [6] und Dür und Bundfuss in [9] entwickelt. Während die Implementierung dieser Algorithmen einige vielversprechende numerische Ergebnisse hervorbrachten, konnten die Autoren nur die copositive Neuformulierung des ($StQP$)s lösen. In [11] präsentierte Burer eine vollständig positive Umformulierung für allgemeine (QP)s, sogar mit binären Nebenbedingungen. Leider konnte er keine Methode zur Lösung für ein solches vollständig positives Problem präsentieren, noch wurde eine copositive Formulierung vorgeschlagen, auf die man die oben erwähnten Algorithmen modifizieren und anwenden könnte, um diese zu lösen.

Diese Arbeit wird einen neuen endlichen Algorithmus zur Lösung eines *standard quadratischen Optimierungsproblems* aufstellen. Desweiteren werden in dieser Thesis copositve Darstellungen für ungleichungsbeschränkte sowie gleichungsbeschränkte quadratische Optimierungsprobleme vorgestellt. Für den ersten Ansatz wurde eine vollständig positive Umformulierung des (QP) entwickelt. Die copositive Umformulierung konnte durch Betrachtung des dualen Problems des vollständig positiven Problems erhalten werden. Ein direkterer Ansatz wurde gemacht, indem das Lagrange-Duale eines äquivalenten quadratischen Optimierungsproblems betrachtet wurde, das durch eine semidefinite quadratische Nebenbedingung beschränkt wurde. In

diesem Zusammenhang werden Bedingungen für starke Dualität vorgeschlagen.

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Contents

Chapter 1

Introduction and Preliminaries

1.1 Introduction

The subject of the present thesis consists of two main topics: the general quadratic optimization problem and the copositive/completely positive program.

By "general quadratic programming problem" we mean an optimization problem, in which all functions involved are quadratic or linear and, in general, local optima can be different from global optima. We also consider the case where variables are required to take values in $\{0, 1\}$ (binary variables). The class of general quadratic programming problems plays a prominent role in the field of nonconvex global optimization because of its theoretical aspects as well as its wide range of applications. On the one hand, many real world problems arising from economies and engineering design can be directly modeled as quadratic programming problems. On the other hand, general quadratic programming includes as special cases the equivalent formulations of many important and well studied optimization problems, e.g., linear zero-one programs, knapsack problems, assignment problems, maximum clique problems, linear complementarity problems, bilinear problems, packing problems, etc. Last but not least, some special quadratic programming problems are used as basic subproblems in trust region methods in nonlinear programming.

A copositive/completely positive program is in general a linear optimization problem in matrix variables X with additional conic constraints of the form $X \in \mathcal{K}$, where $\mathcal{K}$ is either the cone of so-called copositive matrices or its dual cone of so-called completely positive matrices.

It has been shown that there is a close relationship between quadratic optimization problems and copositive/completely positive programs. This relationship enables us, on the one hand, to investigate duality properties of nonconvex quadratic problems and copositive/completely positive programs, and, on the other hand, can be employed in many cases to solve NP-hard quadratic problems by copositive/completely positive programs.

The major contribution of this thesis is outlined as follows:

In Chapter 2, the quadratic problem over the convex hull of finitely many points is investigated. This problem contains some interesting special cases such as the standard and multi-standard quadratic problems. A finite algorithm of branch and bound type is established, which also can be modified to check copositivity of matrices.

In Chapter 3, a general concept of constructing equivalent completely positive programs for quadratic problems is established. The quadratic problem to be considered thereafter has a system of linear inequalities as constraints. Two types of equivalent completely positive programs for these quadratic problems are constructed whose dual problems, which are copositive programs, are strictly feasible under some mild conditions. The strict feasibility of the dual problems guarantees the strong duality and allows to solve copositive programs efficiently by existing algorithms, e.g. the one in [9].

Aspects of Lagrange duality for a wide class of quadratic problems are investigated in Chapter 4. The Lagrange dual problem is constructed, and several duality properties are presented, including strong duality. Following the obtained duality results, an exact penalty method for a special class of quadratic problems is developed in the second part of Chapter 4.

Finally, Chapter 5 contains conclusions and topics of future research.

1.2 Preliminaries

1.2.1 Notation

For given positive integers d and k, we introduce the following notation:
$\mathbb{R}^d$ and $\mathbb{R}^d_+$: the $d-$dimensional real space and its nonnegative orthant;
The inner product on $\mathbb{R}^d$ is $\langle x, y\rangle = x^T y = \sum\limits_{i=1}^{d} x_i y_i$;
$\mathbb{R}^{d\times k}$: The space of $d \times k$ matrices;
The inner product on $\mathbb{R}^{d\times d}$ is the Frobenius product:

$$\langle A, B\rangle = \mathrm{tr}(A^T B) = \sum_{i=1}^{d}\sum_{j=1}^{d} a_{ij} b_{ij};$$

$\mathcal{S}_d := \{S \in \mathbb{R}^{d\times d} \mid S^T = S\}$ denotes the space of symmetric matrices;
$\mathcal{N}_d := \{S \in \mathcal{S}_d \mid S_{ij} \geq 0\ \forall i, j\}$ denotes the space of entrywise nonnegative matrices;
$\mathcal{S}^+_d := \{S \in \mathcal{S}_d \mid x^T S x \geq 0\ \forall x \in \mathbb{R}^d\}$, the positive semidefinite cone;
$\mathcal{D}_d := \mathcal{S}^+_d \cap \mathcal{N}_d$ denotes the cone of doubly nonnegative matrices;
$\Delta_d := \{x \in \mathbb{R}^d \mid e^T x = 1, x \geq 0\}$, the standard simplex, where $e \in \mathbb{R}^d$ denotes the vector of ones. For every subset M of $\mathbb{R}^d$, the notations

$$\mathrm{int}(M),\ \mathrm{cl}(M),\ \partial(M),\ \mathrm{conv}(M) \text{ and } \mathrm{rec}(M)$$

stand for interior, closure, boundary, convex hull and recession cone of M, respectively.
If M is a convex set, then $V(M)$ denotes the set of its extreme points. If M is a convex cone, then $\mathrm{E}(M)$ denotes the set of its extreme rays.

1.2.2 The Copositive and Completely Positive Cones

Definition 1.2.1. *Let A be a $d \times d$ real symmetric matrix. Then A is called copositive if $x^T Ax \geq 0$ for all $x \geq 0$. Strict copositivity of A means that $x^T Ax > 0$ for all $x \geq 0,\ x \neq 0$.*

Let $\mathcal{COP}_d$ be the set of all $d \times d$ copositive matrices. Then we have the following properties.

Proposition 1.2.2. *(See, e.g.,[1], [16], [19], and references given therein)*

(i) $\mathcal{COP}_d$ *is a closed convex pointed cone in* $\mathcal{S}_d$ *with* $\mathrm{int}(\mathcal{COP}_d) \neq \emptyset$.

(ii) $\mathcal{S}_d^+ \subset \mathcal{COP}_d$, $\mathcal{N}_d \subset \mathcal{COP}_d$, *and* $\mathcal{S}_d^+ + \mathcal{N}_d \subset \mathcal{COP}_d$.

(iii) $\mathrm{int}(\mathcal{COP}_d)$ *is the set of strictly copositive matrices, and*

$$\partial(\mathcal{COP}_d) = \{A \in \mathcal{S}_d \mid \ \min\{x^T Ax : e^T x = 1, x \geq 0\} = 0\}.$$

where e denotes the all-ones vector in $\mathbb{R}^d$.

Definition 1.2.3. *Let A be a $d \times d$ real symmetric matrix. One says that A is completely positive if there exists an integer m and a $d \times m$ matrix B with nonnegative entries such that $A = BB^T$. The smallest possible number m is called the CP-rank of A.*

Let $\mathcal{CP}_d$ be the set of all $d \times d$ completely positive matrices. Then we have the following properties.

Proposition 1.2.4. *(See, e.g., [1], [13], [16], [19], and references given therein)*

(i) $\mathcal{CP}_d$ *is a closed convex pointed cone in* $\mathcal{S}_d$ *with* $\mathrm{int}(\mathcal{CP}_d) \neq \emptyset$.

(ii) $\mathcal{CP}_d \subset \mathcal{S}_d^+ \subset \mathcal{COP}_d$.

(iii) $\mathcal{CP}_d = \mathrm{conv}\{xx^T \mid \ x \in \mathbb{R}^d_+\}$.

(iv) $\mathrm{int}(\mathcal{CP}_d) = \{A \in \mathcal{S}_d \mid \mathrm{rank}(A) = d, \ A = BB^T \textit{ with } B > 0\}$, *where* 0 *is the* $d \times d$ *zero matrix.*

(v) $E(\mathcal{CP}_d) = \{xx^T \mid \ x \in \mathbb{R}^d_+\}$.

Definition 1.2.5. *Let* $\mathcal{C}$ *be an arbitrary given cone in* $\mathcal{S}_d$. *The dual cone* $\mathcal{C}^*$ *to* $\mathcal{C}$ *is defined as*

$$\mathcal{C}^* = \{A \in \mathcal{S}_d \mid \ \langle A, B\rangle \geq 0 \textit{ for all } B \in \mathcal{C}\}.$$

Proposition 1.2.6. *(See, e.g.,[1], [16], [19], and references given therein) The cones* $\mathcal{COP}_d$ *and* $\mathcal{CP}_d$ *are dual to each other in the sense that*

$$\mathcal{COP}_d^* = \mathcal{CP}_d \textit{ and } \mathcal{CP}_d^* = \mathcal{COP}_d.$$

1.2.3 Copositive and Completely Positive Programs and their Duals

Let $Q \in \mathcal{S}_d, \ A_i \in \mathcal{S}_d, \ b_i \in \mathbb{R}, \ i = 1, \ldots, m$, and let $\mathcal{K}$ be some closed convex cone. Consider a linear optimization problem in matrix variables with a conic constraint of the following form:

$$\begin{array}{ll} \min & \langle Q, X\rangle \\ \text{s.t.} & \langle A_i, X\rangle = b_i,\ i = 1,\ldots,m \\ & X \in \mathcal{K}. \end{array} \tag{1.1}$$

Definition 1.2.7. *Problem* (1.1) *is called a copositive program if* $\mathcal{K} = \mathcal{COP}_d$*. It is called a completely positive program if* $\mathcal{K} = \mathcal{CP}_d$*.*

The corresponding Lagrangian dual of Problem (1.1) is then

$$\begin{array}{ll} \max & \sum\limits_{i=1}^{m} b_i y_i \\ \text{s.t.} & Q - \sum\limits_{i=1}^{m} y_i A_i \in \mathcal{K}^* \\ & y_i \in \mathbb{R},\ i = 1,\ldots,m. \end{array} \tag{1.2}$$

Since $\mathcal{K}$ and $\mathcal{K}^*$ are convex cones, strong duality requires some constraint qualifications such as Problem (1.1) respectively Problem (1.2) to be strictly feasible, i.e., the existence of a feasible point in $\operatorname{int}(\mathcal{K})$ or $\operatorname{int}(\mathcal{K}^*)$, respectively (see [18]).

1.2.4 Quadratic Optimization Problems and Completely Positive Programs

Two types of quadratic optimization problems are considered in this thesis. The first one is the optimization of a general quadratic function $f : \mathbb{R}^d \to \mathbb{R}$ over the convex hull of a set of finitely many points formulated as

$$\min\{f(x) : x \in \operatorname{conv}\{v^1, \ldots, v^k\}\}, \tag{1.3}$$

where $v^1, \ldots, v^k \in \mathbb{R}^d$. The other type of problem has the form

$$\min\{f(x) : x \in P,\ g_i(x) = b_i,\ i = 1,\ldots,m\}, \tag{1.4}$$

where $P \subset \mathbb{R}^d$ is a polyhedral set, and $f,\ g_i : \mathbb{R}^d \to \mathbb{R},\ i = 1, \dots, m$ are quadratic functions. Note that any binary condition $x_i \in \{0, 1\}$ can be rewritten as a quadratic constraint $x_i(1 - x_i) = 0$, so problems with binary constraints can be written in the form (1.4).

The general form of a quadratic function $f : \mathbb{R}^d \to \mathbb{R}$ is given by

$$f(x) = x^T Q x + q^T x, \tag{1.5}$$

where $Q \in \mathcal{S}_d$, and $q \in \mathbb{R}^d$.

In many cases, a general quadratic function of the form (1.5) can be rewritten as a quadratic form $f(x) = x^T \bar{Q} x$ with $\bar{Q} \in \mathcal{S}_d$, e.g., if the problem under consideration contains a constraint $c^T x = 1$. In this case, by substitution $\bar{Q} = Q + \frac{1}{2}(cq^T + qc^T)$, one obtains

$$f(x) = x^T \bar{Q} x$$

on the feasible set of the optimization problem.

There exits a close relationship between quadratic optimization problems and completely positive/copositive programs. We discuss this relationship by the following two known cases.

First, consider the so-called standard quadratic optimization problem in [5]:

$$\begin{aligned} \min \quad & x^T Q x \\ s.t. \quad & e^T x = 1 \\ & x \geq 0, \end{aligned} \tag{1.6}$$

where $Q \in \mathcal{S}_d$ and e denotes the all-ones vector. From Problem (1.6), one constructs the following completely positive program:

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ s.t. \quad & \langle ee^T, X \rangle = 1 \\ & X \in \mathcal{CP}_d. \end{aligned} \tag{1.7}$$

Problem (1.6) and problem (1.7) are equivalent in the sense, that they have the same optimal values:

$$\min(1.6) = \min(1.7).$$

Furthermore it has been shown in [5] that $X^* = \sum_{k=1}^r \lambda_k (x^k)(x^k)^T$ with $\sum_{k=1}^r \lambda_k = 1$, $\lambda_k \geq 0$ $(k = 1, \ldots, r)$ is an optimal solution of (1.7) if and only if $x^1, \ldots, x^k$ are optimal solutions of (1.6).

The second problem is the mixed-binary quadratic program considered by Burer in [11]:

$$\begin{aligned} \min \quad & x^T Q x + 2q^T x \\ \text{s.t.} \quad & a_i^T x = b_i,\ i = 1, \ldots, m \\ & x \geq 0 \\ & x_j \in \{0, 1\},\ j \in J \subseteq \{1, \ldots, d\}, \end{aligned} \tag{1.8}$$

where $Q \in \mathcal{S}_d$ and $q,\ a_i \in \mathbb{R}^d$ for all $i = 1, \ldots, m$.

Burer considered the following two *Key Assumptions* :

(KA1): The system $a_i^T x = b_i, x \geq 0$ $(i = 1, \ldots, m)$ implies $0 \leq x_j \leq 1$ for all $j \in J$.

(KA2): There exists $\beta \in \mathbb{R}^m$ such that

$$\sum_{i=1}^m \beta_i a_i \geq 0,\ \sum_{i=1}^m \beta_i b_i = 1.$$

Burer [11] showed that under (KA1)-(KA2), by using a vector

$$\alpha = \sum_{i=1}^m \beta_i a_i \geq 0, \tag{1.9}$$

Problem (1.8) can be equivalently reformulated as the following completely positive program:

$$\begin{aligned} \min \quad & \langle Q, X\rangle + 2q^T X\alpha \\ \text{s.t.} \quad & a_i^T X\alpha = b_i,\ i = 1,\dots,m \\ & a_i^T X a_i = b_i^2,\ i = 1,\dots,m \\ & (X\alpha)_j = X_{jj},\ j \in J \\ & \alpha^T X\alpha = 1 \\ & X \in \mathcal{CP}_d. \end{aligned} \tag{1.10}$$

The equivalence between Problem (1.8) and Problem (1.10) is stated as follows (see [11]):

Theorem 1.2.8. *Under (KA1)-(KA2), let α be defined as in (1.9). Then Problem (1.8) is equivalent to Problem (1.10) in the sense that:*

(i) The optimal values of both problems are equal.

(ii) If X^* is an optimal solution of Problem (1.10), then $X^*\alpha$ lies in the convex hull of optimal solutions of Problem (1.8).

1.2.5 Algorithms for Copositive Programs using approximations for $\mathcal{COP}$ and $\mathcal{CP}$

Approximation of $\mathcal{COP}$ with Sum of Squares

In the last part of this chapter we cover the known approximations for the copositve and completely positive cone. After that we discuss the resulting algorithms to solve copostive and completely positive problems.
The first approximation was presented by Bomze and De Klerk in 2002 (see [6]). The main idea was that every $z \in \mathbb{R}^n_+$ can be written as $z = x \circ x$ for

some $x \in \mathbb{R}^n$, where $\circ$ indicates the componentwise (Hadamard) product. Therefore, another condition for copositivity can be formulated as follows. A matrix $A \in \mathcal{S}_n$ is copositive if and only if

$$P(x) := (x \circ x)^T A(x \circ x) = \sum_{i,j=1}^{n} A_{ij} x_i^2 x_j^2 \geq 0 \text{ for all } x \in \mathbb{R}^n. \tag{1.11}$$

Using $\bar{x} := [x_1^2, ..., x_n^2, x_1x_2, x_1x_3, ..., x_{n-1}x_n]$, the polynomial $P(x)$ can be represented as

$$P(x) = \bar{x}^T \bar{A} \bar{x}, \tag{1.12}$$

for a suitable, but not uniquely determined matrix $\bar{A} \in \mathcal{S}_{(n+\frac{1}{2}n(n-1))}$. If the polynomial $P(x)$ has a sum of squares (s.o.s.) decomposition, i.e.

$$P(x) = \sum_{i=1}^{l} f_i(x)^2 \text{ for all } x \in \mathbb{R}^n$$

for some polynomial functions $f_1(x), ..., f_l x$, then clearly we have $P(x) \geq 0$. Therefore, if $P(x)$ has an s.o.s. decomposition, then A is for sure a copositive matrix, but not vice versa.

Parirlo showed in [26], that $P(x) = (x \circ x)^T A(x \circ x)$ has an s.o.s. decomposition if and only if $A \in \mathcal{S}^+ + \mathcal{N} = \mathcal{D}^*$, where $\mathcal{D}^*$ is the dual of the doubly nonnegative cone. Note that $A \in \mathcal{S}^+ + \mathcal{N}$ is a sufficient condition for copositivity of A. In [6], Bomze and de Klerk defined the cone

$$\mathcal{K}^0 := \mathcal{S}^+ + \mathcal{N} \subset \mathcal{COP},$$

and then they gave higher order sufficient conditions for copositivity by considering polynomials of the form

$$P^{(r)}(x) := P(x) \left(\sum_{k=1}^{n} x_k^2 \right)^r, \tag{1.13}$$

and defining the cone $\mathcal{K}^r$ as the cone of matrices for which $P^{(r)}(x)$ has an s.o.s. decomposition. If $P^{(r)}(x) = \sum_{i=1}^{l} [f_i(x)]^2$, then

$$P^{(r+1)}(x) = (\sum_{k=1}^{n} x_k^2) P^{(r)}(x) = \sum_{i=1}^{l} \sum_{k=1}^{n} [f_i(x) x_k]^2 \,, \tag{1.14}$$

which implies that $\mathcal{K}^r \subset \mathcal{K}^{r+1}$.

Furthermore, Bomze and de Klerk [6] defined for $r \in \mathbb{N}$ the cone $\mathcal{C}^r$ of matrices for which $P^{(r)}(x)$ has nonnegative coefficients. Clearly we have again for all $r \in \mathbb{N}$ that $\mathcal{C}^r \subset \mathcal{C}^{r+1}$ and

$$\mathcal{C}^r \subset \mathcal{K}^r \subset \mathcal{COP}. \tag{1.15}$$

From the famous theorem of Póyla [28] follows that every strictly copostive matrix A lies in some cone $\mathcal{C}^r$ for sufficiently large r, and we have the following theorem

Theorem 1.2.9 (De Klerk and Pasechnik [14])**.** *Let $\mathcal{C}^r$ and $\mathcal{K}^r$ be defined as above. Then we have $\mathcal{C}^0 = \mathcal{N}$ and*

$$\mathrm{cl} \bigcup_{r \in \mathbb{N}_0} \mathcal{C}^r = \mathrm{cl} \bigcup_{r \in \mathbb{N}_0} \mathcal{K}^r = \mathcal{COP}.$$

Theoretically, is possible to give conditions for any $r \in \mathbb{N}$ to construct the matrix $\bar{A} \in \mathcal{S}_d$, where $d = \mathcal{O}(n^{r+2})$ such that $P^{(r)}(x)$ has an s.o.s decomposition (see Theorem 2.2 in [6]). Due to the rapidly increasing d even for small $n \in \mathbb{N}$, Bomze and de Klerk in [6] gave explicit conditions for $\mathcal{C}^0, \mathcal{C}^1, \mathcal{K}^0$ and $\mathcal{K}^1$, and point out that problems becomes too large for the SPD-solver at this time for $r \geq 1$, even for small values of n. The authors of [6] implemented algorithms to solve corresponding relaxations for the copositive reformulation of the standard quadratic program (1.6), i.e. instead of solving

$$\begin{array}{ll} \max & \lambda \\ \text{s.t.} & Q - \lambda E \in \mathcal{COP} \\ & \lambda \in \mathbb{R}, \end{array}$$

they solved the program

$$\begin{aligned} \max \quad & \lambda \\ \text{s.t.} \quad & Q - \lambda E \in \mathcal{K} \\ & \lambda \in \mathbb{R}, \end{aligned} \tag{1.16}$$

where $\mathcal{K} \in \{\mathcal{K}^0, \mathcal{K}^1, \mathcal{C}^0, \mathcal{C}^1\}$ and therefore obtained only lower bounds for the optimal value of (1.6). Note that for $\mathcal{K} = \mathcal{K}^0, \mathcal{K}^1$ these relaxations are semi-definite programs (SDP)(see [6] Theorem 2.3), while for $\mathcal{K} = \mathcal{C}^0, \mathcal{C}^1$ (1.16) is a linear program (see [6] Theorem 2.5). We will discuss results of these implementations in Chapter 2, when we compare these algorithms with our method to solve Problem (1.6).

Approximation of $\mathcal{COP}$ and $\mathcal{CP}$ using Simplicial Partitions

We discuss the approach of Bundfuss and Dür given in [9]. The main idea of this approach is the following result.

Lemma 1.2.10. *Let $S_n := \operatorname{conv}\{v^1, ..., v^n\}$ be a simplex and $A \in \mathcal{S}_n$. Assume that*

$$(v^i)^T A v^j \geq 0 \textit{ for all } i, j = 1, ..., n. \tag{1.17}$$

Then $x^T A x \geq 0$ for all $x \in S_n$.

Proof. Let $x \in S_n = \operatorname{conv}\{v^1, ..., v^n\}$, i.e. $x = \sum\limits_{i=1}^n \lambda_i v^i$, where $\lambda \in \mathbb{R}^n_+$ with $e^T \lambda = 1$, then

$$x^T A x = \left(\sum_{i=1}^n \lambda_i v^i \right)^T A \left(\sum_{j=1}^n \lambda_i v^j \right) = \sum_{i,j} \lambda_i \lambda_j (v^i)^T A v^j, \tag{1.18}$$

which implies $x^T A x \geq 0$ for all $x \in S_n$. □

Note that a matrix A is copositive if and only if $x^T Ax \geq 0$ for all $x \in \Delta_n$. The main idea for an outer approximation of $\mathcal{COP}$ is to consider a subset of finitely many points $x^1, ..., x^r$ of the standard simplex, and consider the set of matrices A which fulfill $(x^i)^T Ax^i \geq 0$ for all $i = 1, ..., r$. The more points contained in the subset, the better the approximation will be. For an algorithmic approach of partitioning the standard simplex Δ_n Bundfuss and Dür suggested in [9] a simplicial bisection which was investigated by Horst in [20]. First we will give a definition for a simplical partition.

Definition 1.2.11. *Let S_n be a simplex in $\mathbb{R}^n$. A family $\mathcal{P} = \{S_n^1, ..., S_n^m\}$ of simplices satisfying*

$$S_n = \bigcup_{i=1}^{m} S_n^i \text{ and } \operatorname{int}(S_n^i) \cap \operatorname{int}(S_n^j) = \emptyset \text{ for } i \neq j \tag{1.19}$$

is called a simplical partition of S_n. Furthermore, we denote the set of vertices of the partition by

$$V(\mathcal{P}) = \{v^{i,k} \mid i \in \{1, ..., n\}, k \in \{1, ..., m\}\}, \tag{1.20}$$

and the set of edges by

$$E(\mathcal{P}) = \{(v^{i,k}, v^{j,k}) \mid i, j \in \{1, ..., n\} \text{ with } i < j, k \in \{1, ..., m\}\}, \tag{1.21}$$

where $v^{i,k}$ denotes the i-th vertex of simplex S_n^k.

Note that $(v^{i,k}, v^{j,k}) = (v^{j,k}, v^{i,k})$ for all $i \neq j$, therefore it is redundant to consider these edges twice in $E(\mathcal{P})$. The next definition helps to determine how to obtain a refinement $\mathcal{P}^{k+1}$ from a simplicial partition $\mathcal{P}^k$.

Definition 1.2.12. *Let $\mathcal{P}$ be a simplicial partition of Δ_n. We call the maximum diameter of a simplex in the partion $\mathcal{P}$ the fineness of $\mathcal{P}$ and denote it by*

$$\delta(\mathcal{P}) = \max_{(u,v) \in E(\mathcal{P})} \|u - v\|. \tag{1.22}$$

In order to obtain a refinement $\mathcal{P}^{k+1}$ of $\mathcal{P}^k$ Horst [20] suggested to bisect the simplex S^l in $\mathcal{P}^k$ which contains an edge $(v^{i,l}, v^{j,l})$ with $\delta(\mathcal{P}^k) = \|v^{i,l} - v^{j,l}\|$. Denote by $v^{1,l}, ..., v^{n,l}$ the vertices of S^l, and then define S^{l_1} with the vertex set

$$V(S^{l_1}) = \{v^{1,l}, ..., v^{i-1,l}, u, v^{i+1,l}, ..., v^{n,l}\}$$

and S^{l_2} with the vertex set

$$V(S^{l_2}) = \{v^{1,l}, ..., v^{j-1,l}, u, v^{j+1,l}, ..., v^{n,l}\},$$

where $u = \frac{1}{2}v^{i,l} + \frac{1}{2}v^{j,l}$. Then we have

$$\operatorname{int} S^{l_1} \cap \operatorname{int} S^{l_2} = \emptyset \text{ and } S^l = S^{l_1} \cup S^{l_2}.$$

Then we can define $\mathcal{P}^{k+1} := \mathcal{P}^k \setminus \{S^l\} \cup \{S^{l_1}, S^{l_2}\}$. Using this rule, we can generate a sequence of simplicial partitions $\{\mathcal{P}_k\}_{k\in\mathbb{N}}$ yielding

$$\delta(\mathcal{P}_k) \to 0 \text{ for } k \to \infty \tag{1.23}$$

This kind of subdivision is called simplicial partition along the longest edge and has the nice property that it generates a nested sequence of simplices which converges to a singleton. This property is a necessary condition for convergence of any branch and bound algorithm. Having a nice partition rule for the standard simplex Δ_n (Bundfuss and Dür [9]), define the sets

$$\mathcal{I}_{\mathcal{P}_k} := \{A \in \mathcal{S}_n \mid u^T A v \geq 0, v^T A v \geq 0, v \in V(\mathcal{P}_k), (u, v) \in E(\mathcal{P}_k)\},$$

and

$$\mathcal{O}_{\mathcal{P}_k} := \{A \in \mathcal{S}_n \mid v^T A v \geq 0 \text{ for all } v \in V(\mathcal{P}_k)\}.$$

It is easy to see that $\mathcal{I}_{\mathcal{P}_k}$ and $\mathcal{O}_{\mathcal{P}_k}$ are polyhedral cones for all $k \in \mathbb{N}$ and

$$\mathcal{I}_{\mathcal{P}_k} \subset \mathcal{COP} \subset \mathcal{O}_{\mathcal{P}_k}. \tag{1.24}$$

We also have $\mathcal{O}_{\mathcal{P}_l} \subset \mathcal{O}_{\mathcal{P}_k}$ and $\mathcal{I}_{\mathcal{P}_k} \subset \mathcal{I}_{\mathcal{P}_l}$ for $k \leq l$, and moreover we have

$$\mathrm{cl}\left(\bigcup_{k\in\mathbb{N}} \mathcal{I}_{\mathcal{P}_k}\right) = \mathcal{COP} = \bigcap_{k\in\mathbb{N}} \mathcal{O}_{\mathcal{P}_k}. \tag{1.25}$$

By duality, we have that the dual cone $\mathcal{I}^*_{\mathcal{P}_k}$ of $\mathcal{I}_{\mathcal{P}_k}$,

$$\mathcal{I}^*_{\mathcal{P}_k} = \{ \sum_{(v^i,v^j)\in E(\mathcal{P}_k)} \lambda_{i,j}((v^i)(v^j)^T + (v^j)(v^i)^T) + \sum_{v^i\in V(\mathcal{P}_k)} \lambda_i (v^i)(v^i)^T \mid \lambda_{i,j}, \lambda_i \geq 0\}$$

is an outer approximation of $\mathcal{CP}$ and analogously the dual cone $\mathcal{O}^*_{\mathcal{P}_k}$ of $\mathcal{O}_{\mathcal{P}_k}$,

$$\mathcal{O}^*_{\mathcal{P}_k} = \{ \sum_{v^i\in V(\mathcal{P}_k)} \lambda_i (v^i)(v^i)^T \mid \lambda_i \geq 0\}$$

is an inner approximation of $\mathcal{CP}$, and we also have

$$\mathrm{cl}\left(\bigcup_{k\in\mathbb{N}} \mathcal{O}^*_{\mathcal{P}_k}\right) = \mathcal{CP} = \bigcap_{k\in\mathbb{N}} \mathcal{I}^*_{\mathcal{P}_k}. \tag{1.26}$$

From these results, Bundfuss and Dür presented in [9] the following Algorithm 1 to solve copositive problems of the form

$$\begin{array}{ll} \max & b^T y \\ \text{s.t.} & C - \sum\limits_{i=1}^{m} y_i A_i \in \mathcal{COP} \\ & y \in \mathbb{R}^m. \end{array} \tag{1.27}$$

For a given accuracy $\varepsilon > 0$ Algorithm (1) computes an approximately optimal value μ^* with

$$\frac{\mu - \mu^*}{1 + |\mu| + |\mu^*|} < \varepsilon,$$

where μ denotes the optimal value of Problem (1.27). We call $y^* \in \mathbb{R}^m$ with $b^T y^* = \mu^*$ an approximately optimal solution.

Algorithm 1 ε-approximation for (1.27)

Input:

- Problem data: $A^1, ..., A^m, C \in \mathcal{S}_n, b \in \mathbb{R}^m$
- Tolerance $\varepsilon > 0$

$\mathcal{P} \leftarrow \{\Delta_n\}$

repeat

  solve the inner LP

$$\begin{array}{ll} \max & b^T y \\ \text{s.t.} & C - \sum_{i=1}^{m} y_i A_i \in \mathcal{I}_{\mathcal{P}} \\ & y \in \mathbb{R}^m, \end{array} \tag{1.28}$$

  denote the optimal solution of this problem by $y^{\mathcal{I}}$

  solve the outer LP

$$\begin{array}{ll} \max & b^T y \\ \text{s.t.} & C - \sum_{i=1}^{m} y_i A_i \in \mathcal{O}_{\mathcal{P}} \\ & y \in \mathbb{R}^m, \end{array} \tag{1.29}$$

  denote the optimal solution of this problem by $y^{\mathcal{O}}$

  choose $S \in \mathcal{P}$

  bisect $S = S^1 \cup S^2$

  set $\mathcal{P} \leftarrow \mathcal{P} \setminus \{S\} \cup \{S^1, S^2\}$

until $\frac{b^T y^{\mathcal{O}} - b^T y^{\mathcal{I}}}{1+|b^T y^{\mathcal{O}}|+|b^T y^{\mathcal{I}}|} \leq \varepsilon$

Output: Approximation of an optimal solution of (1.27)

In this algorithm it is not specified how a simplex is selected in line 8 or how the bisection is performed in Line 9. However the partitioning rule suggested by Horst [20] generates cones $\mathcal{I}_{\mathcal{P}_k}$ and $\mathcal{O}_{\mathcal{P}_k}$ that approximate $\mathcal{COP}$ uniformly arbitrarily well, but for optimization purpose it is not very efficient. Bundfuss and Dür [9] used another partition rule which they called "simplicial partion along the longest active edge". First we will recall how Bundfuss and Dür chose an edge $\{u, v\}$ for bisection. For this purpose consider the inner LP

$$\begin{array}{ll} \max & b^T y \\ \text{s.t.} & u^T C v - \sum\limits_{i=1}^{m} y_i (u^T A_i v) \geq 0, \quad \text{for all } (u,v) \in E(\mathcal{P}) \\ & v^T C v - \sum\limits_{i=1}^{m} y_i (v^T A_i v) \geq 0, \quad \text{for all } v \in V(\mathcal{P}) \\ & y \in \mathbb{R}^m, \end{array}$$

and the outer LP

$$\begin{array}{ll} \max & b^T y \\ \text{s.t.} & v^T C v - \sum\limits_{i=1}^{m} y_i (v^T A_i v) \geq 0, \quad \text{for all } v \in V(\mathcal{P}) \\ & y \in \mathbb{R}^m. \end{array}$$

Denote by $y^{\mathcal{I}}$ the optimal solution of (1.28). Assume that the stopping criterion in Line 11 has not been met, i.e. for the optimal solution $y^{\mathcal{I}}$ there exists no vertex vertex $v \in V(\mathcal{P})$ such that

$$v^T C v - \sum_{i=1}^{m} y_i^{\mathcal{I}} (v^T A_i v) = 0,$$

otherwise $y^{\mathcal{I}}$ is also optimal for (1.29). Therefore there exists an edge $(u, v) \in E(\mathcal{P})$ with $u^T C v - \sum\limits_{i=1}^{m} y_i^{\mathcal{I}} (u^T A_i v) = 0$. Such an edge is called *active edge*. Bundfuss and Dür choose in Line 8 the longest of the active edges in $y^{\mathcal{I}}$ for bisection. Once an edge (u, v) is chosen for bisection, Bundfuss and Dür bisect all simplices containing the edge (u, v) at the new point $w := \frac{1}{2}u + \frac{1}{2}v$.

In [9], the authors presented numerical results for the reformulated copositive program from the standard quadratic problem (1.6). Note that while the results are very promising for solving these problems, the algorithm only provides the optimal value, but no optimal solution for the standard quadratic problem (1.6).

It is our purpose to propose the following improvement for the algorithm of Bundfuss and Dür.

We propose a way to obtain an optimal solution of the standard quadratic problem (1.6)

$$\begin{aligned} \min \quad & x^T Q x \\ s.t. \quad & e^T x = 1 \\ & x \geq 0, \end{aligned}$$

which is reformulated as the copositive program

$$\begin{aligned} \max \quad & y \\ \text{s.t.} \quad & Q - yE \in \mathcal{COP} \\ & y \in \mathbb{R}. \end{aligned} \tag{1.30}$$

The outer relaxation (1.29) can be written as

$$\begin{aligned} \max \quad & y \\ \text{s.t.} \quad & y \leq u^T Q u, \quad \text{for all } u \in V(\mathcal{P}) \\ & y \in \mathbb{R}. \end{aligned} \tag{1.31}$$

Again denote by $y^{\mathcal{O}}$ the optimal value and optimal solution of (1.29), and assume that the optimality criterion for ε-accurency has been met, i.e.

$$\frac{y^{\mathcal{O}} - y^{\mathcal{I}}}{1 + |y^{\mathcal{O}}| + |y^{\mathcal{I}}|} < \varepsilon.$$

Note that in this case $y^{\mathcal{O}}$ is also an $\varepsilon-$ optimal value of (1.29), furthermore there exists $u^{\mathcal{O}} \in V(\mathcal{P})$ with

$$y^{\mathcal{O}} = (u^{\mathcal{O}})^T Q (u^{\mathcal{O}}). \tag{1.32}$$

From the equivalence between the problems (1.6) and (1.30), we have

$$y^{\mathcal{O}} - \min_{x \in \Delta_n} x^T Q x \leq y^{\mathcal{O}} - y^{\mathcal{I}},$$

and therefore, $y^{\mathcal{O}}$ can also be considered as an approximately optimal value of Problem (1.6).

Since $u^{\mathcal{O}} \in \Delta_n$, it follows that $u^{\mathcal{O}}$ can be taken as an approximately optimal solution of Problem (1.6).

Using the same reasoning as above, we can also obtain an approximately optimal solution for the completely positive problem

$$\begin{array}{ll} \min & \langle Q, X \rangle \\ \text{s.t.} & \langle A_i, X \rangle = b_i \quad (i = 1, \ldots, m) \\ & X \in \mathcal{CP}. \end{array} \tag{1.33}$$

The dual of (1.33) is the copositive problem

$$\begin{array}{ll} \max & b^T y \\ \text{s.t.} & Q - \sum_{i=1}^m y_i A_i \in \mathcal{COP} \\ & y \in \mathbb{R}^m. \end{array} \tag{1.34}$$

Consider the relaxation problem (1.29)

$$\begin{array}{ll} \max & b^T y \\ \text{s.t.} & (u^k)^T Q u^k - \sum\limits_{i=1}^{m} y_i ((u^k)^T A_i u^k) \geq 0, \quad u^k \in V(\mathcal{P}) \\ & y \in \mathbb{R}^m, \end{array}$$

and its dual LP

$$\begin{array}{ll} \min & \sum_{k=1}^{|V(\mathcal{P})|} x_k \ (u^k)^T Q u^k \\ \text{s.t.} & \sum_{k=1}^{|V(\mathcal{P})|} x_k \ (u^k)^T A_i u^k = b_i \quad (i = 1, \ldots, m) \\ & x \in \mathbb{R}_+^{|V(\mathcal{P})|}, \end{array}$$

which can be written as

$$\begin{array}{ll} \min & \langle Q, \sum_{k=1}^{|V(\mathcal{P})|} x_k (u^k)(u^k)^T \rangle \\ \text{s.t.} & \langle A_i, \sum_{k=1}^{|V(\mathcal{P})|} x_k (u^k)(u^k)^T \rangle = b_i \quad (i = 1, \ldots, m) \\ & x \in \mathbb{R}_+^{|\mathcal{P}|}. \end{array}$$

Obviously, $\sum_{k=1}^{|V(\mathcal{P})|} x_k (u^k)(u^k)^T \in \mathcal{O}_{\mathcal{P}}^* \subset \mathcal{CP}$. Again denote by $y^{\mathcal{O}}$ the optimal solution of (1.29) and assume that the ε-accuracy has been met. Furthermore, denote the optimal solution of the dual LP by $x^{\mathcal{O}^*}$. Then

$$X^* = \sum_{k=1}^{|V(\mathcal{P})|} x_k^{\mathcal{O}^*} (u^k)(u^k)^T$$

is a ε-optimal solution for (1.33).

We want to mention a problem in the simplicial partition rule of the algorithm in [9].

Let (u^*, v^*) be one of the longest active edges, i.e. an edge satisfying

$$\begin{array}{l} (u^*)^T (Q - \sum y_i^{\mathcal{I}} A_i) v^* = 0, \\ \|u^* - v^*\| = \max\{\|u - v\| \mid u^T (Q - \sum y_i^{\mathcal{I}} A_i) v = 0, (u, v) \in E(\mathcal{P})\}, \end{array}$$

where $y^{\mathcal{I}}$ denotes the optimal solution of (1.28).

In [9], the new vertex w is determined by $w := \lambda u^* + (1 - \lambda) v^*$ with $\lambda = \frac{1}{2}$.

By this rule, it can happen that the edges (u^*, w) and (w, v^*) will be considered thereafter such that many other vertices and edges can be generated from the edge (u^*, v^*). Hence this partition rule may not be exhaustive, and therefore convergence is not necessary given for the algorithm in [9].

CHAPTER 2

Quadratic Optimization over the Convex Hull of finitely many Points

2.1 Introduction

In this chapter, we consider a (possibly nonconvex) quadratic optimization problem over the convex hull of finitely many points of a real space, and present an algorithm to solve such a problem. The main idea of the algorithm is to transform this problem into a quadratic optimization problem of the form

$$\begin{aligned} \min \quad & f(x) = x^T Q x + q^T x + c \\ \text{s.t.} \quad & e^T x \leq 1 \\ & x \geq 0, \end{aligned} \tag{2.1}$$

where $Q \in \mathcal{S}_n$, $q \in \mathbb{R}^n$, $c \in \mathbb{R}$. Before going into the details of the transformation we will give some examples for quadratic optimization problems.

Formally, a quadratic, not necessarily convex problem is written by

$$\min\{\bar{f}(\xi) : \ \xi \in S\}, \tag{2.2}$$

where S is the convex hull of $n+1$ given vectors $v^1, \ldots, v^{n+1} \in \mathbb{R}^d$, i.e.,

$$S = \mathrm{conv}\{v^1, \ldots, v^{n+1}\}, \tag{2.3}$$

and $\bar{f} : \mathbb{R}^d \to \mathbb{R}$ a quadratic function given by

$$\bar{f}(\xi) = \xi^T \bar{Q} \xi + \bar{q}^T \xi \tag{2.4}$$

with $\bar{Q} \in \mathbb{R}^{d \times d}$ being a symmetric matrix, and $\bar{q} \in \mathbb{R}^d$.

Note that the feasible set $S = \mathrm{conv}\{v^1, \ldots, v^{n+1}\}$ of Problem (2.2) is a polytope, i.e. a bounded polyhedral set. In general, a polyhedral set P is defined as an intersection of finitely many halfspaces, i.e.

$$P = P(A, b) = \{x \in \mathbb{R}^n \mid Ax \leq b\}, \tag{2.5}$$

where $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. The following well-known theorem stats the equivalence of both representations.

Theorem 2.1.1. *P is a polyhedral set if and only if there exist sets $\mathcal{V}$ and $\mathcal{E}$ of finite many points such that*

$$P = \mathrm{conv}(\mathcal{V}) + \mathrm{cone}(\mathcal{E}). \tag{2.6}$$

The set $\mathrm{cone}(\mathcal{E})$ is called the recession cone of $P(A, b)$. It is well known that for a polytope we have $\mathrm{cone}(\mathcal{E}) = \{0\}$. And hence Problem (2.2) is a quadratic optimization problem over a bounded polyhedral set.

The quadratic optimization problem (2.2) arises in many contexts. We can encounter it in the optimization of nondifferentiable functions, in approximation theory (P. Wolfe [33]), in economics, in computer sciences, etc. Some typical examples for Problem (2.2) are given below.

Example 2.1.2. *For a given point $y \in \mathbb{R}^n$ Wolfe [33] considered the problem of finding the point of smallest Euclidean distance to y in the convex hull of a given finite point set $\{v^1, ..., v^r\}$. Formally the problem can be written as*

$$\min\{\|x - y\|_2^2 \mid \; x \in \operatorname{conv}\{v^1, ..., v^r\}\}. \tag{2.7}$$

Note that for the objective function we have

$$\|x - y\|_2^2 = (x - y)^T(x - y) = x^T x - 2x^T y + y^T y.$$

And therefore to find the nearest point in a polyeder is a quadratic optimization problem.

Example 2.1.3. *Let $G = (V, E)$ be an undirected graph, where V is the vertex set and E is the edge set. A* clique *of G is a subset of mutually adjacent vertices in V. A clique is called* maximal *if it is not contained in any other clique. A clique is called* maximum *if it has maximum cardinality of all cliques in G. The maximum size of a clique in G is called the* clique number *of G and is denoted by $\omega(G)$. Furthermore, let A denote the adjacency matrix of G. Then Motzkin and Strauss [25] showed that*

$$\frac{1}{2}\left[1 - \frac{1}{\omega(G)}\right] = \min\{x^T A x \mid x \in \Delta_n\}. \tag{2.8}$$

Note that the right hand side of (2.8) *is the standard quadratic optimization problem* (1.6).

Example 2.1.4. *The multi-standard quadratic optimization problem (see. Bomze and Schachinger [7]) has the structure of* (2.2)*:*

$$\min\{\bar{f}(\xi) : \; \xi \in S\}, \tag{2.9}$$

where $\bar{f}(\xi)$ is a quadratic function, and

$$S = \bigotimes_{i=1}^{m} \Delta_{d_i} \subset \bigotimes_{i=1}^{m} \mathbb{R}^{d_i} = \mathbb{R}^d. \tag{2.10}$$

For each polytope P, let $V(P)$ denote its vertex set. Then the set S defined in (2.10) *is a polytope having $\prod_{i=1}^{m} d_i$ vertices, i.e., in this case we have $n = \prod_{i=1}^{m} d_i - 1$. More precisely, the set S can be written as*

$$S = \operatorname{conv}\left\{ \begin{pmatrix} e_1 \\ \vdots \\ e_m \end{pmatrix} : \ e_i \in V(\Delta_{d_i}), \ i = 1, \dots, m \right\}. \tag{2.11}$$

It is worth noting that Problem (2.9) *can be naturally generalized in such a way that in the definition of the polytope S, the sets Δ_{d_i} can be generalized to be arbitrary polytopes given by their vertex sets.*

Example 2.1.5. *Let $Q \in \mathcal{S}_n$ and $a, c \in \mathbb{R}^n$. Then the quadratic knapsack problem is*

$$\begin{aligned} \min \quad & x^T Q x - r^T x \\ s.t. \quad & a^T x \le 1 \\ & x \in \{0,1\}^n. \end{aligned} \tag{2.12}$$

One of the most important applications of Problem (2.12) *is the portfolio management problem, which can be formulated as an optimization problem with a quadratic objective function under a knapsack constraint (see, e.g., [23], [15], [27], [29], [30]). The quadratic function measures both the expected return and the risk. The single knapsack constraint represents the budget restriction.*

As mentioned above, for the case of convex quadratic function, Wolfe proposed an efficient method in [33]. An algorithm for the case of any convex objective function is given in [8]. To our knowledge, for nonconvex problems, there exist only a few algorithms for some very special cases (see, e.g. [3], [17], [21], [31], [34]).

The problem to be considered in this chapter has a nonconvex quadratic objective function, which can have local optima different from global optima.

2.2 Transformation into Quadratic Problem over the Origin Simplex

The purpose of this section is to transform the problem defined in (2.2)-(2.4) into an equivalent quadratic optimization problem over the origin simplex of $\mathbb{R}^n$.

The origin simplex, denoted by O_n, is the following subset of $\mathbb{R}^n$:

$$O_n := \operatorname{conv}\{0, e^1, \dots, e^n\} = \{x \in \mathbb{R}^n : x \geq 0,\ \sum_{i=1}^{n} x_i \leq 1\}, \tag{2.13}$$

where $e^1, \dots, e^n$ are unit vectors of $\mathbb{R}^n$. It is clear that O_n, being the convex hull of $n+1$ affinely independent vectors in $\mathbb{R}^n$, is an $n-$simplex in $\mathbb{R}^n$ (i.e., $\dim(O_n) = n$).

By definition of S in (2.3), we have that for any $\xi \in S$ there exist $x_1, \dots, x_{n+1} \geq 0$ with $\sum_{i=1}^{n+1} x_i = 1$ such that $\xi = \sum_{i=1}^{n+1} x_i v^i$. This gives

$$\begin{aligned} \xi &= \sum_{i=1}^{n+1} x_i v^i = v^{n+1} + \underbrace{(x_{n+1} - 1)}_{= -\sum_{i=1}^{n} x_i} v^{n+1} + \sum_{i=1}^{n} x_i v^i \\ &= v^{n+1} + \sum_{i=1}^{n} x_i (v^i - v^{n+1}). \end{aligned} \tag{2.14}$$

Note that $\sum_{i=1}^{n} x_i = 1 - x_{n+1} \leq 1$. Next, let V be a $d \times n$ matrix having the columns $(v^i - v^{n+1})$, $i = 1, \dots, n$, i.e.,

$$V = ((v^1 - v^{n+1}) \dots (v^n - v^{n+1})). \tag{2.15}$$

Then we have that for any $\xi \in S$ there exists $x \in O_n$ with

$$\xi = v^{n+1} + Vx. \tag{2.16}$$

If the vectors $v^1, \dots, v^{n+1}$ are affinely independent, i.e. the vectors $(v^1 - v^{n+1}) \dots (v^n - v^{n+1})$ are linearly independent, then x in (2.16) is uniquely determined. Otherwise for a $\xi \in S$ there can be several points $x \in O_n$ satisfying (2.16).

Next, define a function $f : \mathbb{R}^n \to \mathbb{R}$ by

$$\begin{aligned} f(x) &:= \bar{f}(v^{n+1} + Vx) \\ &= (v^{n+1} + Vx)^T \bar{Q}(v^{n+1} + Vx) + \bar{q}^T(v^{n+1} + Vx) \\ &= x^T V^T \bar{Q} V x + 2(v^{n+1})^T \bar{Q} V x + \bar{q}^T V x \\ &\quad + (v^{n+1})^T \bar{Q} v^{n+1} + \bar{q}^T v^{n+1}. \end{aligned} \tag{2.17}$$

By defining

$$\begin{aligned} Q &:= V^T \bar{Q} V, \\ q^T &:= 2(v^{n+1})^T \bar{Q} V + \bar{q}^T V, \\ c &:= ((v^{n+1})^T \bar{Q} + \bar{q}^T) v^{n+1}, \end{aligned} \tag{2.18}$$

we have

$$f(x) = x^T Q x + q^T x + c. \tag{2.19}$$

Note that the $n \times n$ matrix Q is symmetric, since from the symmetry of $\bar{Q}$ we get that

$$Q^T = (V^T \bar{Q} V)^T = V^T \bar{Q}^T V = V^T \bar{Q} V = Q.$$

Finally, considering the following quadratic optimization problem

$$\min\{f(x) : x \in O_n\}, \tag{2.20}$$

where O_n is the origin simplex defined in (2.13), and the function f is defined in (2.18)-(2.19), we obtain the following equivalence between Problem (2.2) and Problem (2.20).

Lemma 2.2.1. *The problems (2.2) and (2.20) are equivalent in the following sense: If $x^* \in O_n$ is an optimal solution of Problem* (2.20)*, then*

$$\xi^* = v^{n+1} + Vx^*$$

is an optimal solution of Problem (2.2)*, and if ξ^* is an optimal solution of Problem* (2.2)*, then each $x^* \in O_n$ satisfying $\xi^* = v^{n+1} + Vx^*$ is an optimal solution of Problem* (2.20)*.*

Proof. From (2.14) and (2.16) it follows that for all $\xi \in S$ there exists $x \in O_n$ such that

$$\xi = v^{n+1} + Vx.$$

Thus, the equivalence between problems (2.2) and (2.20) follows from the definitions in (2.19)-(2.18). □

As seen above, the dimension of the transformed problem (2.20) depends on the number of the points contained in the set S. As S is a polytope, it can be represented by the convex hull of its vertex set, which is a subset of $\{v^1, \ldots, v^{n+1}\}$. The question arises as to how we can find the vertex set of the polytope S from the set $\{v^1, \ldots, v^{n+1}\}$, or at least, how we can detect and remove points from the set $\{v^1, \ldots, v^{n+1}\}$, which are not vertices of S. This task helps to reduce the dimension of the transformed problem (2.20) and is the topic of the next section.

2.3 Reducing Dimension of Transformed Problem

We present in this section a simple procedure for detecting and removing points from the set $\{v^1, \ldots, v^{n+1}\}$ which are not vertices of S.

Let $v^j \in \{v^1, \dots, v^{n+1}\}$. Define $I^j := \{1, \dots, n+1\} \setminus \{j\}$ and consider the following linear system in variables λ_i $(i \in I^j)$:

$$v^j = \sum_{i \in I^j} \lambda_i v^i, \; \sum_{i \in I^j} \lambda_i = 1, \; \lambda_i \geq 0 \text{ for all } i \in I^j. \tag{2.21}$$

If System (2.21) has no solution, then the point v^j is a vertex of S, otherwise, it is not, and can be excluded from further consideration. Note that checking System (2.21) can easily be performed by using phase 1 of the well known simplex algorithm. We present below a procedure for determining the vertex set of the polytope S from the set $\{v^1, \dots, v^{n+1}\}$.

Algorithm 2 Procedure for determining the vertex set of S:

Input $\mathcal{P} = \{v^1, \dots, v^{n+1}\}$
$V(S) \leftarrow \emptyset$
$l \leftarrow 0$ ▷ l counts the number of points in $V(S)$
for $j = 1, \dots, n+1$ **do**
    solve (2.21)
    if (2.21) in feasible **then**
        $V(S) \leftarrow V(S) \cup \{v^j\}$
        $l \leftarrow l + 1$
    end if
end for
Output Vertex set $V(S)$ and $l = |V(S)|$

Proposition 2.3.1. *The set $V(S)$ generated by Algorithm 2 is the vertex set of polytope S.*

In the rest of this chapter, we establish an algorithm for finding a globally optimal solution of Problem (2.20).

2.4 Main idea of the algorithm

The main idea of our algorithm for solving Problem (2.20) is briefly outlined as follows.

If the matrix Q in the representation of the quadratic function f is positive semidefinite, then Problem (2.20) can be solved by many known efficient algorithms for convex quadratic optimization problems (e.g. Mehrotra's predictor-corrector interior point algorithm [24]).

If Q is negative semidefinite, then we have a concave optimization problem, where an optimal solution x^* of Problem (2.20) is obtained by checking the vertices of the origin simplex O_n, i.e.,

$$x^* \in \operatorname{argmin}\{f(x) : x \in \{0, e^1, \ldots, e^n\}\}.$$

For the case that Q is indefinite, we recall the following well known result with a simple proof.

Lemma 2.4.1. *Let ∂O_n denote the boundary of O_n. Moreover let the matrix Q in the representation of the function f in* (2.19) *be indefinite. Then*

$$\min\{f(x) \mid x \in O_n\} = \min\{f(x) \mid x \in \partial O_n\}. \tag{2.22}$$

Proof. Suppose there exists a globally optimal solution x^* of problem (2.20) such that $x^* \in \operatorname{int} O_n$. Then from $\nabla f(x^*) = 2Qx^* + q = 0$ it follows that $q = -2Qx^*$, and hence we have for all $x \in O_n$ that

$$\begin{aligned} 0 \leq f(x) - f(x^*) &= x^TQx - (x^*)^TQx^* + (x - x^*)^Tq \\ &= x^TQx - (x^*)^TQx^* - 2(x - x^*)^TQx^* \\ &= x^TQx - 2x^TQx^* + (x^*)^TQx^* \\ &= (x - x^*)^TQ(x - x^*). \end{aligned} \tag{2.23}$$

Let $y \in \mathbb{R}^n$. Then there exists $\alpha \geq 0$ and $x \in O_n$ such that $y = \alpha(x - x^*)$. From (2.23) it follows that $y^T Q y \geq 0$ for all $y \in \mathbb{R}^n$, which is a contradiction to the indefiniteness of Q. $\square$

Obviously, the set ∂O_n consists of $n+1$ simplices of dimension $n-1$, (i.e., $(n-1)-$simplices). Denote these simplices by $B_1, \ldots, B_{n+1}$, where

$$\begin{aligned} &B_i = \operatorname{conv}\left(\{0, e^1, \ldots, e^n\} \setminus \{e^i\}\right), \ i = 1, \ldots, n, \ \text{and} \\ &B_{n+1} = \operatorname{conv}\{e^1, \ldots, e^n\}, \end{aligned} \tag{2.24}$$

From Lemma 2.4.1, Problem (2.20) can be replaced by $n+1$ problems of the form

$$\min\{f(x) : x \in B_i\}, \ i = 1, \ldots, n+1. \tag{2.25}$$

Note that every problem in (2.25) has again the form (2.2), however, in a space of lower dimension, and therefore, it can be handled by the same procedure as described above.

First the simplex B_{n+1} is exactly the standard simplex of $\mathbb{R}^n$. Thus the transformation of Problem (2.25) for $i = n+1$ into a quadratic problem over the origin simplex O_{n-1} of $\mathbb{R}^{n-1}$ is performed as presented in Section 2.2.

For other problems in (2.25) we obtain quadratic problems over the origin simplex $O_{n-1} \subset \mathbb{R}^{n-1}$ immediately by the following lemma.

Lemma 2.4.2. *For each $i = 1, \ldots, n$, let Q_i be the $(n-1) \times (n-1)$ matrix obtained from Q by removing the i-th row and the i-th column, let q_i be the vector obtained from q by removing its i-th component, and let $c_i = c$. Then the i-th problem in (2.25) can be written as the problem*

$$\min\{y^T Q_i y + q_i^T y + c_i : y \in O_{n-1}\}. \tag{2.26}$$

Proof. The i-th problem in (2.25) is

$$\min\{f(x) = x^T Qx + q^T x + c : x \in B_i\}.$$

Now let $x \in B_i$. Then $x_i = 0$ and for $I^i := \{1, \ldots, n\} \setminus \{i\}$ we have that

$$f(x) = \sum_{k,j \in I^i} Q_{k,j} x_k x_j + \sum_{k \in I^i} q_k x_k + c. \tag{2.27}$$

Defining $y \in \mathbb{R}^{n-1}$ with $y_k = x_k$ for $k = 1, \ldots, i-1$ and $y_k = x_{k+1}$ for $k = i+1, \ldots, n$. In other words, y can be constructed from x by removing coordinate x_i. Obviously we have that $y \geq 0$ and

$$\sum_{k=1}^{n-1} y_k \leq \sum_{j=1}^{n} x_j \leq 1,$$

i.e. $y \in O_{n-1}$, and with (2.27) we get that

$$x^T Qx + q^T x + c = y^T Q_i y + q_i^T y + c_i,$$

and the results follows. $\square$

The whole procedure for computing an optimal solution of Problem (2.20) is presented in the next Section.

2.5 The algorithm and its finite convergence

Based on the results from he previous sections, we establish an algorithm for globally solving the following quadratic problem over the origin simplex:

$$\begin{array}{ll} \min & x^T Qx + q^T x \\ \text{s.t.} & e^T x \leq 1 \\ & x \geq 0, \end{array} \tag{2.28}$$

where, again, $Q \in \mathcal{S}_n$ and $q \in \mathbb{R}^n$.

Algorithm 3 Solving a quadratic problem over the origin simplex

1: **Input** Problem $P = \min\{x^TQx + q^Tx \mid x \in O_n\}$
2: $\gamma \leftarrow \min\{x^TQx + q^Tx \mid x \in \{0, e^1, \dots, e^n\}\}$
3: $x^* \leftarrow \text{argmin}\{x^TQx + q^Tx \mid x \in \{0, e^1, \dots, e^n\}\}$
4: $\mathcal{P} \leftarrow \{P\}$ ▷ for the 1st iteration $\mathcal{P}$ contains only P
5: **while** $\mathcal{P} \neq \emptyset$ **do**
6:     choose $P \in \mathcal{P}$
7:     **if** P is a convex or concave minimization problem **then**
8:         solve P
9:         **if** $\min P < \gamma$ **then**
10:             $\gamma \leftarrow \min P$
11:             $x^* \leftarrow \text{argmin} P$
12:         **end if**
13:     **else**
14:         construct $n+1$ subproblems $P_1, \dots, P_{n+1}$ as in (2.25)
15:         $\mathcal{P} \leftarrow \mathcal{P} \cup \{P_1, \dots, P_{n+1}\}$
16:     **end if**
17:     $\mathcal{P} \leftarrow \mathcal{P} \setminus \{P\}$
18: **end while**
19: **Output** Optimal value γ and optimal solution x^*

Theorem 2.5.1. *The Algorithm 3 solves Problem* (2.28) *after finite many iterations.*

Proof. The origin simplex has finitely many faces and therefore the algorithm has so solve finitely many subproblems. From Lemma 2.4.1 it follows that γ is the optimal value and x^* is the optimal solution of P. □

To check if P is a convex or concave minimization problem in Line 7, we check the definiteness of the objective matrix Q. Unfortunately from the definiteness of Q we cannot conclude about the definiteness of a submatrix Q_i. Therefore in every subproblem P_i we need to check its convexity (concavity), which means that we have to check definitness of every submatrix of Q.

2.5.1 Improving the algorithm using lower bounds

Idea: Throughout the algorithm, for every indefinite quadratic problem (P) to be handled, we try to compute a lower bound, $\mu(P)$, of its optimal value. If $\mu(P)$ is not smaller than the current best function value, then P is deleted immediately. Therefore we propose a method to compute a lower bound. Let Problem (P) be formulated as

$$\min\{x^T Px + p^T x : x \in O\}, \tag{P}$$

where P and p are a (symmetric indefinite) matrix and a vector of appropriate sizes, and O is the origin simplex. We propose below a simple method for computing a lower bound for the optimal value $\mu(P)$.

Denote by P_{i*} the i-th row of matrix P, by $V(O)$ the vertex set of simplex O, and by a the vector whose components a_i are determined by

$$a_i := \min\{P_{i*}x : x \in V(O)\}. \tag{2.29}$$

Lemma 2.5.2. *A lower bound $\mu(P)$ of the optimal value of Problem* (P) *can be computed by*

$$\mu(P) = \min\{(a+p)^T x : \; x \in O\}. \tag{2.30}$$

Proof. As $x \geq 0$, it follows from (2.29) that $x^T Px \geq a^T x$ for all $x \in O$, which implies that the objective function of Problem (P) is greater than or equal to the one of (2.30) in O, and the theorem follows. $\square$

2.6 Algorithm for checking copositivity via (semi)definiteness

A symmetric matrix $A \in \mathbb{R}^{n\times n}$ is called copositive, if $x^T Ax \geq 0$ for all $x \geq 0$. Checking copositivity is a co-NP-hard problem and therefore much harder than checking definiteness. In the literature, there exist some methods to check a copositivity of a matrix such as Bundfuss and Dür in [10] by using simplicial partions. In [32] Sponsel, Bundfuss and Dür improved that algorithm furthermore. It is worth mentioning that in [4] Bomze and Eichfelder also presented a method to check copositivity by combining difference-of-convex (d.c.) decompositions into a branch-and-bound algorithm of ω-subdivisions. In this section, we apply Algorithm 3 for checking copositivity of a matrix based on successively using the methods for checking definiteness.

Lemma 2.6.1. *A matrix $A \in \mathbb{R}^{n\times n}$ is non-copositive, if and only if*

$$\min\{x^T Ax : x \in O_n\} < 0. \tag{2.31}$$

Proof. The sufficient condition is trivial. For the necessary condition, suppose we do not have (2.31), i.e., $x^T Ax \geq 0$ for all $x \in O_n$. Since

$$\mathbb{R}^n_+ = \{x \in \mathbb{R}^n : x = \alpha y, y \in O_n, \alpha \geq 0\},$$

it follows that $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n_+$, i.e., A is copositive, a contradiction. □

The Problem contained in Condition (2.31) is a quadratic optimization problem over the origin simplex, and therefore, in principle, we can apply Algorithm 3 to solve it. However, as we in fact only need to show whether or not there exists a point $x^* \in O_n$ satisfying $f(x^*) < 0$, we propose the following algorithm, which is a slightly modified version of Algorithm 3.

Algorithm 4 Checking copositivity of a matrix A

Input symmetric matrix $A \in \mathbb{R}^{n\times n}$
$\gamma \leftarrow \min\{x^T Ax \mid x \in \{0, e^1, \ldots, e^n\}\}$
$\mathcal{P} \leftarrow \{\min\{x^T Ax \mid x \in O_n\}\}$
while ($\mathcal{P} \neq \emptyset$) and ($\gamma \geq 0$) **do**
  choose $P \in \mathcal{P}$
  if P is a convex or concave minimization problem **then**
    solve P
    if $\min P < \gamma$ **then**
      $\gamma \leftarrow \min P$
    end if
  else
    construct $n+1$ subproblems $P_1, \ldots, P_{n+1}$ as in (2.25)
    $\mathcal{P} \leftarrow \mathcal{P} \cup \{P_1, \ldots, P_{n+1}\}$
  end if
  $\mathcal{P} \leftarrow \mathcal{P} \setminus \{P\}$
end while
if $\gamma \geq 0$ **then**
  Output: A is copositive
else
  Output: A is not copositive
end if

Theorem 2.6.2. *Algorithm 4 terminates after solving finite many subproblems.*

2.7 Illustrative examples and preliminary computational experiments

2.7.1 The pseudo-code

First we give a pseudo-code of our algorithm for solving the quadratic problem over the origin simplex given in (2.20), i.e. the problem

$$\begin{aligned} \min \quad & f(x) = x^T Qx + q^T x + c \\ \text{s.t.} \quad & e^T x \leq 1 \\ & x \geq 0, \end{aligned} \tag{2.32}$$

where $Q \in \mathcal{S}_n$, $e = (1, \ldots, 1)^T \in \mathbb{R}^n$, $q \in \mathbb{R}^n$, and $c \in \mathbb{R}$.

While in Algorithm 3 no lower bounds were implemented, therefore we have to solve every subproblem of (2.32), which is a not very efficient way to solve the problem. In the following Algorithm 5 a lower bound was introduced to hopefully reduce the number of subproblems the algorithm has to solve. Note that the number of subproblems, which are eliminated, depends on the lower bound. If the lower bound is not good, in worst case we still need to solve all subproblems.

In the following Algorithm 5 in Line 9 we only consider subproblems which has a better lower bound than the best function value γ found so far, i.e. subproblems with worse lower bound than γ are eliminated from further consideration.

Algorithm 5 Algorithm solving Problem 2.32

Input: $n \in \mathbb{N}, Q \in \mathbb{R}^{n\times n}$, $q \in \mathbb{R}^n$, $c \in \mathbb{R}$
$\gamma \leftarrow \min\{Q_{ii} + q_i + c \mid i = 1, \ldots, n\}$
$\mathcal{P}_n \leftarrow \{P\}$.
$\mu(P) = -\infty$
$M \leftarrow \{\mu(P)\}$
call solve$(\mathcal{P}_n, n, M)$
function SOLVE$(\mathcal{P}_k, k, M)$
    while $\mathcal{P}_k \neq \emptyset$ **do**
        $mini \leftarrow \min\{i \in \{1, \ldots, |\mathcal{P}_k|\} \mid \mu(P_i) < \gamma, P_i \in \mathcal{P}_k\}\}$
        if P_{mini} is convex or concave **then**
            solve P_{mini}
            if $\min P_{mini} < \gamma$ **then**
                $\gamma \leftarrow \min P$
                update x^*
            end if
        else
            $\mathcal{P}_{mini,k-1} \leftarrow \{P_{mini,1}, \ldots, P_{mini,k+1}\}$
            for $i = 1, ..., k$ **do**
                compute $\mu(P_i)$
            end for
            $M_{mini} \leftarrow \{\mu(P_{mini,1}), \ldots, \mu(P_{mini,k+1})\}$
            call solve$(\mathcal{P}_{mini,k-1}, k-1, M_{mini})$
        end if
        $\mathcal{P}_k \leftarrow \mathcal{P}_k \setminus \{P_{mini}\}$
    end while
end function
Output: Optimal value: γ, optimal solution: x^*

The pseudo-code is implemented in C++ using the **gsl library** (available at `https://www.gnu.org/software/gsl/`). The test problems are run on an **intel core duo processor @3,2 Ghz and 2 GB RAM memory** on an Ubuntu base system.

In line 19: $\mu(P_i)$ denotes the lower bound of Problem $P_i \in \mathcal{P}_k$ determined by (2.30). Obviously we are only considering subproblems, whose lower bound is not worse than the best upper bound γ found so far. To determine the definiteness of the objective function matrix Q_P of subproblem P, we use the Cholesky decomposition procedure from the **gsl-library** to compute the smallest and greatest eigenvalue of the matrix Q_P.

In line 11: an implementation of Mehrotra's predictor corrector interior point method [24] by Ewgenij Hübner, a former Ph.D. graduate of the Trier University, is used to solve P_{mini}, whenever P_{mini} is a convex quadratic problem. Note that if a subproblem $P \in \mathcal{P}$ is concave, then the optimal solution of P is a vertex of the origin simplex. Since the vertex set of any sub-problem is a subset of the original problem (2.32), for which we already found the optimal value and vertex in the first line, we have that $\min P \geq \gamma$ and hence we do not need to solve P. The main function solve$(\mathcal{P}_k, k, M)$ is a recursive function, which will call itself to solve non-convex and non-concave subproblems.

2.7.2 Illustrative Examples

We present some numerical examples to illustrate the algorithm for solving the quadratic problem over the origin simplex. The examples originate from the test problems considered in [6].

Example 2.7.1. *We discuss here the four examples considered by I.M. Bomze and E. de Klerk in [6]. These are standard quadratic problems of the form*

$$\begin{aligned} \min \quad & x^T Q x \\ s.t. \quad & e^T x = 1 \\ & x \geq 0, \end{aligned}$$

which originated from maximum clique problems (see Example 2.1.3) and are equivalent to completely positive programs of the form:

$$\begin{aligned} \min \quad & \langle Q, X \rangle \\ s.t. \quad & \langle ee^T, X \rangle = 1 \\ & X \in \mathcal{CP}. \end{aligned}$$

The dual of the above completely positive program is the copositive program

$$\begin{aligned} \max \quad & \lambda \\ \text{s.t.} \quad & Q - \lambda E \in \mathcal{COP} \\ & \lambda \in \mathbb{R}. \end{aligned}$$

We point out that in Chapter 5 of this thesis, the equivalence between a class of quadratic problems including the standard quadratic problem and the copositive program will be shown directly.

In [6], Bomze and Klerk present a solution method for the resulting copositive program by using the LP-based approximations $\mathcal{C}^r$, ($r = 0, 1, \ldots$) and semidefinite programming (SDP) approximations $\mathcal{K}^r$, ($r = 0, 1, \ldots$) of the copositive cone, which we have introduced in Section 1.2.5. Note that, as mentioned in [6], these approaches only provide one sided bounds without further information about the quality of the current best optimal value. Furthermore we will compare our numerical results with the results presented in [9] by Bundfuss and Dür.

Problem 1: *This problem has the objective function matrix*

$$Q = \begin{pmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{pmatrix} \in \mathbb{R}^{5\times 5},$$

so the problem corresponds to the maximum clique number in a pentagon. As it is well known, this problem has the optimal value $\frac{1}{2}$*, i.e. the maximum clique number in a pentagon is 2.*

Throughout our algorithm, 12 convex and 4 concave subproblems are solved. The time needed to compute the optimal solution is 0.000443 seconds.

Note that in [6], using the approximation cones $\mathcal{C}^r$ *and* $\mathcal{K}^r$ *for* $r = 0, 1$ *the authors obtain for this problem the following bounds: For* $\mathcal{C}^0$ *and* $\mathcal{C}^1$ *they obtain* $\frac{1}{3}$*. The approximation cones* $\mathcal{K}^0$ *and* $\mathcal{K}^1$ *yield the bounds* $\frac{1}{\sqrt{5}}$ *and* $\frac{1}{2}$*, respectively, i.e.* $\mathcal{K}^1$ *yields the (known) exact optimal solution. With their algorithm in [9], Bundfuss and Dür solved this problem exactly within* 6 *iterations and* 0.01 *seconds.*

Problem 2: *This problem is to determine the maximum clique number of* *an icosahedron. The corresponding matrix* Q *is*

$$Q = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \in \mathbb{R}^{12\times 12}.$$

It is well known that the maximum clique number of such an icosahedron is 3*, i.e., the optimal value of the corresponding standard quadratic problem is* $\frac{1}{3}$.

Our algorithm needs 0.00126 *seconds yielding the optimal value* 0.333333 *after solving* 24 *convex and* 2 *concave subproblems.*

For this problem the bound for the approximation cone $\mathcal{C}^1$ *is* 0 *and the bound for* $\mathcal{K}^1$ *is* 0.309*. In this case* $\mathcal{K}^1$ *does not yield the exact optimal value. The authors in [6] did not report further bounds for* $r > 1$ *due to the difficulties of the approximations in high dimensions. In [9] Bundfuss and Dür solved this problem in* 158 *iterations and needed* 0.54 *seconds to compute the optimal value.*

Problem 3: *This is a mathematical model in population genetics, where the corresponding matrix Q is*

$$Q = \begin{pmatrix} 14 & 15 & 16 & 0 & 0 \\ 15 & 14 & 12.5 & 22.5 & 15 \\ 16 & 12.5 & 10 & 26.5 & 16 \\ 0 & 22.5 & 26.5 & 0 & 0 \\ 0 & 15 & 16 & 0 & 14 \end{pmatrix}, \in \mathbb{R}^{5\times 5}.$$

It is known that the optimal value of this problem is $16\frac{1}{3}$. *In [6] the authors obtained from* $\mathcal{C}^1$ *the bound* 21.0, *and* $\mathcal{K}^1$ *yields the exact optimal value. Bundfuss and Dür's algorithm [9] solved this problem within* 0.03 *seconds and* 44 *iterations. Our algorithm obtained the optimal value* 16.333333 *after* 0.000528 *seconds. The algorithm has solved* 10 *convex subproblems.*

Problem 4: *The fourth and last example arises from portfolio optimization. In this case* $x \in \Delta$ *(the standard simplex) corresponds to a portfolio and* x_i *is the fraction of the capital to be invested in item* i. *Given a portfolio* $x \in \Delta$, *a risk* $x^T \bar{Q} x$ *and a return* $r^T x$, *the optimization problem under consideration is*

$$\min\{x^T(\bar{Q} - rr^T)x \mid x \in \Delta\}$$

(for more details, see [6]). The following matrix has been taken from [6]:

$$Q = \begin{pmatrix} 0.9044 & 0.1054 & 0.5140 & 0.3322 & 0 \\ 0.1054 & 0.8715 & 0.7385 & 0.5866 & 0.9751 \\ 0.5140 & 0.7385 & 0.6936 & 0.5368 & 0.8086 \\ 0.3322 & 0.5866 & 0.5368 & 0.5633 & 0.7478 \\ 0 & 0.9751 & 0.8086 & 0.7478 & 1.2932 \end{pmatrix} \in \mathbb{R}^{5\times 5}.$$

The known optimal value is 0.483933. *After considering* 7 *convex subproblems,* *our algorithm terminated yielding the exact optimal value* 0.483933 *(*0.000672 *seconds needed).*

In [6], the approximation cone $\mathcal{C}^1$ *provides a bound of* 0.3015 *and* $\mathcal{K}^1$ *yields a bound of* 0.4839*. In [9], the algorithm takes* 27 *iterations* (0.001 *seconds*) *to obtain an accuracy of* 10^{-6}.

2.7.3 Computational experiments

In the following we generated random instances of the origin quadratic problem (2.32), where the entries of the symmetric matrix $Q \in \mathbb{R}^{n\times n}$ were uniformly distributed in $[-10, 10]$. For each size we created 40 instances. The algorithm stopped when there were no more subproblems with a lower bound smaller than the best value γ found so far. This can either happen if there are no subproblems left, or the lower bounds of the remaining subproblems are worse than the best value found so far. Note that for testing our algorithm, the accuracy is taken depending on the accuracy of the solver for convex quadratic optimization “sl_cq“ in [18], which is 10^{-6}.

The computational results (in the sense of average) are summarized in the following table.

n	time in sec.	# concave subproblems	# convex subproblems
10	0.000	60.37	53.72
25	0.013	273.5	1,781.25
50	0.127	6,577.2	41,224.37
100	43.876	72,499.37	429,928.72
500	2613.342	1,027,257.72	2,890,735.12

To conclude this chapter, we note that the implementation of this algorithm was not meant to be competitive with other “high-end“ and/or “big data“

algorithms, it is a mere proof-of-concept, that the method introduced in Chapter 2 can work quite well.

It is worth noting that the recursive approach is a very fast method to solve problems of moderate sizes, but for higher dimensional problems the memory needed for such a recursive program can be very big, which even some server computers can not provide. Also there is still room for improvement for this program, e.g. a faster implementation to determine whether a matrix is semidefinite or not, also the convex solver used in this program may not be the best implementation for convex quadratic programming. Therefore we did not test this program for higher dimensional problems on a high-performance server computer.

Note that in [9] the authors presented numerical results for randomly generated instances. However we cannot compare our results with theirs, because Bundfuss and Dür uses the procedure ”.randomize()“ of the CVM Class Library by Sergei Nikolaev (available at `www.cvmlib.com`) to generate the objective function matrix. Unfortunately this procedure generates negative semidefinite matrices. Therefore the problems considered in [9] were all concave minimization problems. Therefore Bundfuss and Dür could present very good numerical results. It is unclear how the algorithm would perform for general quadratic problems.

CHAPTER 3

Completely Positive Modelling of Quadratic Problems

3.1 Introduction

In previous chapter we already showed that quadratic optimization problems (QP) have a wide area of applications. It is well known that the nonconvex (QP) is an NP-hard problem, even for simple cases such as the standard quadratic problem. In the last two decades, the idea of formulating (QP) equivalently as a so called copositive optimization problem or its dual called completely positive program was developed. These are convex programming problems with conic constraints. A survey on them can be found in [16]. The first completely positive reformulation and its dual, a copositive optimization problem, is due to Bomze et al in [5] for the standard quadratic problem. An efficient algorithm to solve the copositive reformulation of the standard quadratic problem is established by Bundfuss and Dür in [9], (see also [10]), using iteratively polyhedral inner and outer approximations of the copositive cone.

In [11], Burer established a general completely positive reformulation for (QP) restricted by equality constraints and even with binary constraints such as in the quadratic knapsack problem (see Example 2.1.5). However unlike the reformulation of the standard quadratic problem, in this reformulation, the resulting completely positive optimization problem is in general not strictly feasible and therefore, there may exist a nonzero duality gap, so that it is not suitable to consider the dual problem, which is a copositive optimization problem.

In this chapter, we consider the quadratic optimization problem with inequality and mixed binary constraints. Our purpose is to construct for this problem two kinds of equivalent completely positive optimization problems, which we call lifted problems, and to show that in many cases, their corresponding dual problems are strictly feasible, so that strong duality holds. The construction consists of two stages. At the first stage, we construct for the given quadratic optimization problem two different equivalent quadratic problems in two different spaces.

The second part of this chapter will deal with the lifting procedure of the resulting quadratic problems into two different kinds of completely positive optimization problems.

The duals of these completely positive optimization problems are then constructed, and it is shown that, under some mild conditions, they are strictly feasible.

3.2 Quadratic Optimization Problem and Concept of Lifted Problem

Consider the following quadratic optimization problem:

$$\begin{array}{ll} \min & x^T Q x \\ \text{s.t.} & x \in F(QP), \end{array} \tag{QP}$$

where $Q \in \mathbb{R}^{d\times d}$ is a real symmetric matrix, and $F(QP)$ is some nonempty feasible set in $\mathbb{R}^d$.

Define the following two sets:

$$\mathcal{C} := \operatorname{conv}\{xx^T : x \in F(QP)\} \tag{3.1}$$

$$\mathcal{R} := \operatorname{conv}\{yy^T : y \in \operatorname{rec} F(QP)\}, \tag{3.2}$$

where for each set D, $\operatorname{rec}(D)$ and $\operatorname{conv}(D)$ are the recession cone and the convex hull of D, respectively. By definition, it is clear that the set $\mathcal{R}$ is a convex cone in $\mathbb{R}^{d\times d}$.

Consider the optimization problem constructed from (QP):

$$\begin{array}{ll} \min & \langle Q, X\rangle \\ \text{s.t.} & X \in \mathcal{C} + \mathcal{R}, \end{array} \tag{CP}$$

which is called the lifted problem according to the original problem (QP). Let $F(CP)$ denote the feasible set of the lifted problem (CP). The following lemma is the basis of all lifting approaches considered in this thesis.

Lemma 3.2.1. *Assume that an optimal solution $\bar{x}$ of* (QP) *exists. Then the problems* (QP) *and* (CP) *are equivalent in the sense that they have the same optimal value, and any optimal solution $\bar{X}$ of* (CP) *is a convex combination of matrices $x^i(x^i)^T$, where x^i are optimal solutions of* (QP)*.*

Proof. Let μ be the optimal value of Problem (QP) and γ be optimal value of Problem (CP), respectively. If $\bar{x}$ exists, then $\mu > -\infty$. This implies $y^T Q y = \langle Q, yy^T \rangle \geq 0$ for all $y \in \operatorname{rec} F(QP)$, since otherwise, from $(\bar{x} + \lambda y) \in F(QP)$ for all $\lambda \geq 0$ it would follow that

$$(\bar{x} + \lambda y)^T Q(\bar{x} + \lambda y) = \bar{x}^T Q \bar{x} + 2\lambda \bar{x}^T Q y + \lambda^2 y^T Q y \to -\infty \text{ for } \lambda \to \infty.$$

The matrix $\bar{x}\bar{x}^T$ is feasible for (CP), and therefore

$$\gamma \leq \langle Q, \bar{x}\bar{x}^T \rangle = \mu.$$

On the other hand let

$$\bar{X} := \sum_{i=1}^{k} \lambda_i x^i (x^i)^T + \sum_{j=1}^{l} \mu_j y^j (y^j)^T$$

be an optimal solution for (CP), where $x^1, \ldots, x^k \in F(QP)$, $y^1, \ldots y^l \in \operatorname{rec} F(QP)$ and $\lambda_1, \ldots, \lambda_k \geq 0$ with $\sum_{i=1}^{k} \lambda_i = 1$ and $\mu_1, \ldots, \mu_l \geq 0$. Then we have

$$\begin{aligned}
\mu \geq \gamma &= \langle Q, \bar{X} \rangle \\
&= \sum_{i=1}^{k} \lambda_i \underbrace{\langle Q, x^i (x^i)^T \rangle}_{\geq \langle Q, \bar{x}\bar{x}^T \rangle} + \sum_{j=1}^{l} \underbrace{\mu_j \langle Q, y^j (y^j)^T \rangle}_{\geq 0} \\
&\geq \langle Q, \bar{x}\bar{x}^T \rangle \sum_{i=1}^{k} \lambda_i = \mu.
\end{aligned}$$

Therefore we have $\mu = \gamma$. Furthermore it also implies that $\langle Q, y^j (y^j)^T \rangle = 0$ for all $j = 1, \ldots, l$ and $\langle Q, x^i (x^i)^T \rangle = \langle Q, \bar{x}\bar{x}^T \rangle$, i.e. x^i is optimal for (QP) for all $i = 1, \ldots, k$. $\square$

Unlike the original Problem (QP) of minimizing a not necessarily convex quadratic function over a not necessarily convex set, the lifted problem (CP) is a convex optimization problem. Moreover, in many cases, (CP) is a completely positive programming problem. Therefore, as every local optimal solution obtained by solving (CP) is a global one, we can obtain global optimal solutions for (QP), by computing local optimal solutions of (CP).

Notice that, we do not try to remove the difficulties of (QP), but we shift these difficulties into the feasible set $F(CP)$, whose representation depends on the definition of the set $F(QP)$. More precisely, from a given problem of type (QP), we try to construct some equivalent representations of the feasible set $F(QP)$ which can then be lifted into suitable forms of feasible sets $F(CP)$ of Problem (CP) so that the latter problem is a completely positive optimization problem. This is the subject of the next section.

3.3 Equivalent Representations of (QP)

In what follows, we consider the case where the feasible set $F(QP)$ of Problem (QP) is defined by linear and binary constraints, i.e. $F(QP)$ can be written as

$$F(QP) = P \cap \{x \mid x_i \in \{0,1\} \text{ for } i \in \mathcal{B}\}, \tag{3.3}$$

where $\mathcal{B}$ is the set of indices of binary variables, and P is a polyhedral subset of the nonnegative orthant $\mathbb{R}^d_+$. In general, P can be represented as the intersection of a finite number of halfspaces, i.e.

$$P = \{x \in \mathbb{R}^d_+ \mid Bx \leq b\}, \tag{3.4}$$

where $B \in \mathbb{R}^{m \times d}$ and $b \in \mathbb{R}^m$, furthermore we assume that there exists $x \in P$ such that $Bx < b$, i.e. there are no hidden equations in the system $Bx \leq b$.

Below we present two equivalent representations of the set $F(QP)$ in $\mathbb{R}^n$ with $n := d + 1$ and $\mathbb{R}^{m+n}$, respectively, in such a way that the resulting quadratic problems can then be lifted into completely positive optimization problems thereafter.

We begin with the equivalent representation of the set $F(QP)$ in $\mathbb{R}^{d+1}$.

First, we add a redundant inequality of the form $\alpha^T x \leq 1$ with $\alpha \in \mathbb{R}^d_+$ to the system defining $P \cap \{x \mid x_i \leq 1,\ i \in \mathcal{B}\}$, i.e., it must fulfil that $\alpha^T x \leq 1$ for all $x \in P \cap \{x \mid x_i \leq 1,\ i \in \mathcal{B}\}$.

Such a vector α always exists, and can be constructed in different ways. Some important examples are given below.

Example 3.3.1. *i) In any case for $\alpha = 0$ we always have $\alpha^T x \leq 1$ for all $x \in P \cap \{x \mid x_i \leq 1,\ i \in \mathcal{B}\}$.*

ii) Let $\mathcal{B} = \emptyset$. If P is bounded, then the following pair of primal and dual problems are solvable

$$\begin{array}{llcll} \max & e^T x & \qquad & \min & b^T y \\ \text{s.t.} & Bx \leq b & & \text{s.t.} & B^T y \geq e \\ & x \geq 0 & & & y \geq 0. \end{array}$$

From the assumption that there exists an $\bar{x} \geq 0$ such that $B\bar{x} < b$, we have $P \neq \{0\}$. And hence we have $\max\{e^T x \mid x \in P\} > 0$. Furthermore by assumption that $P \neq \emptyset$ both problems above are feasible, and therefore there exists $\bar{y} \geq 0$ with $B^T \bar{y} \geq e$ and $b^T \bar{y} > 0$. In this case we choose $\alpha := \frac{B^T \bar{y}}{\bar{y}^T b} > 0$ and obtain for all $x \in P$

$$\alpha^T x = \frac{\bar{y}^T B x}{\bar{y}^T b} \leq \frac{\bar{y}^T b}{\bar{y}^T b} = 1 \tag{3.5}$$

iii) If $\mathcal{B} \neq \emptyset$, then choose any α fulfilling $\begin{cases} 0 < \alpha_j \leq 1/(n-1), & \textit{if } j \in \mathcal{B}, \\ \alpha_j = 0, & \textit{else.} \end{cases}$

Using the redundant constraint, we can write

$$P = \{x \in \mathbb{R}_+^{n-1} \mid Bx \le b, \alpha^T x \le 1\}. \tag{3.6}$$

Once the redundant inequality $\alpha^T x \le 1$ is constructed, define a vector $a \in \mathbb{R}^n$ and a matrix $A \in \mathbb{R}^{(m+n)\times n}$ by

$$a^T := (\alpha^T, 1) \in \mathbb{R}^n, \text{ and } A := \begin{pmatrix} ba^T - (B,0) \\ I_n \end{pmatrix} \in \mathbb{R}^{(m+n)\times n}, \tag{3.7}$$

with I_n being the $n \times n$ identity matrix. Furthermore define the set $P_{iq} \subset \mathbb{R}^n$ by

$$P_{iq} := \{x \in \mathbb{R}^n \mid Ax \ge 0, \ a^T x = 1\}. \tag{3.8}$$

And we have the following relationship between P and P_{iq}.

Lemma 3.3.2. *Let P and P_{iq} be defined as above. Then we have*

$$x \in P \textit{ if and only if } \begin{pmatrix} x \\ 1 - \alpha^T x \end{pmatrix} \in P_{iq}.$$

Proof. First let $x \in P$. Then $1 - \alpha^T x \ge 0$ and

$$a^T \begin{pmatrix} x \\ 1 - \alpha^T x \end{pmatrix} = \alpha^T x + 1 - \alpha^T x = 1.$$

Furthermore we have

$$A \begin{pmatrix} x \\ 1 - \alpha^T x \end{pmatrix} = \begin{pmatrix} ba^T - (B,0) \\ I_n \end{pmatrix} \begin{pmatrix} x \\ 1 - \alpha^T x \end{pmatrix} = \begin{pmatrix} b - Bx \\ \begin{pmatrix} x \\ 1 - \alpha^T x \end{pmatrix} \end{pmatrix} \ge 0, \tag{3.9}$$

i.e. $\begin{pmatrix} x \\ 1 - \alpha^T x \end{pmatrix} \in P_{iq}$.

To show the reverse inclusion let $\begin{pmatrix} x \\ 1 - \alpha^T x \end{pmatrix} \in P_{iq}$. Then it follows from (3.9) that $b - Bx \ge 0$ and $x \ge 0$, i.e. $x \in P$.

□

With this equivalent representation for P we obtain an equivalent representation, denoted by $F(QP_{iq})$, for the set $F(QP)$ in $\mathbb{R}^n$.

$$F(QP_{iq}) := \{x \in \mathbb{R}^n \mid \ Ax \geq 0,\ a^T x = 1,\ x_i \in \{0,1\},\ i \in \mathcal{B}_{iq}\}, \tag{3.10}$$

where

$$\mathcal{B}_{iq} = \mathcal{B}. \tag{3.11}$$

To construct the next equivalent representation for $F(QP)$ we will introduce an equivalent representation for $F(QP_{iq})$. For this purpose we use the fact that every inequality constraint can be written as an equality constraint using a nonnegative slack variable. Let $x \in F(QP_{iq})$ which implies that $Ax \geq 0$, i.e. $(B,0)x \leq 1$ and we have

$$(B,0)x \leq b \text{ if and only if } s + (B,0)x = b \text{ for } s \geq 0.$$

Let

$$\begin{aligned} P_e &:= \left\{ \begin{pmatrix} s \\ x \end{pmatrix} \in \mathbb{R}_+^{m+n} \mid s + (B,0)x = b,\ 0^T s + a^T x = 1 \right\} \\ &= \left\{ \begin{pmatrix} s \\ x \end{pmatrix} \in \mathbb{R}_+^{m+n} \mid (I_m, B, 0) \begin{pmatrix} s \\ x \end{pmatrix} = b,\ 0^T s + a^T x = 1 \right\}. \end{aligned} \tag{3.12}$$

Define

$$\begin{aligned} c^T &:= (0, \ldots, 0, a^T) \in \mathbb{R}^{m+n}, \\ C &:= (bc^T - (I_m, B, 0)) \in \mathbb{R}^{m \times (m+n)}, \end{aligned} \tag{3.13}$$

Note that

$$bc^T = \begin{pmatrix} b_1 c^T \\ \vdots \\ b_m c^T \end{pmatrix} \in \mathbb{R}^{m \times m+n}.$$

Then we have

$$P_e = \{y \in \mathbb{R}^{m+n}_+ \mid Cy = 0, c^T y = 1\}, \tag{3.14}$$

Actually, we simply get P_e from P_{iq} by using m nonnegative slack variables. The equivalence between these two sets, P_{iq} and P_e, is given in the following lemma.

Lemma 3.3.3. *Let P_{iq} and P_e be defined as in* (3.8) *and* (3.14)*, respectively. Then*

$$Ax \in P_e \text{ if and only if } x \in P_{iq}.$$

Proof. First, we show that for all $y \in P_e$ there exists an $x \in P_{iq}$ such that $y = Ax$. Therefore let $y := \begin{pmatrix} s \\ x \end{pmatrix} \in P_e$. From $y \geq 0$ it follows that $x \geq 0$ and $s \geq 0$. Then by construction of c we have $1 = c^T y = 0s + a^T x = a^T x$, and furthermore we have

$$0 = Cy = (bc^T - (I_m, B, 0))y = ba^T x - s - (B, 0)x,$$

therefore $0 \leq s = (ba^T - (B, 0))x$ and it follows that

$$0 \leq y = \begin{pmatrix} (ba^T - (B,0)) \\ I_n \end{pmatrix} x = Ax, \text{ i.e. } x \in P_{iq}.$$

To show the other direction, let $x \in P_{iq}$ and $y = Ax$. Then, again by construction we have

$$y \geq 0, \; c^T y = c^T Ax = (0, \ldots, 0, a^T) \begin{pmatrix} ba^T - (B,0) \\ I_n \end{pmatrix} x = a^T x = 1.$$

Furthermore, we have

$$\begin{aligned}
Cy = C(Ax) \quad &= C\begin{pmatrix} ba^T - (B,0) \\ I_n \end{pmatrix} x = (bc^T - (I_m, B, 0))\begin{pmatrix} b - (B,0)x \\ x \end{pmatrix} \\
&= bc^T \begin{pmatrix} b - (B,0)x \\ x \end{pmatrix} - (I_m, B, 0)\begin{pmatrix} b - (B,0)x \\ x \end{pmatrix} \\
&= (0, ba^T)\begin{pmatrix} b - (B,0)x \\ x \end{pmatrix} - (I_m, B, 0)\begin{pmatrix} b - (B,0)x \\ x \end{pmatrix} \\
&= ba^T x - (b - (B,0)x + (B,0)x) \\
&= b - b = 0,
\end{aligned}$$

which implies that $y = Ax \in P_e$.

□

Using the set P_e defined in (3.14), we obtain the following equivalent representation of $F(QP)$ in $\mathbb{R}^{m+n}$.

$$F(QP_e) = \{y \in \mathbb{R}^{m+n}_+ \mid Cy = 0, c^T y = 1, y_i \in \{0,1\} \text{ for } i \in \mathcal{B}_e\}, \quad (3.15)$$

where the index set $\mathcal{B}_e$ is defined as

$$\mathcal{B}_e := \{i \mid i = m + j,\ j \in \mathcal{B}\}. \quad (3.16)$$

Remark 3.3.4. *By construction of the index sets $\mathcal{B}_{iq}$ and $\mathcal{B}_e$ in* (3.11) *and* (3.16)*, respectively, it follows from Lemma 3.3.3 that*

$$Ax \in F(QP_e) \Leftrightarrow x \in F(QP_{iq}).$$

As seen above, from the given feasible set $F(QP)$ in $\mathbb{R}^d_+$ of the original mixed binary quadratic optimization problem (QP), we have constructed two equivalent sets $F(QP_{iq})$ in $\mathbb{R}^n$ and $F(QP_e)$ in $\mathbb{R}^{m+n}$. As a result, we obtain the following two equivalent problems, denoted by (QP_{iq}) and (QP_e), respectively.

$$\begin{aligned} \min \quad & x^T Q_{iq} x \\ \text{s.t.} \quad & x \in F(QP_{iq}) \end{aligned} \tag{QP_{iq}}$$

with

$$Q_{iq} := \begin{pmatrix} Q & 0 \\ 0^T & 0 \end{pmatrix} \in \mathbb{R}^{n \times n}, \tag{3.17}$$

and

$$\begin{aligned} \min \quad & y^T Q_e y \\ \text{s.t.} \quad & y \in F(QP_e) \end{aligned} \tag{QP_e}$$

with

$$Q_e := \begin{pmatrix} 0 & 0 \\ 0 & Q_{iq} \end{pmatrix} \in \mathbb{R}^{(m+n)\times(m+n)}. \tag{3.18}$$

The next step of our purpose is to construct two lifting problems, (CP_{iq}) and (CP_e), corresponding to (QP_{iq}) and (QP_e), respectively.

3.4 The Lifted Problems

3.4.1 Lifting of the feasible sets

The main task of lifting the problems (QP_{iq}) and (QP_e) into suitable matrix spaces is the construction of lifted sets according to the feasible sets $F(QP_{iq})$ and $F(QP_e)$. The first lifting procedure was presented by Burer in [11] for feasible sets of type $F(QP_e)$. Some modifications of this method are given by Burer in [12] and Lieder in [22], in order to reduce the number of constraints in the lifted problem. In [11] Burer stated that his lifting can not work for sets restricted by inequality constraints like $F(QP_{iq})$, and suggested to formulate $F(QP_{iq})$ into $F(QP_e)$ by adding m slack variables. However this will increase the dimension of the quadratic problem from n to $n+m$.

In this subsection, we first construct the lifted set directly for the set $F(QP_{iq})$, without using slack variables. A lifted set, in which only two linear equality constraints are needed, is then given for the set $F(QP_e)$.

We start with lifting the set

$$F(QP_{iq}) = \{x \in \mathbb{R}^n \mid Ax \geq 0, a^T x = 1, x_i \in \{0,1\} \text{ for } i \in \mathcal{B}_{iq}\}$$

as defined in (3.10). Clearly we have

$$\operatorname{rec} F(QP_{iq}) = \{x \in \mathbb{R}^n \mid Ax \geq 0, a^T x = 0, x_i = 0 \text{ for } i \in \mathcal{B}_{iq}\}.$$

Similar as Burer [11], we make the following key assumption:

$$\begin{aligned} &\text{For all } i \in \mathcal{B}_{iq}, \text{ we assume that } a_i > 0 \text{ and that} \\ &0 \leq x_i \leq 1 \text{ for all } x \in \mathbb{R}^n \text{ satisfying } Ax \geq 0, a^T x = 1. \end{aligned} \tag{3.19}$$

It is worth noting that the assumption (3.19) is immediately fulfilled for the cases considered in Example 3.3.1 *iii*).

The following result is the basis for our first lifting approach.

Theorem 3.4.1. *Let $\mathcal{C}_{iq}$ and $\mathcal{R}_{iq}$ be defined by* (3.1)–(3.2) *according to $F(QP_i)$, i.e.,*

$$\mathcal{C}_{iq} := \operatorname{conv}\{xx^T : x \in F(QP_{iq})\},$$

$$\mathcal{R}_{iq} := \operatorname{conv}\{xx^T : x \in \operatorname{rec} F(QP_{iq})\}.$$

Further, define an $n \times n$ matrix B_{iq} by

$$B_{iq} := \sum_{i \in \mathcal{B}_{iq}} \frac{1}{2}(e^i(a-e^i)^T + (a-e^i)(e^i)^T)$$

with e^i being the i-th unit vector for each index i. Then, under Assumption (3.19)*, we have*

$$\begin{aligned} &\mathcal{C}_{iq} + \mathcal{R}_{iq} = \\ &\{X \in \mathcal{CP}_n \mid \langle aa^T, X\rangle = 1, \langle B_{iq}, X\rangle = 0, AXA^T \in \mathcal{CP}_{m+n}\} =: \mathcal{Z}. \end{aligned} \tag{3.20}$$

Proof. We first show that $\mathcal{C}_{iq} + \mathcal{R}_{iq} \subseteq \mathcal{Z}$: To this end, take $X \in \mathcal{C}_{iq}$ and $Y \in \mathcal{R}_{iq}$. Then there exist $x^1, \dots, x^r \in F(QP_{iq})$ and $\lambda_1, \dots, \lambda_r \geq 0$ with $\sum_{k=1}^r \lambda_k = 1$ as well as $y^1, \dots, y^l \in \operatorname{rec} F(QP_{iq})$ and $\mu_1, \dots, \mu_l \geq 0$ such that

$$X = \sum_{k=1}^r \lambda_k x^k (x^k)^T \quad \text{ and } \quad Y = \sum_{j=1}^l \mu_j y^j (y^j)^T.$$

Then it is easy to see that $a^T(X+Y)a = 1$, and for each $k \in \{1, ..., r\}$ and $i \in \mathcal{B}_{iq}$, the fact that $x_i^k \in \{0,1\}$ implies

$$(e^i)^T x^k (x^k)^T e^i = [x^k (x^k)^T]_{ii} = (x_i^k)^2 = x_i^k = a^T x^k (x^k)^T e^i,$$

whence $(a - e^i)^T X e^i = 0$.

Similarly, $y_i^j = 0$ for $j \in \{1, ..., l\}$ and $i \in \mathcal{B}_{iq}$ implies that

$$(e^i)^T y^j (y^j)^T e^i = 0 = a^T y^j (y^j)^T e^i.$$

From this, we get

$$(a - e^i)^T Y e^i = 0,$$

and hence,

$$(a - e^i)^T (X + Y) e^i = 0 \text{ for all } i \in \mathcal{B}_{iq},$$

which is a different way of writing $\langle B_{iq}, X + Y\rangle = 0$.
Finally,

$$A(X+Y)A^T = \sum_{k=1}^r \lambda_k \underbrace{(Ax^k)}_{\geq 0} \underbrace{(Ax^k)^T}_{\geq 0} + \sum_{j=1}^l \mu_j \underbrace{(Ay^j)}_{\geq 0} \underbrace{(Ay^j)^T}_{\geq 0} \in \mathcal{CP}_{m+n}.$$

Therefore, $X + Y \in \mathcal{Z}$ and the inclusion $\mathcal{C}_{iq} + \mathcal{R}_{iq} \subseteq \mathcal{Z}$ is shown.

To show the reverse inclusion, take $X \in \mathcal{Z}$. We append m zero rows and columns to obtain a matrix

$$\widehat{X} := \begin{pmatrix} X & 0 \\ 0 & 0 \end{pmatrix} \in \mathrm{I\!R}^{(n+m)\times(n+m)}.$$

Likewise, we append to A any matrix D such that

$$\widehat{A} := (A, D) \in \mathrm{I\!R}^{(m+n)\times(m+n)}$$

is nonsingular, and we add m zeros to a to obtain $\widehat{a} := (a, 0)^T \in \mathrm{I\!R}^{n+m}$. Note that $\widehat{A}\widehat{X}\widehat{A}^T = AXA^T \in \mathcal{CP}_{m+n}$ and $\widehat{a}^T\widehat{X}\widehat{a} = a^T X a = 1$.

Since $\widehat{A}\widehat{X}\widehat{A}^T \in \mathcal{CP}_{m+n}$, there exist $\hat{z}^1, \ldots, \hat{z}^r \in \mathrm{I\!R}^{n+m}_+$ such that

$$\widehat{A}\widehat{X}\widehat{A}^T = \sum_{k=1}^{r} \hat{z}^k (\hat{z}^k)^T.$$

Define $\hat{y}^k := \widehat{A}^{-1}\hat{z}^k$ for $k = 1, \ldots, r$. Then clearly

$$\widehat{A}\hat{y}^k = \hat{z}^k \geq 0 \text{ and } \widehat{X} = \sum_{k=1}^{r} \hat{y}^k (\hat{y}^k)^T.$$

For any $j = n+1, \ldots, n+m$ it follows from $\widehat{X}_{jj} = 0$ that $\hat{y}^k_j = 0$ for all $k = 1, \ldots r$. Let $y^k \in \mathrm{I\!R}^n$ denote the vector containing the first n components of $\hat{y}^k$.

By construction,

$$X = \sum_{k=1}^{r} y^k (y^k)^T \text{ and } Ay^k = \widehat{A}\hat{y}^k \geq 0,$$

which implies by construction of

$$A = \begin{pmatrix} ba^T - (B, 0) \\ I_n \end{pmatrix}$$

that $y^k \geq 0$ for all k. As $a \geq 0$ by assumption, we have $a^T y^k \geq 0$ for all k.

Define

$$K^+ := \{k \in \{1, \dots, r\} \mid a^T y^k > 0\} \text{ and}$$
$$K^= := \{k \in \{1, \dots, r\} \mid a^T y^k = 0\}.$$

For $k \in K^+$, let $\lambda_k := a^T y^k > 0$ and $x^k := \frac{1}{\lambda_k} y^k$. With this, we get that

$$X = \sum_{k=1}^{r} y^k (y^k)^T = \sum_{k \in K^+} \lambda_k^2 x^k (x^k)^T + \sum_{k \in K^=} y^k (y^k)^T. \tag{3.21}$$

We now show that $y^k \in \operatorname{rec} F(QP_{iq})$ for all $k \in K^=$, and $x^k \in F(QP_{iq})$ for all $k \in K^+$, as well as $\sum_{k \in K^+} \lambda_k^2 = 1$. This will prove that $X \in \mathcal{C}_{iq} + \mathcal{R}_{iq}$ and hence $\mathcal{Z} \subseteq \mathcal{C}_{iq} + \mathcal{R}_{iq}$, as desired.

For $k \in K^=$, we have that $a^T y^k = 0$ and $A y^k \geq 0$. For $i \in \mathcal{B}_{iq}$, Assumption (3.19) and $a^T y^k = 0$ imply that $y_i^k = 0$, so $y^k \in \operatorname{rec} F(QP_{iq})$.

To see that $x^k \in F(QP_{iq})$ for $k \in K^+$, note that $a^T x^k = \frac{1}{\lambda_k} a^T y^k = 1$ and from $\lambda_k > 0$ and $\lambda_k A x^k = A y^k = \widehat{A} y^k \geq 0$ it follows that $A x^k \geq 0$. Using (3.21) we can rewrite the equation

$$\langle B_{iq}, X \rangle = \sum_{i \in \mathcal{B}_{iq}} (a - e^i)^T X e^i = 0$$

as

$$\begin{aligned}
0 &= \sum_{i \in \mathcal{B}_{iq}} \left(\sum_{k \in K^+} \lambda_k^2 (a - e^i)^T x^k (x^k)^T e^i + \sum_{k \in K^=} (a - e^i)^T y^k \underbrace{(y^k)^T e^i}_{= y_i^k = 0} \right) \\
&= \sum_{i \in \mathcal{B}_{iq}} \sum_{k \in K^+} \lambda_k^2 \left[\underbrace{a^T x^k}_{=1} (x^k)^T e^i - (e^i)^T x^k (x^k)^T e^i \right] \\
&= \sum_{i \in \mathcal{B}_{iq}} \sum_{k \in K^+} \lambda_k^2 \left[x_i^k - (x_i^k)^2 \right]
\end{aligned}$$

Since by Assumption (3.19) we have $0 \leq x_i^k \leq 1$ for all $i \in \mathcal{B}_{iq}$ and $k \in K^+$, the last equation holds true if and only if $x_i^k \in \{0, 1\}$ for all $i \in \mathcal{B}_{iq}, k \in K^+$. This shows that $x^k \in F(QP_{iq})$ for all $k \in K^+$.

Finally, we have

$$1 = a^T X a = \sum_{k=1}^{r} a^T y^k (y^k)^T a = \sum_{k \in K^+} \lambda_k^2 + \sum_{k \in K^=} \underbrace{\left(a^T y^k\right)^2}_{=0} = \sum_{k \in K^+} \lambda_k^2,$$

which concludes the proof.

□

Example 3.4.2. *In this example we will apply Theorem 3.4.1 to the multidimensional quadratic knapsack problem. In Example 2.12 we only considered a quadratic knapsack problem with one capacity constraint. In this example we will lift a quadratic knapsack problem subject to multiple capacity constraints, which is formulated as*

$$\begin{aligned} \min \quad & x^T Q x + q^T x \\ \text{s.t.} \quad & (a^i)^T x \leq 1 \qquad i = 1, \ldots, m \\ & x \in \{0,1\}^d, \end{aligned} \tag{3.22}$$

where $Q \in \mathcal{S}_d, q \in \mathbb{R}^d, a^i \in \mathbb{R}^d_+$ *for all* $i = 1, ..., m$. *In the first step we will add a redundant inequality constraint to the problem. We are using the definition for* α *proposed in Example 3.3.1 iii), i.e.* $\alpha_j := \frac{1}{d}$ *for all* $j = 1, \ldots, d$. *Problem* (3.22) *can be written as*

$$\begin{aligned} \min \quad & x^T Q x + q^T x \\ \text{s.t.} \quad & (a^i)^T x \leq 1 \qquad i = 1, \ldots, m \\ & \alpha^T x \leq 1 \\ & x \in \{0,1\}^d. \end{aligned} \tag{3.23}$$

In the second step we add a slack variable $s \geq 0$ *to the constraint* $\alpha^T x \leq 1$

and obtain

$$
\begin{aligned}
\min \quad & x^T Q x + q^T x \\
\text{s.t.} \quad & (a^i)^T x \leq 1 \qquad i = 1, \ldots, m \\
& \alpha^T x + s = 1 \\
& x \in \{0,1\}^d \\
& s \geq 0.
\end{aligned}
\tag{3.24}
$$

Define $n := d + 1$, $a := \begin{pmatrix} \alpha \\ 1 \end{pmatrix} \in \mathbb{R}^n_+ \setminus \{0\}$, *and* $\bar{q} := (q^T, 0)$, *then we obtain the equivalent problem in* $\mathbb{R}^n$

$$
\begin{aligned}
\min \quad & x^T \begin{pmatrix} Q & 0 \\ 0^T & 0 \end{pmatrix} x + \bar{q}^T x \\
\text{s.t.} \quad & ((a^i)^T, 0) x \leq 1 \qquad && i = 1, \ldots, m \\
& a^T x = 1 \\
& x_i \in \{0,1\} && i = 1, ..., n-1 \\
& x_n \geq 0.
\end{aligned}
\tag{3.25}
$$

In the next step we want to get rid of the linear term $\bar{q}^T x$ *in the objective function. From the constraint* $a^T x = 1$ *it follows that*

$$\bar{q}^T x = x^T a \bar{q}^T x.$$

Therefore defining

$$Q_{iq} := \begin{pmatrix} Q & 0 \\ 0 & 0 \end{pmatrix} + \frac{1}{2}(a\bar{q}^T + \bar{q}a^T),$$

and we obtain

$$x^T \begin{pmatrix} Q & 0 \\ 0 & 0 \end{pmatrix} x + (q^T, 0)x = x^T Q_{iq} x.$$

Note that the matrix $Q_{iq} \in \mathbb{R}^{n\times n}$ *is again symmetric. In general we cannot assume that the system*

$$\begin{array}{rcll} ((a^i)^T,0)x & \leq & 1 & i=1,\dots,m \\ a^Tx & = & 1 & \\ x_i & \in & \{0,1\} & i=1,...,n-1 \\ x_n & \geq & 0 & \end{array}$$

implies that $x_i \leq 1$ *for all* $i = 1,...,n-1$*, which is needed for the Key Assumption 3.19, therefore we need to add the trivial constraints*

$$0 \leq x_j \leq 1 \text{ for all } j = 1,\dots,n-1.$$

With these constraints we obtain the following equivalent problem

$$\begin{array}{lll} \min & x^TQ_{iq}x & \\ \text{s.t.} & ((a^i)^T,0)x \leq 1 & i=1,\dots,m \\ & (I_{n-1},0)x \leq e & \\ & a^Tx = 1 & \\ & x \geq 0 & \\ & x_i \in \{0,1\} & i=1,...,n-1. \end{array} \tag{3.26}$$

Since $((a^i)^T,0)x \leq 1$ *is equivalent to* $0 \leq \underbrace{a^Tx}_{=1} - ((a^i)^T,0)x = (a^T - ((a^i)^T,0))x$ *we define*

$$A := \begin{pmatrix} (a^T - ((a^1)^T,0)) \\ \vdots \\ (a^T - ((a^m)^T,0)) \\ ea^T - (I_{n-1},0) \\ I_n \end{pmatrix} \in \mathbb{R}^{(m+n-1+n)\times n}.$$

With this definition of A we can formulate Problem (3.22) *equivalently as*

$$\begin{aligned} \min \quad & x^T Q_{iq} x \\ \text{s.t.} \quad & Ax \geq 0 \\ & a^T x = 1 \\ & x_i \in \{0,1\} \quad i = 1, ..., n-1. \end{aligned} \tag{3.27}$$

Note that Problem (3.27) *fulfills the Key Assumption 3.19, hence we can apply Theorem 3.4.1 to Problem* (3.27) *and obtain the equivalent completely positive problem*

$$\begin{aligned} \min \quad & \langle Q_{iq}, X\rangle \\ & \langle aa^T, X\rangle = 1 \\ & AXA^T \in \mathcal{CP}_{m+2n-1} \\ & \langle B, X\rangle = 0, \end{aligned} \tag{3.28}$$

where $B := \sum_{i=1}^{n-1} \frac{1}{2}(e^i(a-e^i)^T + (a-e^i)(e^i)^T)$ *with* $e^1, \ldots, e^{n-1}$ *being the first* $(n-1)$ *unit vectors of* $\mathbb{R}^n$*.*

We now present the method for lifting the set $F(QP_e) \subset \mathbb{R}_+^{m+n}$. Recall that $F(QP_e)$ is defined by

$$F(QP_e) = \{y \in \mathbb{R}_+^{m+n} \mid Cy = 0,\ c^T y = 1,\ y_i \in \{0,1\} \text{ for } i \in \mathcal{B}_e\},$$

and the index set $\mathcal{B}_e$ is defined in (3.16).

Here we also make the key assumption that

$$\begin{aligned} &\text{For all } i \in \mathcal{B}_e, \text{ it holds } c_i > 0 \text{ and} \\ &0 \leq y_i \leq 1 \text{ for all } y \in \mathbb{R}^{m+n} \text{ satisfying } Cy = 0, c^T y = 1, \end{aligned} \tag{3.29}$$

which is also fulfilled immediately for the cases considered in Example 3.3.1 *iii*).

Theorem 3.4.3. *Let $\mathcal{C}_e$ and $\mathcal{R}_e$ be respectively defined by* (3.1)–(3.2) *corresponding to the set $F(QP_e)$, i.e.,*

$$\mathcal{C}_e := \operatorname{conv}\{yy^T : y \in F(QP_e)\},$$

$$\mathcal{R}_e := \operatorname{conv}\{yy^T : y \in \operatorname{rec} F(QP_e)\}.$$

Further, assume that (3.29) *is fulfilled. Then we have*

$$\begin{aligned} &\mathcal{C}_e + \mathcal{R}_e = \\ &\{Y \in \mathcal{CP}_{m+n} \mid \langle cc^T, Y\rangle = 1, \langle C^TC, Y\rangle = 0, \langle B_e, Y\rangle = 0\} =: \mathcal{Y}, \end{aligned} \tag{3.30}$$

where

$$B_e := \sum_{i \in \mathcal{B}_e} \frac{1}{2}(e^i(c - e^i)^T + ((c - e^i)(e^i)^T)$$

with e^i being the i-th unit vector for each index i.

Proof. Let

$$Y = \sum_{k=1}^{r} y^k (y^k)^T \in \mathcal{Y}.$$

Since C^TC is positive semidefinite, it follows that

$$\begin{aligned} &\sum_{k=1}^{r} (y^k)^T C^T C (y^k) = \langle C^TC, Y\rangle = 0 \text{ if and only if} \\ &(Cy^k)^T Cy^k = 0, \text{ i.e. } Cy^k = 0 \text{ for all } k. \end{aligned}$$

Similar to the proof of Theorem 3.4.1, we define the sets

$$\begin{aligned} K^+ &:= \{k \in \{1, \ldots, r\} \mid c^T y^k > 0\} \text{ and} \\ K^= &:= \{k \in \{1, \ldots, r\} \mid c^T y^k = 0\}. \end{aligned}$$

For $k \in K^+$, let $\lambda_k := c^T y^k > 0$ and $\hat{y}^k := \frac{1}{\lambda_k} y^k$. Then again we have

$$Y = \sum_{k=1}^{r} y^k (y^k)^T = \sum_{k \in K^+} \lambda_k^2 \hat{y}^k (\hat{y}^k)^T + \sum_{k \in K^=} y^k (y^k)^T.$$

The statement of this theorem follows then analogously to the proof of Theorem 3.4.1. $\square$

Remark 3.4.4. *In [11], Burer established for the set*

$$F(QP_e) = \{x \in \mathbb{R}^n_+ \mid Cx = 0, c^T x = 1, x_i \in \{0,1\} \text{ for all } i \in \mathcal{B}_e\},$$

the following lifted set:

$$\{X \in \mathcal{CP}_n \mid c_i^T X c_i = 0, c_i^T X c = 0, [Xc]_j = X_{jj} \ \forall\ j \in \mathcal{B}_e, c^T X c = 1\},$$

where c_i^T is the i-th row of C. In his representation, Burer needed $2m + |\mathcal{B}_e| + 1$ linear constraints. In our representation, we modified Burer's idea in such a way that we only need three linear equations.

Example 3.4.5. *Similar to Example 3.4.2 we can apply Theorem 3.4.3 to the multidimensional quadratic knapsack problem*

$$\begin{array}{lll} \min & x^T Q x + q^T x & \\ \text{s.t.} & (a^i)^T x \leq 1 & i = 1, \dots, m \\ & x \in \{0,1\}^d. & \end{array} \tag{3.31}$$

As mentioned in Example 3.4.2 the system $(a^i)^T x \leq 1$ for all $i = 1, ..., m$ in general does not imply that $0 \leq x_j \leq 1$ for all $j = 1, ..., d$. Therefore we need to add these constraints to the inequality system, i.e.

$$\begin{array}{lll} \min & x^T Q x + q^T x & \\ \text{s.t.} & (a^i)^T x \leq 1 & i = 1, \dots, m \\ & x_j \leq 1 & j = 1, ..., d \\ & x \geq 0 & \\ & x \in \{0,1\}^d. & \end{array} \tag{3.32}$$

Next we add $m + d$ slack variables to transform the inequality constraints into *equality constraints and obtain with* $\bar{q} := \begin{pmatrix} 0 \\ q \end{pmatrix} \in \mathbb{R}^{m+2d}$

$$\begin{array}{ll} \min & x^T \begin{pmatrix} 0 & 0 \\ 0 & Q \end{pmatrix} x + \bar{q}x \\ \text{s.t.} & ((e^i_{m+d})^T, (a^i)^T)x = 1 \quad i = 1, \ldots, m \\ & ((e^{m+j}_{m+d})^T, (e^j_d)^T)x = 1 \quad j = 1, ..., d \\ & x \in \mathbb{R}^{m+2d}_+ \\ & x_{j+m+d} \in \{0, 1\} \qquad j = 1, ..., d, \end{array} \tag{3.33}$$

where $e^i_{m+d} \in \mathbb{R}^{m+d}$ *is the* i*-th unit vector in* $\mathbb{R}^{m+d}$*,* $e^j_d \in \mathbb{R}^d$ *is the* j*-th unit vector in* $\mathbb{R}^d$*. Next we want to add a redundant constraint* $c^T x = 1$ *with* $c > 0$*. It follows from*

$$\sum_{i=1}^{m} ((e^i_{m+d})^T, (a^i)^T)x + \sum_{j=1}^{d} ((e^{m+j}_{m+d})^T, (e^j_d)^T)x = m + d,$$

that for

$$c := \frac{1}{m+d} \sum_{i=1}^{m} \begin{pmatrix} (e^i_{m+d}) \\ (a^i) \end{pmatrix} + \sum_{j=1}^{d} \begin{pmatrix} (e^{m+j}_{m+d}) \\ (e^j_d) \end{pmatrix},$$

we have $c > 0$ *and* $c^T x = 1$ *is a redundant constraint. Define the matrices*

$$Q_e := \begin{pmatrix} 0 & 0 \\ 0 & Q \end{pmatrix} + \frac{1}{2}(c\bar{q}^T + \bar{q}c^T) \in \mathcal{S}_{m+2d}$$

and

$$C := \begin{pmatrix} c^T - ((e^1_{m+d})^T, (a^1)^T) \\ \vdots \\ c^T - ((e^m_{m+d})^T, (a^m)^T) \\ c^T - ((e^{m+1}_{m+d})^T, (e^1_d)^T) \\ \vdots \\ c^T - ((e^{m+d}_{m+d})^T, (e^d_d)^T) \end{pmatrix} \in \mathbb{R}^{(m+d)\times(m+2d)},$$

and

$$B_e := \sum_{i=1}^{d} \frac{1}{2}(e^{m+d+i}(c - e^{m+d+i})^T + (c - e^{m+d+i})(e^{m+d+i})^T) \in \mathrm{I\!R}^{(m+2d)\times(m+2d)}.$$

Then we can write Problem (3.22) *equivalently as*

$$\begin{aligned} \min \quad & x^T Q_e x \\ \text{s.t.} \quad & Cx = 0 \\ & c^T x = 1 \\ & x^T B_e x = 0 \\ & x \in \mathrm{I\!R}_+^{m+2d}. \end{aligned} \tag{3.34}$$

Using Theorem 3.4.3 we can formulate the equivalent completely positive problem of Problem (3.34) *as*

$$\begin{aligned} \min \quad & \langle Q_e, X \rangle \\ \text{s.t.} \quad & \langle C^T C, X \rangle = 0 \\ & \langle cc^T, X \rangle = 1 \\ & \langle B_e, X \rangle = 0 \\ & X \in \mathcal{CP}_{m+2d}. \end{aligned} \tag{3.35}$$

It is worth noting that, independent from the numbers of constraints and variables in Problem (3.22)*, Problem* (3.35) *only has three linear equality constraints and one complete positivity constraint.*

We have constructed above two lifted sets $\mathcal{Z} = \mathcal{C}_{iq} + \mathcal{R}_{iq}$ and $\mathcal{Y} = \mathcal{C}_e + \mathcal{R}_e$ by (3.20) and (3.30), respectively. The relationship between these liftings is shown below.

Lemma 3.4.6. *It holds that*

$$X \in \mathcal{Z} \text{ if and only if } AXA^T \in \mathcal{Y}.$$

Proof. Using Lemma 3.3.3 and Remark 3.3.4 we have the following equivalences:

$$\begin{aligned}
X \in \mathcal{Z} \ \Leftrightarrow \ & \exists x^1, \cdots, x^r \in F(QP_{iq}), y^1, ..., y^l \in \operatorname{rec} F(QP_{iq}) : \\
& X = \sum_{k=1}^{r} \lambda_k (x^k)x^k)^T + \sum_{j=1}^{l} (y^j)(y^j)^T, \lambda_k \geq 0 \ \forall k, \sum_{k=1}^{r} \lambda_k = 1 \\
\Leftrightarrow \ & \exists x^k \in F(QP_{iq}), y^j \in \operatorname{rec} F(QP_{iq}) : \\
& Ax^k \in F(QP_e) \ \forall k = 1, \ldots, r, Ay^j = 0; \forall j = 1, ..., l \\
& \sum_{k=1}^{r} \lambda_k (Ax^k)(Ax^k)^T + \sum_{j=1}^{l} (Ay^j)(Ay^j)^T \in \mathcal{C}_e + \mathcal{R}_e = \mathcal{Y} \\
\Leftrightarrow \ & \exists x^1, \cdots, x^r \in F(QP_{iq}), y^1, ..., y^l \in \operatorname{rec} F(QP_{iq}) : \\
& A(\sum_{k=1}^{r} \lambda_k (x^k)(x^k)^T + \sum_{j=1}^{l} (y^j)(y^j)^T)A^T \in \mathcal{Y} \\
\Leftrightarrow \ & AXA^T \in \mathcal{Y}.
\end{aligned}$$

□

3.4.2 The Resulting Completely Positive Optimization Problems

Now that we have representations for the feasible sets of the quadratic problems (QP_{iq}) and (QP_e), we can reformulate these problems as completely positive optimization problems as follows.

$$(CP_{iq}) \quad \begin{array}{ll} \min & \langle Q_{iq}, X \rangle \\ \text{s.t.} & X \in \mathcal{Z} \end{array} \qquad \text{and} \qquad (CP_e) \quad \begin{array}{ll} \min & \langle Q_e, Y \rangle \\ \text{s.t.} & Y \in \mathcal{Y}, \end{array} \tag{3.36}$$

where the matrices Q_{iq} and Q_e are defined in (3.17) and (3.18), respectively.

Theorem 3.4.7. *For quadratic Problems (QP_{iq}), (QP_e) considered in previous section and Problems (CP_{iq}), (CP_e) defined in* (3.36) *we have:*

(i) $\min(QP_{iq}) = \min(CP_{iq}) = \min(CP_e) = \min(QP_e)$,
where $\min(QP_{iq})$, $\min(CP_{iq})$, $\min(CP_e)$ *and* $\min(QP_e)$ *are the optimal values of the problems (QP_{iq}), (CP_{iq}), (CP_e) and (QP_e), respectively.*

(ii) Let $\bar{X} \in \mathcal{Z}$ with $\bar{X} = \sum_{i=1}^{r} \lambda_i (\bar{x}^i)(\bar{x}^i)^T$, where $\sum_{i=1}^{r} \lambda_i = 1, \lambda_i \geq 0$ and $\bar{x}^i \in F(QP_{iq})$ for all i. Then the following statements are equivalent:

(a) $\bar{X}$ is optimal for Problem (CP_{iq}).

(b) $\bar{Y} := A\bar{X}A^T$ is optimal for Problem (CP_e).

(c) $\bar{y}^i := A\bar{x}^i$ is optimal for Problem (QP_e) for all i.

(d) $\bar{x}^i$ is optimal for Problem (QP_{iq}) for all i.

Proof. First, remember that from (3.7), (3.17) and (3.18) we have

$$A = \begin{pmatrix} ba^T - (B, 0) \\ I_n \end{pmatrix} \in \mathbb{R}^{(m+n)\times n}, \; Q_{iq} = \begin{pmatrix} Q & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{R}^{n\times n} \text{ and}$$
$$Q_e = \begin{pmatrix} 0 & 0 \\ 0 & Q_{iq} \end{pmatrix} \in \mathbb{R}^{(m+n)\times(m+n)}.$$

Therefore, we have

$$A^T Q_e A = \begin{pmatrix} ba^T - (B, 0) \\ I_n \end{pmatrix}^T \begin{pmatrix} 0 & 0 \\ 0 & Q_{iq} \end{pmatrix} \begin{pmatrix} ba^T - (B, 0) \\ I_n \end{pmatrix} = Q_{iq}. \qquad (3.37)$$

First, we prove (i): From Lemma 3.2.1, we have that $\min(QP_{iq}) = \min(CP_{iq})$ and $\min(CP_e) = \min(QP_e)$, and therefore we need only show that $\min(QP_{iq}) = \min(QP_e)$. For this, let $\bar{x}$ be an optimal solution of (QP_{iq}). From Remark 3.3.4 we have $A\bar{x} \in F(QP_e)$, which implies by (3.37) that

$$\min(QP_{iq}) = \bar{x}^T Q_{iq} \bar{x} = \bar{x}^T A^T Q_e A \bar{x} \geq \min(QP_e).$$

Conversely let $\hat{y}$ be an optimal solution of (QP_e). Then there exists a point $\hat{x} \in F(QP_{iq})$ such that $\hat{y} = A\hat{x}$. Thus,

$$\min(QP_e) = \hat{y}^T Q_e \hat{y} = \hat{x}^T A^T Q_e A \hat{x} = \hat{x}^T Q_{iq} \hat{x} \geq \min(QP_{iq}).$$

Next, we prove (ii): From Lemma 3.2.1, we have $(a) \Leftrightarrow (d)$ and $(b) \Leftrightarrow (c)$. We only need to show $(c) \Leftrightarrow (d)$. For this, let $\bar{x}$ be an optimal solution of (QP_{iq}). Then it follows from (3.37) that

$$\bar{x}^T Q_{iq} \bar{x} = \bar{x}^T A^T Q_e A \bar{x} = \bar{y}^T Q_e \bar{y},$$

which implies by (i) that $\bar{y}$ is an optimal solution of (QP_e). In order to show the other direction, let $\bar{y}$ be an optimal solution of (QP_e). Then there exists $\bar{x} \in F(QP_{iq})$ such that $\bar{y} = A\bar{x}$ and we have, again by using (3.37), that

$$\bar{y}^T Q_e \bar{y} = \bar{x}^T A^T Q_e A \bar{x} = \bar{x}^T Q_{iq} \bar{x},$$

which implies by (i) that $\bar{x}$ is optimal solution of (QP_{iq}). $\square$

3.5 The Duals of Resulting Completely Positive Problems and their Strict Feasibility

While the reformulation of the quadratic optimization problem as a completely positive optimization problem is a theoretically important result with many advantages, there is a catch, however: up to now, there do not exist any practical approaches for solving completely positive problems in reasonable time. As mentioned in the introduction and in Chapter 1, an efficient method was developed in [9] to solve its dual problem, which is a copositive optimization program. Unfortunately, unlike duality in linear optimization, there can exist a non-zero duality gap in conic duality. In order to guarantee strong duality for the primal-dual pair under consideration, we need either the completely positive optimization problem or the copositive optimization problem to be strictly feasible.

In what follows, we focus on finding strictly feasible formulations for the copositive problems, which are the dual problems of (CP_{iq}) and (CP_e), respectively. These formulations have superior characteristics as they, on the one hand, fulfill the conditions for strong duality and, on other hand, can be solved by the algorithm developed in [9] for strictly feasible copositive programs.

First we consider the problem

$$\begin{array}{ll} \min & \langle Q_{iq}, X\rangle \\ \text{s.t.} & \langle aa^T, X\rangle = 1 \\ & \langle B_{iq}, X\rangle = 0 \\ & AXA^T \in \mathcal{CP}_{m+n}. \end{array} \tag{CP$_{iq}$}$$

Note that

$$\begin{aligned} AXA^T &= \begin{pmatrix} ba^T - (B,0) \\ I_n \end{pmatrix} X \begin{pmatrix} ba^T - (B,0) \\ I_n \end{pmatrix}^T \\ &= \begin{pmatrix} (ba^T - (B,0))X(ba^T - (B,0))^T & (ba^T - (B,0))X \\ X(ba^T - (B,0)) & X \end{pmatrix} \in \mathcal{CP}_{m+n} \end{aligned}$$

also implies that $X \in \mathcal{CP}_n$. By using an additional variable $Z = AXA^T \in \mathcal{CP}_{m+n}$ we obtain the Lagrangian function

$$L(X, Z, U, \lambda, \sigma) = \langle Q_{iq}, X\rangle + \langle Z - AXA^T, U\rangle + \lambda(1 - \langle aa^T, X\rangle) + \sigma\langle B_{iq}, X\rangle.$$

Therefore, the dual problem of (CP_{iq}), denoted by $(D)_{iq}$, is

$$\begin{aligned} & \max_{U,\lambda,\sigma} \min_{X,Z} \langle Q_{iq}, X\rangle + \langle Z - AXA^T, U\rangle + \lambda(1 - \langle aa^T, X\rangle) + \sigma\langle B_{iq}, X\rangle \\ = \; & \max_{U,\lambda,\sigma} \; \{\lambda + \min_{X,Z}\{\langle Q_{iq} - A^TUA - \lambda aa^T + \sigma B_{iq}, X\rangle + \langle U, Z\rangle\}\}, \end{aligned}$$

where we optimize with respect to $U \in \mathcal{S}_{m+n}$, $\lambda, \sigma \in \mathbb{R}$, $X \in \mathcal{S}_n$ and $Z \in \mathcal{CP}_{m+n}$.

For given U, λ, σ, the conditions for

$$\min_{X,Z}\{\langle Q_{iq} - A^TUA - \lambda aa^T + \sigma B_{iq}, X\rangle + \langle Z, U\rangle\} > -\infty \tag{3.38}$$

are

$$Q_{iq} - A^T U A - \lambda a a^T + \sigma B_{iq} = 0 \text{ and } \langle Z, U \rangle \geq 0.$$

Therefore, from $Z \in \mathcal{CP}$ it follows that $U \in \mathcal{COP}$ and the first condition gives

$$Q_{iq} - \lambda a a^T + \sigma B_{iq} \quad = \quad A^T U A \ .$$

By construction A has full column rank. Denote A^+ as the Moore-Penrose-pseudoinverse of A, we have $AA^+ = I_n$, and the equation above is equivalent to

$$(A^+)^T (Q_{iq} - \lambda a a^T + \sigma B_{iq}) A^+ = U$$

Thus, the dual problem (D_{iq}) can now be formulated as

$$\begin{array}{ll} \max & \lambda \\ \text{s.t.} & (A^+)^T (Q_{iq} - \lambda a a^T + \sigma B_{iq}) A^+ \in \mathcal{COP}_{n+m} \\ & \lambda \in \mathbb{R}, s \in \mathbb{R} \end{array} \qquad (\mathrm{D}_{iq})$$

In general, there may or may not exist a strictly feasible point for (D_{iq}), therefore there can be a non-zero duality gap between (D_{iq}) and (CP_{iq}). In this case the feasible set of (D_{iq}) may be too small. We can restrict the feasible set of the primal problem a bit more, by adding the constraint $X \in \mathcal{CP}_n$ to (CP_{iq}), which gives the known formulation

$$\begin{array}{ll} \min & \langle Q_{iq}, X \rangle \\ \text{s.t.} & \langle a a^T, X \rangle = 1 \\ & \langle B_{iq}, X \rangle = 0 \qquad . \\ & A X A^T \in \mathcal{CP}_{m+n} \\ & X \in \mathcal{CP}_n \end{array} \qquad (CP_{iq})$$

For the minimization problem in (3.38) to be solvable in this case we need

$$Q_{iq} - A^T U A - \lambda a a^T + \sigma B_{iq} \in \mathcal{COP}_n \text{ and } U \in \mathcal{COP}_{m+n}.$$

In this case the dual problem of (CP_{iq}) is

$$\begin{array}{ll} \max & \lambda \\ \text{s.t.} & Q_{iq} - A^T U A - \lambda a a^T + \sigma B_{iq} \in \mathcal{COP}_n \\ & U \in \mathcal{COP}_{m+n} \\ & \lambda \in \mathbb{R}, \sigma \in \mathbb{R} \end{array} \tag{D'$_{iq}$}$$

For the case considered in (3.5) where the key assumption (3.19) is fulfilled it is easy to construct a strictly feasible point as follows. Choose $\hat{U} \in \operatorname{int} \mathcal{COP}_{m+n}$.

Next, set $\hat{\sigma} = 0$. Then choose $\hat{\lambda} < 0$ (sufficiently negative) such that the matrix

$$Q_{iq} - A^T \hat{U} A - \lambda a a^T$$

has strictly positive entries. The point $(\hat{U}, \hat{\lambda}, 0)$ is then strictly feasible to Problem (D'_{iq}). As a result, we have strong duality, and moreover, we can, in principle, apply the algorithm in [9] to solve the dual problem (D'_{iq}). However, since Problem (D'_{iq}) contains two conic constraints, one needs some suitable modifications while implementing the original algorithm. We will deal with these modifications at another occasion.

Example 3.5.1. *We want to give a strictly feasible copositive formulation of Problem* (3.22) *and Problem* (3.28)*. Recall the problems*

$$\begin{array}{lll} \min & x^T Q x + q^T x & \\ \text{s.t.} & (a^i)^T x \leq 1 & i = 1, \dots, m \\ & x \in \{0,1\}^d, & \end{array} \qquad \begin{array}{ll} \min & \langle Q_{iq}, X \rangle \\ \text{s.t.} & \langle a a^T, X \rangle = 1 \\ & A X A^T \in \mathcal{CP}_{m+2n-1} \\ & \langle B_{iq}, X \rangle = 0. \end{array}$$

Then the copositive problem can be formulated as

$$\begin{array}{ll} \max & \lambda \\ & Q_{iq} - \lambda a a^T + \sigma B_{iq} + A^T U A \in \mathcal{COP}_n \\ & \lambda, \sigma \in \mathbb{R} \\ & U \in \mathcal{COP}_{m+2n-1}. \end{array} \tag{3.39}$$

Note that for the constraint

$$Q_{iq} - \lambda aa^T + \sigma B_{iq} + A^T U A \in \mathcal{COP}_n$$

we need B_{iq} to be symmetric. The strict feasibility of Problem (3.39) *is shown as follows. Choose $\hat{U} = ee^T$, i.e. $\hat{U} \in \operatorname{int} \mathcal{COP}_{m+n}$. Furthermore, choosing $\hat{s} = 0$ and $\hat{\lambda} < 0$ small enough we obtain the matrix $Q_{iq} - \hat{\lambda} aa^T + A^T \hat{U} A$ with all positive entries, i.e.*

$$Q_{iq} - \hat{\lambda} aa^T + A^T \hat{U} A \in int\, \mathcal{COP}_n.$$

Notice that under some circumstances the original algorithm in [9] can solve strictly feasible copositive programs with only one copositive variable very efficiently. In order to use this advantage, the problem formulation (CP$_e$) could be considered as a good alternative. To this purpose, we formulate Problem (CP$_e$) explicitly as

$$\begin{aligned} \min \quad & \langle Q_e, X \rangle \\ \text{s.t.} \quad & \langle cc^T, X \rangle = 1 \\ & \langle C^T C, X \rangle = 0 \\ & \langle B_e, X \rangle = 0 \\ & X \in \mathcal{CP}_{m+n}. \end{aligned} \tag{CP$_e$}$$

By the same idea of construction as above, we obtain the following dual problem of (CP$_e$), which is a copositive program with only one copositive variable:

$$\begin{aligned} \max \quad & \lambda \\ \text{s.t.} \quad & Q_e - \lambda cc^T + \sigma C^T C + \tau B_e \in \mathcal{COP}_{m+n} \\ & \lambda, \sigma, \tau \in \mathbb{R}. \end{aligned} \tag{D$_e$}$$

In general, (D$_e$) is not strictly feasible. However since $c^T x = 1$ is a redundant equality constraint for (QP$_e$), we can add another redundant constraint $\hat{c}^T x = 1$ with $\hat{c} > 0$ instead of $c^T x = 1$ whenever the feasible set of (QP$_e$) is bounded. Let $\hat{C}$ be the corresponding matrix defined by (3.13), then we obtain the equivalent problems

$$\begin{array}{ll} \min & \langle Q_e, X\rangle \\ \text{s.t.} & \langle \hat{c}\hat{c}^T, X\rangle = 1 \\ & \langle \hat{C}^T\hat{C}, X\rangle = 0 \\ & \langle B_e, X\rangle = 0 \\ & X \in \mathcal{CP}_{m+n} \end{array} \tag{CP$_e$}$$

and its dual

$$\begin{array}{ll} \max & \lambda \\ \text{s.t.} & Q_e - \lambda\hat{c}\hat{c}^T + \sigma\hat{C}^T\hat{C} + \tau B_e \in \mathcal{COP}_{m+n} \\ & \lambda \in \mathbb{R}, \sigma \in \mathbb{R}, \tau \in \mathbb{R}. \end{array} \tag{D$_e$}$$

In order to construct a strictly feasible point for (D$_e$), choose $\hat{\sigma} = \hat{\tau} = 0$. Then choose $\hat{\lambda} < 0$ (sufficiently negative) such that the matrix

$$Q_e - \hat{\lambda}\hat{c}\hat{c}^T$$

has strictly positive entries and hence $Q_e - \hat{\lambda}\hat{c}\hat{c}^T \in \operatorname{int}\mathcal{COP}_{m+n}$. Then the point $(\hat{\lambda}, \hat{\sigma}, \hat{\tau})$ is a strictly feasible point for (D$_e$).

Remark 3.5.2. *Note that we wanted to solve the Problem* (D$_e$) *with the algorithm from Bundfuss and Dür in [9]. Unfortunately the simplex partition chosen in this paper is not exhaustive for these kinds of problems, therefore convergence is not guaranteed. To find an exhaustive bisection rule is no easy task and require some effort to establish such a exhaustive rule. Which we will not cover in this thesis.*

CHAPTER 4

Duality and Exact Penalty Method

4.1 Introduction

The subjects of this chapter are the following quadratic optimization problems:

$$\begin{aligned} \min \quad & x^T Q x \\ \text{s.t.} \quad & Cx = 0 \\ & c^T x = 1 \\ & x \geq 0, \end{aligned} \tag{P1}$$

and

$$\begin{aligned} \min \quad & x^T Q x \\ \text{s.t.} \quad & x^T A x \leq b \\ & c^T x = 1 \\ & x \geq 0, \end{aligned} \tag{P2}$$

where $Q \in \mathcal{S}_n$, $C \in \mathbb{R}^{m \times n}$, $A \in \mathcal{COP}_n$, $b > 0$, and $c \in \mathbb{R}^n_+ \setminus \{0\}$.

Our purpose consists of two points. Firstly, we construct the Lagrange dual problem of an equivalent formulation of Problem (P1) and investigate duality properties for the resulting primal-dual pair, including strong duality, and secondly, following the obtained duality results, we develop an exact penalty method for globally solving Problem (P2).

Two known special cases of Problem (P1) are the problem with the feasible set P_e given in (3.14), and the standard quadratic problem, where $m = 0$. The feasible set of Problem (P1) is one of the standard forms of polyhedral sets used in interior point algorithms (e.g., in Karmarkar-type algorithms). See Section 3.3 for how to obtain Problem (P1) from quadratic problems over polyhedral sets.

4.2 Equivalent Form of Problem (P1) and its Dual Problem

We notice that

$$Cx = 0 \Leftrightarrow (Cx)^T(Cx) = 0,$$

and since $c \geq 0$, it follows that $c^T x \geq 0$ for $x \geq 0$.
Therefore, for $x \geq 0$ we have

$$c^T x = 1 \Leftrightarrow (x^T c)(c^T x) = 1.$$

Thus, we can formulate Problem (P1) equivalently as the following problem

$$\begin{array}{ll} \min & x^T Q x \\ \text{s.t.} & x^T C^T C x = 0 \\ & x^T c c^T x = 1 \\ & x \geq 0, \end{array} \tag{QP}$$

In the following, Problem (QP) is considered instead of Problem (P1). We begin with the construction of the Lagrangian dual problem of (QP).

Proposition 4.2.1. *The Lagrangian dual problem of the quadratic optimization problem (QP) is the following copositive program:*

$$\begin{aligned} \max \quad & \lambda \\ & Q - \lambda cc^T + \sigma C^T C \in \mathcal{COP}_n \\ & \lambda \in \mathbb{R},\ \sigma \in \mathbb{R}. \end{aligned} \tag{D}$$

Proof. The Lagrangian function for (QP) is:

$$L(x, \lambda, \sigma) = x^T Q x + \sigma(x^T C^T C x) + \lambda(1 - x^T cc^T x).$$

The Lagrangian dual problem has then the form

$$\begin{aligned} &\max_{\lambda,\sigma\in\mathbb{R}} \ \min_{x\geq 0} \left\{ x^T Q x + \sigma(x^T C^T C x) + \lambda(1 - x^T cc^T x) \right\} = \\ &\max_{\lambda,\sigma\in\mathbb{R}} \ \left\{ \lambda + \min_{x\geq 0} \left\{ x^T Q x - \lambda(x^T cc^T x) + \sigma(x^T C^T C x) \right\} \right\} = \\ &\max_{\lambda,\sigma\in\mathbb{R}} \ \left\{ \lambda + \min_{x\geq 0} \ x^T \left(Q - \lambda cc^T + \sigma C^T C \right) x \right\}. \end{aligned}$$

If for some $\bar{\lambda}, \bar{\sigma} \in \mathbb{R}$, there is $\bar{x} \geq 0$ such that

$$\bar{x}^T \left(Q - \bar{\lambda} cc^T + \bar{\sigma} C^T C \right) \bar{x} < 0,$$

then for every real number $\gamma \geq 0$, we also have

$$\gamma \bar{x}^T \left(Q - \bar{\lambda} cc^T + \bar{\sigma} C^T C \right) \gamma \bar{x} < 0.$$

Thus, it follows that

$$\begin{aligned} &\min_{x\geq 0} \ x^T \left(Q - \bar{\lambda} cc^T + \bar{\sigma} C^T C \right) x \leq \\ &\gamma \bar{x}^T \left(Q - \bar{\lambda} cc^T + \bar{\sigma} C^T C \right) \gamma \bar{x} \longrightarrow -\infty \text{ for } \gamma \to +\infty. \end{aligned}$$

Moreover, note that for every pair

$$(\lambda, \sigma) \in \mathbb{R}^2 \text{ satisfying } x^T \left(Q - \lambda cc^T + \sigma C^T C\right) x \geq 0 \text{ for all } x \geq 0,$$

we obtain

$$\min_{x \geq 0} \; x^T \left(Q - \lambda cc^T + \sigma C^T C\right) x = 0.$$

Therefore, the dual problem of (QP) is

$$\begin{array}{ll} \max & \lambda \\ & x^T \left(Q - \lambda cc^T + \sigma C^T C\right) x \geq 0 \text{ for all } x \geq 0 \\ & \lambda, \sigma \in \mathbb{R}, \end{array}$$

which is by definition the copositive program (D).

□

Before investigating relationships between the primal-dual pair (QP) and (D) in the the next sections, we present the following result, which is the basis of an equivalent representation of the constraint system of Problem (D).

Proposition 4.2.2. *Let $c \in \mathbb{R}^n_+$. Then for a matrix $B \in \mathcal{S}_n$ we have*

$$\begin{array}{lll} B \in \mathcal{COP}_n & \Leftrightarrow & x^T Bx \geq 0 \textit{ for all} \\ & & x \in \left\{ \{x \in \mathbb{R}^n_+ : c^T x = 1\} \cup \{x \in \mathbb{R}^n_+ : c^T x = 0\} \right\}. \end{array} \tag{4.1}$$

Proof. The first direction follows immediately from the definition of copositive matrices. To show the opposite direction, suppose that $B \notin \mathcal{COP}_n$, i.e., there exists $y \in \mathbb{R}^n_+$ such that $c^T y \neq 0$, $c^T y \neq 1$ and $y^T By < 0$. Then, since $c \geq 0$, the point $x = \alpha y$ with $\alpha = \frac{1}{c^T y}$ would satisfy $x \in \mathbb{R}^n_+$, $c^T x = 1$ and $x^T Bx < 0$, a contradiction. □

From Proposition 4.2.2, it follows that the constraint

$$Q + \sigma C^T C - \lambda cc^T \in \mathcal{COP}_n$$

in Problem (D) is equivalently written as

$$\begin{aligned} & x^T(Q + \sigma C^T C - \lambda cc^T)x \geq 0 \text{ for all} \\ & x \in \left\{ \{x \in \mathbb{R}^n_+ : c^T x = 1\} \cup \{x \in \mathbb{R}^n_+ : c^T x = 0\} \right\}, \end{aligned} \tag{4.2}$$

or in two groups of constraints:

$$\begin{aligned} \lambda &\leq x^T Q x + \sigma(x^T C^T C x) \text{ for all } x \geq 0,\ c^T x = 1 \\ 0 &\leq x^T Q x + \sigma(x^T C^T C x) \text{ for all } x \geq 0,\ c^T x = 0. \end{aligned} \tag{4.3}$$

4.3 Necessary Conditions for Insolvability of Problem (QP)

Proposition 4.3.1. *We have the following relationship between Problems* (QP) *and* (D).

(i) If Problems (QP) *is infeasible, then Problem* (D) *is either infeasible or unbounded.*

(ii) If Problem (QP) *is unbounded, then Problem* (D) *is infeasible.*

Proof. (i) Infeasiblity of (QP) implies that for $x \geq 0$, $c^T x = 1$, we must have $Cx \neq 0$. In view of (4.3), we can therefore write (D) equivalently as

$$\begin{array}{llll} \max & \lambda & & \\ \text{s.t.} & \lambda & \leq & x^T Q x + \sigma(x^T C^T C x), \text{ for all } x \geq 0, c^T x = 1, Cx \neq 0 \\ & 0 & \leq & x^T Q x + \sigma(x^T C^T C x), \text{ for all } x \geq 0, c^T x = 0, Cx \neq 0 \\ & 0 & \leq & x^T Q x + \sigma(x^T C^T C x), \text{ for all } x \geq 0, c^T x = 0, Cx = 0. \end{array}$$

If (D) is feasible, then clearly the third condition must be fulfilled, and in this case it does not imply any restriction on λ and σ. In this case, we get from $Cx \neq 0$ that $x^T C^T Cx > 0$, and hence

$$x^T Qx + \sigma(x^T C^T Cx) \to \infty \text{ as } \sigma \to \infty.$$

If follows that (D) is unbounded.

(ii) Assume that (QP) is unbounded. Then there exists a descending recession direction $\bar{x}$ satisfying

$$\bar{x} \geq 0,\ C\bar{x} = 0,\ c^T\bar{x} = 0, \text{ and } \bar{x}^T Q\bar{x} < 0.$$

Plugging $\bar{x}$ into (4.3), $\bar{x}$ generates the constraint

$$0 \leq \bar{x}^T Q\bar{x} + \sigma \cdot 0.$$

Since $\bar{x}^T Q\bar{x} < 0$, we see that this constraint cannot be satisfied, so (D) is infeasible.

□

4.4 Necessary Conditions for Insolvability of Problem (D)

For the investigation of further duality properties, we introduce the following quadratic optimization problem, denoted by (PQP_σ), which is defined depending on a parameter $\sigma \geq 0$:

$$\min\{x^T Qx + \sigma x^T C^T Cx : x^T cc^T x = 1,\ x \geq 0\}. \qquad (\mathrm{PQP}_\sigma)$$

Proposition 4.4.1. *Under the assumption that there exists $\bar{\sigma} \geq 0$ such that the problem $(PQP_{\bar{\sigma}})$ is solvable, we have the following relationship between Problems* (QP) *and* (D)*:*

(i) If Problem (D) *is infeasible, then Problem* (QP) *is insolvable.*

(ii) If Problem (D) *is unbounded, then Problem* (QP) *is insolvable.*

Proof. (i) Suppose that Problem (QP) is solvable. Define

$$\bar{\lambda} = \min\{x^T Qx + \bar{\sigma} x^T C^T Cx : x^T cc^T x = 1, x \geq 0\}. \tag{4.4}$$

We show that $(\bar{\lambda}, \bar{\sigma})$ is a feasible solution of Problem (D), which is a contradiction to the infeasibility of Problem (D).

It follows that

$$\bar{\lambda} \leq x^T Qx + \bar{\sigma} x^T C^T Cx \text{ for all } x \geq 0, \quad c^T x = 1. \tag{4.5}$$

Moreover,

$$0 \leq x^T Qx + \bar{\sigma} x^T C^T Cx \text{ for all } x \geq 0, \quad c^T x = 0, \tag{4.6}$$

since otherwise, there exists a descending recession direction $\bar{x}$ satisfying

$$\bar{x} \geq 0, \ c^T \bar{x} = 0, \ \bar{x}^T Q\bar{x} + \bar{\sigma} \bar{x}^T C^T C\bar{x} < 0,$$

contradicting the existence of $\bar{\lambda}$ in (4.4). The systems (4.5) and (4.6) imply that $(\bar{\lambda}, \bar{s})$ satisfies (4.3) and hence it is a feasible solution of Problem (D).

(ii) Suppose Problem (QP) is solvable. Then, as the constraint system (4.3) of (D) contains the following constraint group

$$\lambda \leq x^T Qx \text{ for all } x \text{ satisfying } x \geq 0, \ c^T x = 1, \ Cx = 0,$$

it follows that

$$\lambda \leq \min\{x^T Qx : Cx = 0, c^T x = 1, x \geq 0\}.$$

Since the right hand side equals the optimal value of (QP) this is a contradiction to the unboundedness of (D).

□

4.5 Main Duality Properties

We are now in a position to present the main duality properties of the primal-dual pair (QP) and (D). For this, let $\varepsilon > 0$ be any given real number and consider the following quadratic problem

$$\begin{array}{ll} \min & x^T Q x \\ \text{s.t.} & x^T C^T C x \le \varepsilon \\ & x^T c c^T x = 1 \\ & x \ge 0, \end{array} \tag{QP$_\varepsilon$}$$

which is a perturbation problem of (QP) by using the perturbation parameter $\varepsilon > 0$ for the constraint $x^T C^T C x = 0$.

Theorem 4.5.1. *Under the assumption that there exists $\bar{\sigma} \ge 0$ such that Problem $(PQP_{\bar{\sigma}})$ is solvable, we have the following duality properties of the primal-dual problem pair* (QP) *and* (D)*.*

(dp1) For every feasible solution x of Problem (QP) *and every feasible solution (λ, σ) of Problem* (D) *we have*

$$\lambda \le x^T Q x. \tag{4.7}$$

(dp2) Problem (QP) *is solvable if and only if Problem* (D) *is solvable. In this case, the following holds true for every $\varepsilon > 0$:*

$$\min(QP_\varepsilon) \le \max(D) \le \min(QP). \tag{4.8}$$

Proof. (dp1) Let x be any feasible solution of Problem (QP) and (λ, σ) any feasible solution of Problem (D). Then, as $x^T C^T C x = 0$, $x^T c c^T x = 1$, $x \ge 0$ in (D), and (λ, σ) fulfills the constraint

$$\lambda (c^T x)^2 \le x^T Q x + \sigma (x^T C^T C x)$$

in (D), it follows that

$$\lambda \leq x^T Q x.$$

(dp2) From Proposition 4.3.1 and Proposition 4.4.1, it follows that Problem (QP) is solvable if and only if Problem (D) is solvable.

To show the property (4.8), let (λ^*, σ^*) be an optimal solution of Problem (D) with optimal value λ^*. Then from Assertion ($dp1$), it follows that

$$\lambda^* \leq x^T Q x \text{ for all } x \text{ satisfying } x^T C^T C x = 0,\ x^T c c^T x = 1,\ x \geq 0,$$

or

$$\begin{aligned} \lambda^* &\leq \min\{x^T Q x : x^T C^T C x = 0,\ x^T c c^T x = 1,\ x \geq 0\} \\ &= \min(QP), \end{aligned} \tag{4.9}$$

which is the right inequality in (4.8). For the left inequality in (4.8), notice that as (QP) is solvable, (QP$_\varepsilon$) is feasible. If (QP$_\varepsilon$) is unbounded, the left inequality is fulfilled trivially. Now let (QP$_\varepsilon$) be solvable. Furthermore, let $\bar{x}$ be an optimal solution of Problem ($PQP_{\bar{\sigma}}$) and define

$$\begin{aligned} \lambda_\varepsilon &:= \min(QP_\varepsilon), \\ \sigma_\varepsilon &:= \tfrac{1}{\varepsilon}(\lambda_\varepsilon - \min(\mathrm{PQP}_{\bar{\sigma}})). \end{aligned} \tag{4.10}$$

For $\sigma_\varepsilon < 0$, i.e. $\lambda_\varepsilon < \min(\mathrm{PQP}_{\bar{\sigma}})$ consider the following problems:

$$\begin{array}{ll} \min & \langle Q + \bar{\sigma} C^T C, X \rangle \\ \text{s.t.} & \langle c c^T, X \rangle = 1 \\ & X \in \mathcal{CP}_n, \end{array} \tag{CP$_{\bar{\sigma}}$}$$

and

$$\begin{array}{ll} \max & \lambda \\ \text{s.t.} & (Q+\bar{\sigma}C^TC)-\lambda cc^T \in \mathcal{COP}_n \\ & \lambda \in \mathbb{R}. \end{array} \tag{$\mathrm{D}_{\bar{\sigma}}$}$$

Then Problem ($\mathrm{CP}_{\bar{\sigma}}$) is the completely positve reformulation of ($\mathrm{PQP}_{\bar{\sigma}}$) and Problem ($\mathrm{D}_{\bar{\sigma}}$) its copositve dual. Since ($\mathrm{PQP}_{\bar{\sigma}}$) contains only one equality constraint, we have that ($\mathrm{CP}_{\bar{\sigma}}$) is strictly feasible and hence strong duality with

$$\min(\mathrm{CP}_{\bar{\sigma}}) = \max(\mathrm{D}_{\bar{\sigma}}).$$

Furthermore we have $\max(\mathrm{D}_{\bar{\sigma}}) \leq \max(\mathrm{D})$, and it follows that

$$\min(\mathrm{QP}_{\varepsilon}) = \lambda_{\varepsilon} < \min(PQP_{\bar{\sigma}}) = \max(\mathrm{D}_{\bar{\sigma}}) \leq \max(\mathrm{D}). \tag{4.11}$$

In case $\sigma_{\varepsilon} \geq 0$, we have

$$\begin{aligned} \lambda_{\varepsilon} &= \sigma_{\varepsilon}\varepsilon + \min(\mathrm{PQP}_{\bar{\sigma}}) \\ &= \sigma_{\varepsilon}\varepsilon + \bar{x}^TQ\bar{x} + \bar{\sigma}\bar{x}^TC^TC\bar{x} \\ &\leq x^TQx + \bar{\sigma}x^TC^TCx + \sigma_{\varepsilon}\varepsilon \text{ for all } x \geq 0 \text{ satisfying} \\ &\qquad x^Tcc^Tx = 1 \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (4.12) \\ &\leq x^TQx + (\bar{\sigma}+\sigma_{\varepsilon})x^TC^TCx \text{ for all } x \geq 0 \text{ satisfying} \\ &\qquad x^Tcc^Tx = 1, x^TC^TCx \geq \varepsilon, \end{aligned}$$

and on the other hand, as $\sigma x^T C^T Cx \geq 0$ for all $\sigma \geq 0$ and for all x:

$$\begin{aligned}
\lambda_\varepsilon &= \min(\mathrm{QP}_\varepsilon) \\
&\leq x^T Qx \text{ for all } x \geq 0 \text{ satisfying} \\
&\quad\; x^T cc^T x = 1,\; x^T C^T Cx \leq \varepsilon \qquad (4.13) \\
&\leq x^T Qx + (\bar{\sigma} + \sigma_\varepsilon) x^T C^T Cx \text{ for all } x \geq 0 \text{ satisfying} \\
&\quad\; x^T cc^T x = 1, x^T C^T Cx \leq \varepsilon.
\end{aligned}$$

From the assumption that ($\mathrm{PQP}_{\bar{\sigma}}$) is solvable, there exists no vector $x_{\bar{\sigma}} \geq 0$ with $x_{\bar{\sigma}}^T cc^T x_{\bar{\sigma}} = 0$ such that

$$x_{\bar{\sigma}} Q x_{\bar{\sigma}} + \bar{\sigma} x_{\bar{\sigma}}^T CC^T x_{\bar{\sigma}} < 0,$$

i.e. $x_{\bar{\sigma}}$ is a descending recession direction of $(PQP_{\bar{\sigma}})$. Hence for all $x \geq 0$ with $x^T cc^T x = 0$ we have

$$0 \;\leq\; x^T Qx + (\bar{\sigma} + \sigma_\varepsilon) x^T C^T Cx \qquad (4.14)$$

In sum, the inequalities (4.12)-(4.14) imply that $(\lambda_\varepsilon, (\bar{\sigma} + \sigma_\varepsilon))$ fulfills System (4.3), i.e., it is a feasible solution of Problem (D) and hence we have

$$\min(QP_\varepsilon) = \lambda_\varepsilon \leq \max\,(\mathrm{D}). \qquad (4.15)$$

Finally, from (4.9),(4.11) and (4.15), we obtain (4.8).

□

The next result gives us another duality property by using the problem (PQP_σ).

Theorem 4.5.2. *Under the assumption that the Problems (PQP_0),* (QP) *and* (D) *are solvable, we have the following duality property of the primal-dual problem pairs* (QP) *and* (D)*:*

(dp3) For given $\varepsilon > 0$ there exists $\sigma_\varepsilon > 0$ such that for all $\sigma \geq \sigma_\varepsilon$ we have

$$\min(PQP_\sigma) \leq \max(\mathrm{D}) \leq \min(\mathrm{QP}). \tag{4.16}$$

Proof. From Assertion ($dp2$) of Theorem 4.5.1, the right inequality follows immediately. To show the left inequality, we show that for given $\varepsilon > 0$ there exists $\sigma_\varepsilon > 0$ such that for all $\sigma \geq \sigma_\varepsilon$ we have

$$\min(\mathrm{PQP}_\sigma) = \min(\mathrm{QP}_\varepsilon).$$

Note that Problem (PQP_0) has the form

$$\min\{x^T Qx : x^T cc^T x = 1,\ x \geq 0\}.$$

We can assume without loss of generality that

$$\min(\mathrm{QP}_\varepsilon) > \min(\mathrm{PQP}_0), \tag{4.17}$$

since otherwise both problems (QP_ε) and (PQP_0) are equivalent.

From the solvability of Problems (QP) and (PQP_0), it follows that Problem (QP_ε) is solvable for every given $\varepsilon > 0$. For given $\varepsilon > 0$ let define

$$\begin{aligned} \lambda_\varepsilon &= \min(QP_\varepsilon), \\ \sigma_\varepsilon &= \tfrac{1}{\varepsilon}(\lambda_\varepsilon - \min(PQP_0)). \end{aligned} \tag{4.18}$$

From (4.17) we have $\sigma_\varepsilon > 0$, and from (4.18) it follows for every $\sigma \geq \sigma_\varepsilon$ that

$$\lambda_\varepsilon \leq \min(PQP_0) + \sigma\varepsilon.$$

Thus, for every $\lambda \leq \lambda_\varepsilon$ we have on the one hand

$$\begin{aligned} &\lambda \leq \lambda_\varepsilon \leq x^T Qx + \sigma x^T C^T Cx \\ &\text{for all } x \geq 0 \text{ satisfying } x^T cc^T x = 1,\ x^T C^T Cx \geq \varepsilon, \end{aligned}$$

and on the other hand, as $\sigma x^T C^T C x \geq 0$ for all $x \geq 0$,

$$\lambda \leq \lambda_\varepsilon \leq x^T Q x + \sigma x^T C^T C x$$
$$\text{for all } x \geq 0 \text{ satisfying } x^T c c^T x = 1,\ x^T C^T C x \leq \varepsilon.$$

Therefore, we obtain that for all $\sigma \geq \sigma_\varepsilon$, we have

$$\begin{aligned} \min(QP_\varepsilon) &= \lambda_\varepsilon \\ &= \max\{\lambda : \lambda \leq x^T Q x + \sigma x^T C^T C x \text{ for all } x \geq 0 \text{ satisfying} \\ &\qquad\qquad x^T c c^T x = 1,\ \lambda \in \mathbb{R}\} \\ &= \min\{x^T Q x + \sigma x^T C^T C x : x \geq 0,\ x^T c c^T x = 1\} \\ &= \min(PQP_\sigma). \end{aligned}$$

□

The following result gives us a strong duality property of the pair (QP)-(D).

Theorem 4.5.3. *Assume that $c > 0$, i.e., $c_i > 0,\ i = 1, ..., n$, and Problem (QP) is solvable. Then we have strong duality property for the pair* (QP)-(D), *i.e.,*

$$\min\,(\mathrm{QP}) = \max\,(\mathrm{D}).$$

Proof. From $c > 0$ it follows that (PQP_0) is solvable and from (QP) is feasible it follows from Theorem 4.5.1 that (D) is feasible and for $\varepsilon > 0$ we have

$$\min(\mathrm{QP}_\varepsilon) \leq \max\,(\mathrm{D}) \leq \min\,(\mathrm{QP}).$$

For the strong duality property, denote by

$$\varphi : \mathbb{R}_+ \to \mathbb{R},\ \varphi(\varepsilon) := \min(\mathrm{QP}_\varepsilon)$$

the optimal value function of the parametric optimization problem (QP_ε). Since $c > 0$, the set

$$\{x \in \mathbb{R}^n : x^T c c^T x = 1,\ x \geq 0\}$$

is compact. Thus, since the quadratic function $x^T Qx$ is continuous and Problem (QP_0) (i.e., (QP)) is solvable, it follows that the function φ is both upper and lower semicontinuous at 0 (see Corollary 4.2.1.1 and Theorem 4.2.2 in [2]), which implies that

$$\varphi(\varepsilon) \to \varphi(0) = \min(\mathrm{QP}) \text{ as } \varepsilon \to +0.$$

From (4.8), it follows then $\max(\mathrm{D}) = \min(\mathrm{QP})$. □

Remark 4.5.4. *(i) Theorem 4.5.1 and Theorem 4.5.2 provide computable duality gaps between the primal and dual problems* (QP) *and* (D)*.*

(ii) Theorem 4.5.3 provides a direct reformulation of the quadratic optimization problem (P1) *into a copositive program. By taking the dual of the resulting copositive program, we obtain a completely positive program reformulation of Problem* (P1)*.*

4.6 An Exact Penalty Algorithm for Solving Problem (P2)

Following the duality results obtained above, we develop an exact penalty method for solving Problem (P2), which is written as

$$\min\{x^T Qx : \ x^T Ax \le b, \ c^T x = 1, \ x \ge 0\}, \tag{P}$$

where $Q \in \mathcal{S}_n$, $A \in \mathcal{COP}_n$, $b > 0$, and $c \in \mathbb{R}^n_+$. Notice that the problem class (P) contains Problem (QP_ε) as a special case where $A = C^T C$ and $b = \varepsilon$.

According to (P) we construct the following penalized problem by using the penalty function $\sigma x^T Ax$ with the penalty parameter $\sigma > 0$:

$$\min\{x^T Qx + \sigma x^T Ax : \ c^T x = 1, \ x \ge 0\}. \tag{PP_σ}$$

The following result provides an exact penalty method for globally solving Problem (P).

Theorem 4.6.1. *Assume that Problem* (P) *as well as Problem*

$$\min\{x^T Qx : \ c^T x = 1, \ x \geq 0\}, \tag{SP}$$

are solvable. Moreover, assume that the constraint $x^T Ax \leq b$ is essential for Problem (P)*, i.e.,*

$$\min\,(\mathrm{P}) > \min\,(\mathrm{SP}). \tag{4.19}$$

Then there exists $\bar{\sigma} > 0$ such that for all $\sigma \geq \bar{\sigma}$ we have

(i)

$$\min\,(\mathrm{P}) = \min\,(\mathrm{PP}_\sigma); \tag{4.20}$$

(ii) Every optimal solution x^σ of Problem (PP_σ) *satisfies*

$$(x^\sigma)^T Ax^\sigma \leq b.$$

Proof. (*i*) Define

$$\begin{aligned} \bar{\lambda} &:= \min\,(\mathrm{P}), \\ \bar{\sigma} &:= \tfrac{1}{b}(\bar{\lambda} - \min\,(\mathrm{SP})). \end{aligned} \tag{4.21}$$

From (4.19) we have $\bar{\sigma} > 0$, and from (4.21) it follows for every $\sigma \geq \bar{\sigma}$ that

$$\bar{\lambda} \leq \min\,(\mathrm{SP}) + \sigma b.$$

Thus, for every $\lambda \leq \bar{\lambda}$ we have on the one hand

$$\lambda \leq \bar{\lambda} \leq x^T Qx + \sigma x^T Ax \text{ for all } x \geq 0 \text{ satisfying } c^T x = 1, \ x^T Ax \geq b,$$

and on the other hand, as $\sigma x^T Ax \geq 0$ for all $x \geq 0$,

$$\lambda \leq \bar{\lambda} \leq x^T Qx + \sigma x^T Ax \text{ for all } x \geq 0 \text{ satisfying } c^T x = 1,\ x^T Ax \leq b.$$

Therefore, we obtain that for all $\sigma \geq \bar{\sigma}$ we have

$$\begin{aligned}
\bar{\lambda} &= \max\{\lambda : \lambda \leq x^T Qx + \sigma x^T Ax \text{ for all } x \geq 0 \text{ satisfying} \\
&\qquad\qquad\qquad\qquad\qquad\qquad c^T x = 1,\ \lambda \in \mathbb{R}\} \\
&= \min\{x^T Qx + \sigma x^T Ax : x \geq 0,\ c^T x = 1\} \\
&= \min(PP_\sigma).
\end{aligned}$$

(ii) To show this assertion, suppose that $(x^\sigma)^T Ax^\sigma > b$, i.e.,

$$\frac{(x^\sigma)^T Ax^\sigma}{b} > 1.$$

Then from (4.21) and Assertion (i) we have

$$\begin{aligned}
\bar{\lambda} &= (x^\sigma)^T Qx^\sigma + \sigma (x^\sigma)^T Ax^\sigma \\
&\geq (x^\sigma)^T Qx^\sigma + \tfrac{(\bar{\lambda} - \min(SP))}{b} (x^\sigma)^T Ax^\sigma \\
&> (x^\sigma)^T Qx^\sigma + (\bar{\lambda} - \min(\mathrm{SP})) \\
&= \bar{\lambda} + ((x^\sigma)^T Qx^\sigma - \min(\mathrm{SP})) \\
&\geq \bar{\lambda},
\end{aligned}$$

which is a contradiction. Note that the last inequality follows from the fact that x^σ is feasible for (SP), and hence

$$(x^\sigma)^T Qx^\sigma - \min(\mathrm{SP}) \geq 0.$$

$\square$

In particular, we consider the case where in Problem (P), the vector c satisfies $c > 0$, i.e., $c_i > 0, i = 1, \cdots, n$.

Let Δ^c be the simplex defined by

$$\Delta^c := \{x \in \mathbb{R}^n : c^T x = 1,\ x \geq 0\}. \tag{4.22}$$

Then the problem (PQP$_0$) is

$$\min\{x^T Q x : x \in \Delta^c\}, \tag{4.23}$$

which is clearly solvable.

For a given $\varepsilon > 0$, the problem (QP$_\varepsilon$) is

$$\min\{x^T Q x : x^T C^T C x \leq \varepsilon,\ x \in \Delta^c\}. \tag{4.24}$$

From Theorem 4.6.1, there exists $\sigma_\varepsilon \geq 0$ such that Problem (4.24) can be replaced by the problem (PP$_\sigma$)

$$\min\{x^T (Q + \sigma C^T C) x :\ x \in \Delta^c\}, \tag{4.25}$$

with $\sigma \geq \sigma_\varepsilon$. Problem (4.25) belongs to the problem class considered in Chapter 2, and can be solved by the algorithm given there. From the proof of Theorem 4.5.1 we can construct a $\sigma \geq \sigma_\varepsilon$. For this define

$$\begin{aligned} \lambda_\varepsilon &:= \min(\mathrm{QP}_\varepsilon), \\ \sigma_\varepsilon &:= \tfrac{1}{\varepsilon}(\lambda_\varepsilon - \min(\mathrm{PP}_0)). \end{aligned}$$

For computational efficiency we do not need to exactly compute σ_ε. It suffice to obtain a feasible point λ of (QP$_\varepsilon$) and a good lower bound μ for (PP$_0$) and define $\sigma := \frac{1}{\varepsilon}(\lambda - \mu)$. Clearly we have $\sigma \geq \sigma_\varepsilon$.

Chapter 5

Conclusions and Outlook

In this final chapter we address the questions *"What have we done in this thesis?"* (Section 5.1) and *"What remains open for future research?"* (Section 5.2).

5.1 Summary

In this thesis, we have done the following.

Chapter 1 introduces notations and background knowledge required in this thesis. All symbols and spaces are listed in Subsection 1.2.1. The definitions of the copositive and completely positive cone was introduced in Subsection 1.2.2. Subsection 1.2.3 and 1.2.4 was devoted to the copositive and completely positive programs and their duals. Finally in Subsection 1.2.5, known algorithms to solve copositive problems were discussed.

In **Chapter 2**, based on Lemma 2.4.1 that optimal solutions of a non convex quadratic optimization problem over a compact convex set can be obtained on the *boundary* of the feasible set, a *finite* algorithm to solve quadratic optimization problems over the origin simplex was established. An implementation of the algorithm in C++ and the comparison of the numerical results for some chosen problems were performed.

The main subject of **Chapter 3** was to reformulate *general quadratic optimization problems* as *completely positive problems* similar to the case of the *Standard Quadratic Problem* considered in [5]. The resulting problems were called *lifted problems* which are in general convex programs with matrix variables and conic constraints. The general concept of constructing lifting problems was discussed in Subsection 3.2. Subsection 3.3 was devoted to an equivalent reformulation of the feasible set of a given *general quadratic optimization problem*, which is suitable to be lifted into the space of completely positive cone. In Subsection 3.4, two lifted completely positive representations for *general quadratic optimization problems* were constructed, one for quadratic optimization problems restricted by *inequalities* and the other one for *equality-restricted* quadratic optimizations problems. Subsection 3.5 was concerned with the copositive duals of the completely positive problems introduced in Subsection 3.4 and the question of strong duality for primal-dual problem pairs, i.e. *strict feasibility* of the primal or/and the dual problem.

We have taken the multidimensional knapsack problem as an example for performing our reformulation technique.

In **Chapter 4**, we were concerned with two topics: duality and penalty method for respectively two classes of quadratic optimization problems. For the first class, which contains standard forms of polyhedral sets as special cases, we constructed the Lagrange dual problem and investigated different duality properties including strong duality for the resulting primal-dual pair. Following these results, we developed an exact penalty method for solving another problem class, which is a generalized form of a perturbation problem of the first class. Using this penalty method, we can solve the latter class by applying the algorithm given in Chapter 2.

To sum up, the novelties of this thesis are as follows:

- In Chapter 2, a new finite algorithm to solve a quadratic optimization problem over the origin simplex has been established (Algorithm 5). Preliminary computational results show that this algorithm can work well for problems of moderate dimensions.

- In Chapter 3, completely positive program representations for respectively two classes of quadratic problems were constructed. The first class contains inequality constrains (Theorem 3.4.1), while the second one contains equality constraints (Theorem 3.4.3). For both cases, the resulting completely positive program contains only one conic constraint. Two copositive dual problems were respectively formulated for two resulting completely positive problems, and one condition for the case of strong duality was given (Subsection 3.5).

- In the first part of Chapter 4, Lagrangian dual of a wide class of quadratic problem over polyhedral set and duality properties including strong duality were presented. These results provide on the one hand computable duality gaps between the primal and dual problems, and on the other hand, a direct reformulation of the primal problem into a copositive program.

  An exact penalty method for a special class of quadratic problems was developed in the second part of Chapter 4. As a result, the algorithm given in Chapter 2 can be used for solving the standard quadratic problem with an additional quadratic constraint.

5.2 Future Work

The following research topics are subjects of our next works:

1. To investigate whether the results obtained in Chapter 4 can be generalized for quadratic optimization problems of the form

$$\begin{aligned} \min \quad & x^T Q x \\ \text{s.t.} \quad & Cx = 0 \\ & x^T A_i x = b_i, \quad i = 1, ..., m \\ & c^T x = 1 \\ & x \geq 0, \end{aligned} \tag{QP}$$

where $Q \in \mathcal{S}_n$, $C \in \mathbb{R}^{m \times n}$, $A_i \in \mathcal{S}_n$, and $c \in \mathbb{R}^n_+ \setminus \{0\}$.

In particular, to investigate the relationships between problem (QP) and the following copositive program

$$\begin{aligned} \max \quad & \lambda + \sum_{i=1}^{m} b_i \beta_i \\ \text{s.t.} \quad & Q - \lambda c c^T + \delta C - \textstyle\sum_{i=1}^m \beta_i A_i \in \mathcal{COP}_n \\ & \lambda, \delta \in \mathbb{R}, \beta = (\beta_1, \cdots, \beta_m) \in \mathbb{R}^m. \end{aligned} \tag{COP}$$

2. To develop algorithms for solving Problem (COP) and its dual based on following ideas:

2.a. Solving Problem (COP) and its dual simultaneously within a framework of primal-dual algorithms.

2.b. Solving Problem (COP) by an outer approximation method using the algorithm given in Chapter 2 for checking copositivity of matrices.

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