Reformulation of the Quadratic Multidimensional Knapsack Problem as Copositive/Completely Positive Prorams

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Abstract. The general (nonconvex) quadratic multidimensional knapsack problem (QMKP) is one of the most important combinatorial optimization problems with many practical applications. The purpose of this article is to establish equivalent formulations of (QMKP) as so called copositive programs and completely positive programs. The resulting programs can then be handled by copositive programming methods, which are completely different from classical algorithms for directly solving quadratic knapsack problems.

Keywords: Knapsack problem · Quadratic multidimensional knapsack problem · Copositive programming · Completely positive program

1 Introduction

Let $\mathbb{R}^d$ and $\mathbb{R}^d_+$ be the d dimensional real space and its nonnegative orthant, respectively, $\mathbb{R}^{d\times k}$ the space of $d \times k$ matrices, and

$$\mathcal{S}_d := \{S \in \mathbb{R}^{d\times d} \mid S^T = S\}$$

the space of symmetric matrices.

The subject of this article is the general (nonconvex) quadratic multidimensional knapsack problem, which is formally formulated as follows (see [7,16]).

$$(QMKP) \begin{cases} \min \; x^T\bar{Q}x + \bar{c}^Tx & \\ \text{s.t. } \; \bar{a}_i^Tx \le \bar{b}_i & \text{for all } i = 1,\ldots,m \\ \qquad x \in \{0,1\}^d, & \end{cases}$$

where $\bar{Q} \in \mathcal{S}_d, \bar{c} \in \mathbb{R}^d$, $\bar{a}_i \in \mathbb{R}^d_+$ and $\bar{b}_i > 0$ for all $i = 1,\ldots,m$.

A well known special case of $(QMKP)$ is the quadratic knapsack problem, (QKP), containing only one capacity constraint, i.e., the case where $m = 1$.

One of the most important applications of Problem (QKP) 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., [11]).

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The quadratic function measures both the expected return and the risk. The single knapsack constraint represents the budget restriction. By using only one knapsack constraint, it is not allowed to consider the possibility of investing into assets of different risk levels. Therefore, several knapsack constraints should be considered, each of them represents a budget allocated to assets of a given risk level. More details about this capital budgeting model can be found in Faaland [9] and Djerdjour et al. [7].

While the Quadratic Knapsack Problem (QKP) is a much-studied combinatorial optimization problem, (see, e.g. [2,3,13] and a survey of Pisinger in [14] and references given therein), there are only a few methods for handling some specific cases of the quadratic multidimensional knapsack problem (QMKP), see e.g., [7,15,16].

In the last two decades, a relatively young field in mathematical optimization called copositive programming has received a great deal of attention from researchers. This is a class of linear programs with matrix variables and additional conic constraints defined by the cones of copositive or completely positive matrices. It has been shown that there is a close relationship between (continuous or binary) quadratic problems and copositive programs, see e.g. [4–6,8,10,12] and references given therein.

The purpose of this paper is to establish equivalent formulations of (QMKP) as copositive programs and completely positive programs. The resulting problems can then be handled by solution methods (see, e.g., [5,8,12] and references given therein), which are completely different from known algorithms for directly solving quadratic knapsack problems.

In the next section we give some preliminaries on copositive programs and completely positive programs. Equivalent Reformulations of (QMKP) as copositive programs and completely positive programs are established thereafter.

2 Preliminaries

2.1 Copositive and Completely Positive Cones

Definition 1. *Let A be a $d \times d$ real symmetric matrix. One says that A is 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 (see, e.g.,[1,8,10]) $\mathcal{COP}_d$ is a closed convex pointed cone in the space of symmetric matrices $\mathcal{S}_d$ with $\mathrm{int}(\mathcal{COP}_d) \neq \emptyset$.

Definition 2. *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 non-negative 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 $d \times d$ copositive matrices. Then $\mathcal{CP}_d$ is a closed convex pointed cone in $\mathcal{S}_d$ with $\mathrm{int}(\mathcal{CP}_d) \neq \emptyset$ (see, e.g.,[1,8,10]).

Definition 3. *Let $\mathcal{C}$ be an arbitrary given cone in $\mathcal{S}_d$, the dual cone $\mathcal{C}^*$ to $\mathcal{C}$ is defined as*

$$\mathcal{C}^* = \{A \in \mathcal{S}_d \mid \langle A, B\rangle \geq 0 \; \forall B \in \mathcal{C}\},$$

where

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

It is well known (see, e.g., [1,8,10], and references given therein) that the cones $\mathcal{COP}_d$ and $\mathcal{CP}_d$ are dual to each other in the sense that

$$\mathcal{COP}_d^* = \mathcal{CP}_d \text{ and } \mathcal{CP}_d^* = \mathcal{COP}_d. \tag{1}$$

2.2 Copositive and Completely Positive Programs and Their Duals

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

$$\begin{array}{ll} \min & \langle Q, X\rangle \\ \text{s.t.} & \langle A_i, X\rangle = b_i,\ i = 1, \cdots, m \\ & X \in \mathcal{K}. \end{array} \tag{2}$$

Definition 4. *Problem (2) is called copositive program if $\mathcal{K} = \mathcal{COP}_d$. It is called completely positive program if $\mathcal{K} = \mathcal{CP}_d$.*

The corresponding Lagrangian dual of Problem (2) is then

$$\begin{array}{ll} \max & \sum\limits_{i=1}^{m} b_i y_i \\ \text{s.t.} & Q - \sum\limits_{i=1}^{m} y_i A_i \in \mathcal{K}^* \\ & y_i \in \mathbb{R},\ i = 1, \cdots, m. \end{array} \tag{3}$$

Since $\mathcal{K}$ and $\mathcal{K}^*$ are convex cones, the strong duality requires some constraint qualifications such as Problem (2) respectively Problem (3) to be strict feasible, i.e., there exists a feasible point in $\mathrm{int}(\mathcal{K})$ or $\mathrm{int}(\mathcal{K}^*)$, respectively.

2.3 Quadratic Optimization Problems and Completely Positive Programs

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 [4]:

$$\begin{array}{ll} \min & x^T Q x \\ s.t. & e^T x = 1 \\ & x \geq 0, \end{array} \tag{4}$$

where $Q \in \mathcal{S}_d$ and e denotes the all-ones vector. The authors of [4] showed that Problem 4 is equivalent to the following completely positive program:

$$\begin{array}{rl} \min & \langle Q, X\rangle \\ s.t. & \langle ee^T, X\rangle = 1 \\ & X \in \mathcal{CP}_d. \end{array} \tag{5}$$

The equivalence between Problem 4 and Problem 5 is that each extreme optimal solution of 5 has the form $X^* = x^*(x^*)^T$, where x^* is an optimal solution of Problem 4 and both problems have the same optimal values.

The second problem is the mixed-binary quadratic program considered by Burer in [6],

$$\begin{array}{rl} \min & x^T Qx + 2q^T x \\ \text{s.t.} & a_i^T x = b_i,\ i = 1, \cdots, m \\ & x \geq 0 \\ & x_j \in \{0, 1\},\ j \in J \subseteq \{1 \cdots, d\}, \end{array} \tag{6}$$

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

Under the following two *Key Assumptions*:

(KA1) It holds: $x \in L \Longrightarrow 0 \leq x_j \leq 1, j = 1, \cdots, d$, where

$$L = \{x \geq 0 : a_i^T x = b_i,\ i = 1, \cdots, m\},$$

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

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

Burer [6] showed that under (KA1)–(KA2), by using a vector

$$\alpha = \sum_{i=1}^m \beta_i a_i \geq 0, \tag{7}$$

Problem (6) can then be equivalently reformulated as the following completely positive program:

$$\begin{array}{rl} \max & \langle Q, X\rangle + 2q^T X\alpha \\ \text{s.t.} & a_i^T X\alpha = b_i,\ i = 1, \cdots, m \\ & a_i^T X a_i = b_i^2,\ i = 1, \cdots, m \\ & (X\alpha)_j = X_{jj},\ j \in J \\ & \alpha^T X\alpha = 1 \\ & X \in \mathcal{CP}_d. \end{array} \tag{8}$$

The equivalence between Problem (6) and Problem (8) is stated as follows (see [6]):

Proposition 1. *Under (KA1)–(KA2), let α be defined as in (7). Then Problem (6) is equivalent to Problem (8) in the sense that:*

(i) The optimal values of both problems are equal;
(ii) If X^* is an optimal solution of Problem (8), then $X^*\alpha$ lies in the convex hull of optimal solutions for Problem (6).

3 Construction of Equivalent Completely Positive and Copositive Optimization Problems

Based on the reformulation principle developed in [12], we present two copositive/completely positive optimization problem models for Problem $(QMKP)$. Moreover, we also show that the resulting primal-dual pairs have strong duality property.

Model I

The first completely positive optimization problem model is constructed by the following steps.

Step 1. Add a redundant constraint $\bar{a}^T x \leq 1$ with $\bar{a} > 0$ to the system of linear inequalities. There are two simple ways to construct such a vector $\bar{a}$.

(i) If there exists $y \in \mathbb{R}^m_+$ with $\sum_{i=1}^m y_i \bar{a}_i > 0$. Then set

$$\bar{a} := \frac{1}{\bar{b}^T y} \sum_{i=1}^m y_i \bar{a}_i > 0,$$

where $\bar{b}^T = (\bar{b}_1, \cdots, \bar{b}_m) > 0$.

(ii) Set

$$\bar{a} := \frac{1}{n-1} e,$$

where e is the vector with all components equal to 1.

As a result, we have a slightly modified problem

$$(QMKP) \begin{cases} \min\ x^T \bar{Q} x + \bar{c}^T x & \\ \text{s.t. } \bar{a}_i^T x \leq \bar{b}_i & \text{for all } i = 1, \ldots, m \\ \quad\ \ \bar{a}^T x \leq 1 & \\ \quad\ \ x \in \{0,1\}^d. & \end{cases}$$

Step 2. Add a slack variable s to the constraint $\bar{a}^T x \leq 1$, obtaining

$$(QMKP) \begin{cases} \min\ x^T \bar{Q} x + \bar{c}^T x & \\ \text{s.t. } \bar{a}_i^T x \leq \bar{b}_i & \text{for all } i = 1, \ldots, m \\ \quad\ \ \bar{a}^T x + s = 1 & \\ \quad\ \ x \in \{0,1\}^d & \\ \quad\ \ s \geq 0. & \end{cases}$$

Define $n := d + 1$ and

$$Q' := \begin{pmatrix} \bar{Q} & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{R}^{n \times n},\ c := \begin{pmatrix} \bar{c} \\ 0 \end{pmatrix},\ b := \begin{pmatrix} \bar{b}_1 \\ \vdots \\ \bar{b}_m \end{pmatrix} > 0,$$

$$a := \begin{pmatrix} \bar{a} \\ 1 \end{pmatrix} > 0,\ A' := \begin{pmatrix} (\bar{a}_1^T, 0) \\ \vdots \\ (\bar{a}_m^T, 0) \end{pmatrix} \in \mathbb{R}^{m \times n}_+.$$

Then we obtain the following equivalent problem in $\mathbb{R}^n$, i.e., the vector of variables is now $x \in \mathbb{R}^n$.

$$(QMKP) \begin{cases} \min x^T Q' x + c^T x \\ \text{s.t. } A'x \le b \\ \qquad a^T x = 1 \\ \qquad x_i \in \{0,1\}, \; i = 1, \cdots, n-1 \\ \qquad x_n \ge 0. \end{cases}$$

Step 3. (Getting rid of the linear term $c^T x$ in the objective function) From the constraint $a^T x = 1$ we have

$$c^T x = x^T a c^T x = \frac{1}{2} x^T (ac^T + ca^T) x.$$

Therefore, defining

$$Q := Q' + \frac{1}{2}(ac^T + ca^T),$$

we obtain

$$x^T Q' x + c^T x = x^T Q x.$$

Note that the matrix $Q \in \mathbb{R}^{n \times n}$ is again symmetric.

Thus, using the trivial constraints

$$0 \le x_j \le 1 \text{ for all } j = 1, \ldots, n-1,$$

we get the following equivalent problem.

$$(QMKP) \begin{cases} \min x^T Q x \\ \text{s.t. } A'x \le b \\ \qquad 0 \le x_j \le 1 \text{ for all } j = 1, \ldots, n-1 \\ \qquad a^T x = 1 \\ \qquad x_i \in \{0,1\}, \; i = 1, \cdots, n-1 \\ \qquad x_n \ge 0. \end{cases}$$

Step 4. Define matrix

$$A := (b)a^T - A'ea^T - I_{n-1}I_n \in \mathbb{R}^{(m+n-1+n)\times n}.$$

Then the above problem can be written as

$$(QMKP) \begin{cases} \min x^T Q x \\ \qquad a^T x = 1 \\ \qquad Ax \ge 0 \\ \qquad x_i \in \{0,1\}, \; i = 1, \cdots, n-1. \end{cases} \tag{9}$$

Note that for the last formulation of $(QMKP)$ in (9) the following key assumption is fulfilled:

$$\begin{aligned} &\text{For all } i = 1, \cdots, n-1, \text{ we have} \\ &a_i > 0, \text{ and } 0 \le x_i \le 1 \text{ for all } x \in \mathbb{R}^n \text{ satisfying } Ax \ge 0, a^T x = 1. \end{aligned} \tag{10}$$

Step 5. From the reformulation principle (Theorem 3.3 in [12]), the equivalent completely positive problem is

$$(CPMKP)\begin{cases}\min \langle Q, X\rangle \\ \qquad \langle aa^T, X\rangle = 1 \\ \qquad AXA^T \in \mathcal{CP}_{m+2n-1} \\ \qquad \langle B, X\rangle = 0,\end{cases}$$

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

Step 6. The coposivite program, which is the dual of $(CPMKP)$ is

$$(COPMKP)\begin{cases}\max \lambda \\ \qquad Q - \lambda aa^T + sB + A^TUA \in \mathcal{COP}_n \\ \qquad A^TUA \in \mathcal{COP}_n \\ \qquad \lambda, s \in \mathbb{R} \\ \qquad U \in \mathcal{COP}_{m+2n-1}.\end{cases}$$

The strict feasibility of Problem $(COPMKP)$ is shown as follows.

Choose $\hat{U} = ee^T$, so $\hat{U} \in \mathrm{int}\mathcal{COP}_{m+n}$. Furthermore, choosing $\hat{s} = 0$ and $\hat{\lambda} < 0$ small enough, we obtain the matrix $Q - \hat{\lambda}aa^T + A^T\hat{U}A$ with all positive entries, i.e.,

$$Q - \hat{\lambda}aa^T + A^T\hat{U}A \in \mathrm{int}\ \mathcal{COP}_n.$$

Model II

Consider again the quadratic multidimensional knapsack problem

$$(QMKP)\begin{cases}\min x^T\bar{Q}x + \bar{c}^Tx \\ \text{s.t. } \bar{a}_i^Tx \le \bar{b}_i \qquad \text{for all } i = 1, \ldots, m, \\ \qquad x \in \{0,1\}^{n-1},\end{cases}$$

Step 1. Add constraints $0 \le x_j \le 1$ for all $j = 1, \ldots, n-1$ to the problem, obtaining

$$(QMKP)\begin{cases}\min x^T\bar{Q}x + \bar{c}^Tx \\ \text{s.t. } \bar{a}_i^Tx \le \bar{b}_i\ \forall i = 1, \ldots, m, \\ \qquad x_j \le 1\ \forall j = 1, \cdots, n-1 \\ \qquad x \in \{0,1\}^{n-1} \\ \qquad x \ge 0.\end{cases}$$

Step 2. Add $m+n-1$ slack variables to transform the inequality constraints into equality constraints, obtaining

$$(QMKP)\begin{cases}\min x^T\bar{Q}x + \bar{c}^Tx \\ \text{s.t. } \bar{a}_i^Tx + s_i = \bar{b}_i \quad \forall i = 1, \ldots, m, \\ \qquad x_j + s_{m+j} = 1\ \forall j = 1, \ldots, n-1 \\ \qquad x_j \in \{0,1\} \qquad \forall j = 1, \cdots, n-1 \\ \qquad x, s \ge 0.\end{cases}$$

Step 3. For each $i = 1, \dots, m$, set

$$a_i := \frac{1}{\bar{b}_i} \begin{pmatrix} \bar{a}_i \\ e^i_{m+n-1} \end{pmatrix},$$

where $e^i_{m+n-1} \in \mathbb{R}^{m+n-1}$ is the i-th unit vector in $\mathbb{R}^{m+n-1}$.

For each $j = 1, \dots, n-1$, set

$$a_{m+j} := \begin{pmatrix} e^j_{n-1} \\ e^{m+j}_{m+n-1} \end{pmatrix},$$

where $e^j_{n-1} \in \mathbb{R}^{n-1}$ is the j-th unit vector of $\mathbb{R}^{n-1}$ and $e^i_{m+n-1} \in \mathbb{R}^{m+n-1}$ is the i-th unit vector in $\mathbb{R}^{m+n-1}$.

Define

$$Q := \begin{pmatrix} \bar{Q} & O \\ O & O \end{pmatrix} \in \mathbb{R}^{(m+2n-2)\times(m+2n-2)} \text{ and } c := \begin{pmatrix} \bar{c} \\ 0 \end{pmatrix} \in \mathbb{R}^{m+2n-2}.$$

Then we can rewrite (QMKP) as a problem in $\mathbb{R}^{m+2n-2}$ with the vector of variables $y = \begin{pmatrix} x \\ s \end{pmatrix} \in \mathbb{R}^{(n-1)+(m+n-1)}$, where s is the vector of slack variables:

$$(QMKP) \begin{cases} \min\ y^T Q y + c^T y \\ \text{s.t. } \ a_i^T y = 1 \quad \forall i = 1, \dots, m+n-1, \\ \qquad y_j \in \{0, 1\} \quad \forall j = 1, \dots, n-1 \\ \qquad y \geq 0. \end{cases}$$

Step 4. Adding a redundant equality constraint $a^T y = 1$ with

$$a := \frac{1}{m+n-1} \sum_{i=1}^{m+n-1} \bar{a}_i,$$

we obtain

$$(QMKP) \begin{cases} \min\ y^T Q y + c^T y \\ \text{s.t. } \ a_i^T y = 1 \quad \forall i = 1, \dots, m+n-1, \\ \qquad y_j \in \{0, 1\} \quad \forall j = 1, \dots, n-1 \\ \qquad a^T y = 1 \\ \qquad y \geq 0. \end{cases}$$

Note that by construction, we have $a > 0$.

Step 5. Define following matrices:

$$\Omega := Q + \frac{1}{2}(ca^T + ac^T) \in \mathbb{R}^{(m+2n-2)\times(m+2n-2)},$$

$$C := (a)^T - a_1 \vdots a^T - a_{m+n-1} \in \mathbb{R}^{(m+n-1)\times(m+2n-2)}$$

and

$$B := \sum_{i=1}^{n-1} e^i (a - e^i)^T + \sum_{i=1}^{n-1} (a - e^i)(e^i)^T \in \mathbb{R}^{(m+2n-2)\times(m+2n-2)},$$

where e^i is the i-th unit vector in $\mathbb{R}^{m+2n-2}$. Then Problem $(QMKP)$ is lifted into the following completely positive problem:

$$(CPMKP) \begin{cases} \min \ \langle \Omega, Y \rangle \\ \text{s.t.} \ \ \langle CC^T, Y \rangle = 0 \\ \qquad \langle B, Y \rangle = 0 \\ \qquad \langle aa^T, Y \rangle = 1 \\ \qquad Y \in \mathcal{CP}_{m+2n-2} \end{cases}$$

It is worth noting that, independently from the numbers of constraints and variables in Problem $(QMKP)$, Problem $(CPMKP)$ has only two linear equality constraints and one completely positive constraint.

Step 6. The dual problem of $(CPMKP)$ is the following copositive program:

$$(COPMKP) \begin{cases} \max \ \lambda \\ \text{s.t.} \ \ \Omega - \lambda aa^T + sCC^T + tB \in \mathcal{COP}_{m+2n-2} \\ \qquad \lambda, s, t \in \mathbb{R} \end{cases}$$

A strictly feasible point of Problem $(COPMKP)$ is easily determined as follows.

As the vector a defined in Step 4 satisfies $a > 0$, one can choose $\hat{s} = 0$ and $\hat{\lambda} < 0$ small enough, such that the matrix $(\Omega - \hat{\lambda} aa^T)$ has all (strictly) positive entries, i.e. this matrix is an interior point of the copositive cone.

Remark 1. Using the formulation of Burer in [6] for the last problem $(QMKP)$ constructed in Step 4, we obtain the following completely positive problem:

$$(CPMKP)_B \begin{cases} \min \ \langle Q, Y \rangle + c^T Y a \\ \text{s.t.} \ \ a_i^T Y a_i = 1 & \forall i = 1, \ldots, m+n-1, \\ \qquad a_i^T Y a = 1 & \forall i = 1, \ldots, m+n-1 \\ \qquad a^T Y a = 1 \\ \qquad [Ya]_i = Y_{ii} & \forall i = 1, \ldots, n-1 \\ \qquad Y \in \mathcal{CP}_{m+2n-2}. \end{cases}$$

Note that this problem has $2(m+n-1)+n$ linear equality constraints and one completely positive constraint. Thus, its dual problem has more variables than Problem $(COPMKP)$ has. Moreover, it is also not clear, whether or not its dual problem is strictly feasible.

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