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Research Article

A two-phase method for solving continuous rank-one quadratic knapsack problems

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Abstract

We propose a two-phase algorithm for solving continuous rank-one quadratic knapsack problems (R1QKPs). In particular, we study the solution structure of the problem without the knapsack constraint. In fact an $O(n \log n)$ algorithm is suggested in this case. We then use the solution structure to propose an $O(n^2 \log n)$ algorithm that finds an interval containing the optimal value of the Lagrangian dual of R1QKP. In the second phase, we solve the Lagrangian dual problem using a traditional single-variable optimization method. We perform a computational test on random instances and compare our algorithm with the general solver CPLEX.

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Keywords: Quadratic Knapsack Problem; Line-Sweep Algorithm

1 Introduction

The quadratic knapsack problem (QKP) deals with minimizing a quadratic function over one allocation constraint together with simple bounds on decision variables. Formally, this problem can be written as

$$\text{minimize} \quad \frac{1}{2}\bar{x}^\top Q y - \bar{c}^\top \bar{x}, \tag{1a}$$

$$\text{subject to} \quad \bar{a}^\top \bar{x} = b, \tag{1b}$$

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$$0 \leq \bar{x} \leq \bar{u}, \tag{1c}$$

where Q is a symmetric $n \times n$ matrix, $\bar{a}, \bar{c}, \bar{u} \in \mathbb{R}^n$, and $b \in \mathbb{R}$. The QKP as a quadratic optimization problem is polynomially solvable when Q is positive definite matrix [12].

When Q is diagonal with strictly positive diagonal entries, then QKP can be viewed as a strictly convex separable optimization problem that has many applications (e.g., resource allocation [1, 13, 14] and multicommodity network flows [9]). The solution methods for solving this type of QKPs usually rely on the fact that the optimal solution to the Lagrangian dual subproblems can be explicitly obtained in terms of the Lagrange multiplier λ of (1b). Therefore, the problem reduces to find a value for λ such that the solution to the corresponding Lagrangian subproblem is satisfied equality constraint (1b).

Helgason, Kennington, and Lall [9] proposed an $O(n \log n)$ algorithm for solving the equation based on searching breakpoints of the Lagrangian dual problem. Brucker [2] found an $O(n)$ bisection algorithm based on the properties of the Lagrangian dual function. Dai and Fletcher [4] proposed a two-phase method. A bracketing phase determines an interval containing the solution followed by the secant phase that approximates the solution within the promising interval. This method is modified by Comminetti, Mascarenhas, and Silva [3] by ignoring the bracketing phase and using a semi-smooth Newton method instead of the secant method. Liu and Liu [11] considered a special case of the strictly convex form of the problem. They found the solution structure of the subproblems and used it in a modified secant algorithm.

Robinson, Jiang, and Lerme [15] used the geometric interpretation of the problem and proposed an algorithm that works in the primal space rather than the dual space. This algorithm iteratively fixes variables and terminates after at most n iterations.

In a more general case, when Q is positive semidefinite in (1), Dussault, Ferland, and Lemaire [7] proposed an iterative algorithm in which a QKP with diagonal Q should be solved in each iteration. Paradalos, Ye, and Han [12] suggested a potential reduction algorithm to solve this class of QKP. di Serafino et al. [6] proposed a two-phase gradient projection with acceptable numerical performance compared to similar gradient-based methods.

QKPs with positive definite Q are also solved by a gradient projection method [4] and an augmented-Lagrangian approach [8].

In this paper, we suppose that Q is a rank-one symmetric matrix, that is, $Q = qq^\top$ for some $q \in \mathbb{R}^n$. Moreover, we assume that $0 < \bar{u}$. Without loss of generality, we assume that $q_i \neq 0$ for each i. By the changing variables

$$x_i \leftarrow q_i \bar{x}_i, \quad c_i \leftarrow \frac{\bar{c}_i}{q_i}, \quad a_i \leftarrow \frac{\bar{a}_i}{q_i}, \quad u_i \leftarrow \max\{0, q_i \bar{u}_i\},$$

problem (1) is reduced to

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}(\mathbf{1}^\top x)^2 - c^\top x, && \text{(2a)} \\ \text{subject to} \quad & a^\top x = b, && \text{(2b)} \\ & 0 \le x \le u. && \text{(2c)} \end{aligned}$$

Sharkey and Romeijn [16] studied a class of nonseparable nonlinear knapsack problems in which one has to

$$\begin{aligned} \text{minimize} \quad & g(s^\top x) - c^\top x, \\ \text{subject to} \quad & a^\top x = b, \\ & l \le x \le u, \end{aligned} \tag{3}$$

where $g : \mathbb{R} \to \mathbb{R}$ is an arbitrary real-valued function, and $s \in \mathbb{R}^n$ is given. They introduced an algorithm for solving (3) that runs in $O(n^2 \max\{\log n, \phi\})$, where ϕ is the time required to solve a single-variable optimization problem $\min\{g(S) - \alpha S \ : \ L \le S \le U\}$ for given $\alpha, L, U \in \mathbb{R}$. With $g(t) = t^2$ and s equal to the all-one vector, problem (2) is a special case of problem (3). That is, there exists an $O(n^2 \max\{\log n, 1\}) = O(n^2 \log n)$ algorithm for solving problem (2).

In this paper, we consider a two-phase algorithm for solving problem (2). In Section 2, we study the solution structure of the relaxed version of the problem in which the equality constraint (2b) is excluded. We show that the relaxed version could be solved in $O(n \log n)$ time. In Section 3, in phase I, we use the solution structure of the relaxed version to find an interval that may contain the optimal value of the Lagrangian dual function. This is done in $O(n^2 \log n)$ time in the worst case. Then, we perform phase II, in which we explore the interval by a single-variable optimization method to find the optimal Lagrangian multiplier with the desired precision. In Section 4, we perform a computational test. In particular, we compare the algorithm with the general quadratic programming solver CPLEX.

2 Solution structure of the relaxed version

In this section, we consider the following relaxed version of the problem (2):

$$\begin{aligned} \text{minimize} \quad & f(x) = \frac{1}{2}(\mathbf{1}^\top x)^2 - c^\top x, && \text{(4a)} \\ \text{subject to} \quad & 0 \le x \le u. && \text{(4b)} \end{aligned}$$

We propose a characterization of the solution in the primal space. Note that most of algorithms for such problems use the so-called KKT conditions to study the solution structure.

Without loss of generality, we assume that $c_1 \ge c_2 \ge \cdots \ge c_n \ge 0$, and that $l_i = 0$, $i = 1, \ldots, n$. Given two vectors $a, b \in \mathbb{R}^n$, we denote the

set $\{x \ : \ a \leq x \leq b\}$ by $[a, b]$. Finally, given a vector $u \in \mathbb{R}^n$, we define $U_k := \sum_{i=1}^{k} u_i$ for $k = 1, \ldots, n$, and $U_0 := 0$.

Now consider the following preliminary lemmas:

Lemma 1. For $k = 1, \ldots, n$ define $x^{(k)}$ as

$$x_i^{(k)} = \begin{cases} u_i, & i = 1, \ldots, k, \\ 0, & i = k+1, \ldots, n, \end{cases}$$

and $x^{(0)}$ as the all-zero vector, and define G_k as

$$G_k = \frac{1}{2}\left(U_k + U_{k-1}\right) - c_k = U_{k-1} + \frac{1}{2}u_k - c_k.$$

Then the following assertions hold:

(i) If $\bar{n}$ is the smallest index in $\{1, \ldots, n\}$ such that $G_{\bar{n}} \geq 0$, then $\min_{i=1,\ldots,n} f(x^{(i)}) = f(x^{(\bar{n}-1)})$.

(ii) If $G_k < 0$ for all $k = 1, \ldots, n-1$, then $\min_{i=1,\ldots,n} f(x^{(i)}) = f(x^{(n)})$.

Proof. (i) For $1 \leq k \leq n-1$, we have

$$\begin{aligned} G_k - G_{k+1} &= \frac{1}{2}\left(U_k + U_{k-1}\right) - c_k - \frac{1}{2}\left(U_{k+1} + U_k\right) + c_{k+1} \\ &= -\frac{1}{2}\left(u_k + u_{k+1}\right) + \left(c_{k+1} - c_k\right) \\ &< 0. \end{aligned}$$

Thus

$$G_1 < G_2 < \cdots < G_{\bar{n}-1} < 0 \leq G_{\bar{n}} < G_{\bar{n}+1} < \cdots < G_n.$$

On the other hand, for $1 \leq k \leq n-1$, we have

$$\begin{aligned} f(x^{(k+1)}) - f(x^{(k)}) &= \frac{1}{2}U_{k+1}^2 - \sum_{i=1}^{k+1} u_i c_i - \frac{1}{2}U_k^2 + \sum_{i=1}^{k} u_i c_i \\ &= \frac{1}{2}U_{k+1}^2 - u_{k+1}c_{k+1} - \frac{1}{2}U_k^2 \\ &= \frac{1}{2}(U_{k+1}^2 - U_k^2) - u_{k+1}c_{k+1} \\ &= \frac{1}{2}(U_{k+1} - U_k)(U_{k+1} + U_k) - u_{k+1}c_{k+1} \\ &= u_{k+1}\left(\frac{1}{2}(U_{k+1} + U_k) - c_{k+1}\right) \\ &= u_{k+1}G_{k+1}. \end{aligned} \tag{5}$$

Now let $m > \bar{n} - 1$. Then

$$\begin{aligned} f(x^{(m)}) - f(x^{(\bar{n}-1)}) &= f(x^{(m)}) - f(x^{(m-1)}) + f(x^{(m-1)}) + \cdots + f(x^{(\bar{n})}) - f(x^{(\bar{n}-1)}) \\ &= u_m G_m + \cdots + u_{\bar{n}} G_{\bar{n}} > G_{\bar{n}}(u_m + \cdots + u_{\bar{n}+1}) \\ &\geq 0. \end{aligned}$$

Similarly, if $m < \bar{n} - 1$, then $f(x^{(m)}) - f(x^{(\bar{n}-1)}) \geq 0$.

(ii) The second part can be easily proved by considering (5). □

We need the following result for two-dimensional version of problem (4).

Lemma 2. Consider the following optimization problem:

$$\begin{aligned} \text{minimize} \quad & f(x_1, x_2) = \frac{1}{2}(x_1 + x_2)^2 - c_1 x_1 - c_2 x_2, \\ \text{subject to} \quad & 0 \leq x_1 \leq u_1, \\ & 0 \leq x_2 \leq u_2, \end{aligned} \tag{6}$$

where $c_1 \geq c_2 \geq 0$ and u_1 and u_2 are real positive constants. Define set $I := I_1 \cup I_2$, where $I_1 = \{(u_1, x_2) \ : \ 0 \leq x_2 \leq u_2\}$, and $I_2 = \{(x_1, 0) \ : \ 0 \leq x_1 \leq u_1\}$. Then, problem (6) has no optimal solution outside of I.

Proof. If $c_1 = c_2$, then $f(x_1, x_2) = \frac{1}{2}(x_1 + x_2)^2 - c_1(x_1 + x_2) = \frac{1}{2}z^2 - c_1 z = g(z)$, where $z = x_1 + x_2$. It is easy to see that $x^* = (x_1^*, x_2^*)$ with $x_1^* = \min\{c_1, u_1\}$ and $x_2^* = \min\{c_1 - x_1^*, u_2\}$, is the optimal solution to the problem, and we have $x^* \in I$. Assume that $c_1 \neq c_2$. The feasible region of (6) is equal to $I_1 \cup I_2 \cup I_3 \cup I_4$, where $I_3 = \{(x_1, x_2) \ : \ 0 < x_1 < u_1, 0 < x_2 < u_2\}$ and $I_4 = \{(0, x_2) \ : \ 0 < x_2 < u_2\} \cup \{(x_1, u_2) \ : \ 0 < x_1 < u_1\}$. We show that there is no optimal solution in I_3 and I_4. Indeed, we write the KKT optimality conditions as follows:

$$x_1 + x_2 - c_1 + \alpha_1 - \alpha_2 = 0, \tag{7}$$

$$x_1 + x_2 - c_2 + \beta_1 - \beta_2 = 0, \tag{8}$$

$$\alpha_1(x_1 - u_1) = 0, \quad \alpha_2 x_1 = 0, \tag{9}$$

$$\beta_1(x_2 - u_2) = 0, \quad \beta_2 x_2 = 0, \tag{10}$$

$$0 \leq x_1 \leq u_1, \tag{11}$$

$$0 \leq x_2 \leq u_2, \tag{12}$$

$$\alpha_1, \alpha_2, \beta_1, \beta_2 \geq 0, \tag{13}$$

where α_i and β_i, $i = 1, 2$ are KKT multipliers corresponding to the bound constraints. If $(x_1, x_2) \in I_3$, then from (9) and (10), we have $\alpha_1 = \alpha_2 = \beta_1 = \beta_2 = 0$. Substituting these values in (7) and (8) implies that $c_1 = c_2$, which contradicts our assumption. On the other hand, if $(x_1, x_2) \in I_4$ and $x_1 = 0$, then $\alpha_1 = 0$. Now, (7) implies that $x_2 = c_1 + \alpha_2 > 0$. Thus $\beta_2 = 0$. From (8), we have $x_2 = c_2 - \beta_1$. Therefore, $c_2 = c_1 + \alpha_2 + \beta_1 \geq c_1$. This contradicts our assumption on c_i's. That is, problem (6) has no optimal solution with

$x_1 = 0$. Now, if $x_2 = u_2$, then $\alpha_1 = 0$ and β_2. It implies from (7) and (8) that $0 \leq \alpha_2 + \beta_1 = c_2 - c_1 \leq 0$. That is, $c_2 = c_1$, a contradiction. □

Theorem 1. Suppose that $x^{(k)}$ and G_k, $k = 1, \ldots, n$, and $\bar{n}$ are defined as in Lemma 1. Then the following assertions hold:

(i) For $\bar{n} > 1$, define δ_1 and δ_2 as $\delta_1 := \min\{c_{\bar{n}-1} - U_{\bar{n}-2}, u_{\bar{n}-1}\}$ and $\delta_2 := \max\{c_{\bar{n}} - U_{\bar{n}-1}, 0\}$. Also, define $\bar{x}$ and $\tilde{x}$ as

$$\bar{x} = x^{(\bar{n}-2)} + \delta_1 e_{\bar{n}-1}, \quad \tilde{x} = x^{(\bar{n}-1)} + \delta_2 e_{\bar{n}},$$

where e_i is the ith column of the identity matrix of dimension n. Then $\min\{f(\bar{x}), f(\tilde{x})\}$ is the optimal value of the following optimization problem:

$$\begin{aligned} \text{minimize} \quad & f(x), \\ \text{subject to} \quad & x^{(\bar{n}-2)} \leq x \leq x^{(\bar{n})}. \end{aligned} \tag{14}$$

(ii) For $\bar{n} = 1$, define $\delta := \min\{c_1, u_1\}$ and $\tilde{x} := \delta e_1$. Then $f(\tilde{x})$ is the optimal value of the following optimization problem:

$$\begin{aligned} \text{minimize} \quad & f(x), \\ \text{subject to} \quad & x^{(0)} \leq x \leq x^{(1)}. \end{aligned}$$

(iii) For $G_k < 0$ for all $k = 1, \ldots, n$, define $\delta := \min\{c_n - U_{n-1}, u_n\}$ and $\tilde{x} := x^{(n-1)} + \delta e_n$. Then $f(\tilde{x})$ is the optimal value of the following optimization problem:

$$\begin{aligned} \text{minimize} \quad & f(x), \\ \text{subject to} \quad & x^{(n-1)} \leq x \leq x^{(n)}. \end{aligned}$$

Proof. (i) By Lemma 2, we can partition the optimal solution set as $I_1 \cup I_2$, where $I_1 = [x^{(\bar{n}-2)}, x^{(\bar{n}-1)}]$ and $I_2 = [x^{(\bar{n}-1)}, x^{(\bar{n})}]$. We show that $f(\bar{x}) = \min\{f(x) : x \in I_1\}$ and $f(\tilde{x}) = \min\{f(x) : x \in I_2\}$. Indeed, we use a simple technique of single-variable calculus. Let $x \in I_1$. Then $x = x(\delta)$, for some $\delta \in [0, u_{\bar{n}-1}]$, where $x(\delta) = x^{(\bar{n}-2)} + \delta e_{\bar{n}-1}$. Thus the problem $\min\{f(x) : x \in I_1\}$ reduces to $\min\{f(x(\delta)) : 0 \leq \delta \leq u_{\bar{n}-1}\}$. On the other hand, one can write

$$f(x(\delta)) = \frac{1}{2}\left(U_{\bar{n}-2} + \delta\right)^2 - \sum_{i=1}^{\bar{n}-2} c_i u_i - c_{\bar{n}-1}\delta.$$

We have $df(x(\delta))/d\delta = U_{\bar{n}-2} + \delta - c_{\bar{n}-1}$. Thus $df(x(\delta))/d\delta = 0$ only if $\delta = \delta' = c_{\bar{n}-1} - U_{\bar{n}-2}$. Since $d^2 f(x(\delta))/d\delta^2 > 0$ and $\delta' > \frac{1}{2}u_{\bar{n}-1}$ the optimal value is achieved at δ_1.

To prove $f(\tilde{x}) = \min\{f(x) : x \in I_2\}$, by the same argument as the previous paragraph, it suffices to solve single optimization problem

$\min\{f(x(\delta)) : 0 \le \delta \le u_{\bar{n}}\}$, where $x(\delta) = x^{(\bar{n}-1)} + \delta e_{\bar{n}}$. It is easy to see that if $\delta = \delta' = c_{\bar{n}} - U_{\bar{n}-1}$, then $df(x(\delta))/d\delta = 0$. Since $\delta' \le \frac{1}{2}u_{\bar{n}}$, by the definition of $\bar{n}$, then $f(\tilde{x})$ is the optimal value of $\min\{f(x) : x \in I_2\}$.

The proof of parts (ii) and (iii) is similar. □

The following Corollary 1 presents simple conditions under which the optimal solution to the problem in Theorem 1(i) is $\bar{x}$ or $\tilde{x}$.

Corollary 1. In Theorem 1(i),

(i) if $\delta_1 = u_{\bar{n}-1}$, then $\min\{f(\bar{x}), f(\tilde{x})\} = f(\tilde{x})$, and

(ii) if $\delta_2 = 0$, then $\min\{f(\bar{x}), f(\tilde{x})\} = f(\bar{x})$.

Proof. For brevity, we just prove part (i). The proof of the second part is similar. Under the assumption of part (i), we have

$$f(\bar{x})-f(\tilde{x}) = \frac{1}{2}U_{\bar{n}-1}^2-\sum_{i=1}^{\bar{n}-1} c_i u_i-\frac{1}{2}c_{\bar{n}}^2+\sum_{i=1}^{\bar{n}-1} c_i u_i+c_{\bar{n}}(c_{\bar{n}}-U_{\bar{n}-1}) = \frac{1}{2}\left(U_{\bar{n}-1} - c_{\bar{n}}\right)^2 \ge 0.$$

□

Theorem 1 solves a relaxed version of problem (2). In Theorem 2, we show that the solution to the relaxed version is the solution to the original problem.

Theorem 2. Define G_k's, $x^{(k)}$'s, $\bar{n}$, $\bar{x}$, and $\tilde{x}$ as in Theorem 1. Then, the following assertions hold:

(i) If $1 < \bar{n} \le n$, then $\min\{f(\bar{x}), f(\tilde{x})\}$ is the optimal value of (4), where $\tilde{x}$ and $\bar{x}$ are defined as in Theorem 1(i).

(ii) If $\bar{n} = 1$, then $f(\tilde{x})$ is the optimal value of (4), where $\tilde{x}$ is defined as in Theorem 1(ii).

(iii) If $G_k < 0$ for all $k = 1, \ldots, n$, then $f(\tilde{x})$ is the optimal solution to (4), where $\tilde{x} = x^{(n-1)} + \delta' e_n$ and $\delta' = \min\{c_n - U_{n-1}, u_n\}$.

Proof. For two vectors $x, z \in \mathbb{R}^n$, we have

$$f(z) - f(x) = \frac{1}{2}(\mathbf{1}^\top z + \mathbf{1}^\top x)(\mathbf{1}^\top z - \mathbf{1}^\top x) - c^\top(z - x). \tag{15}$$

Let x be a feasible solution to (4). If $x = u = x^{(n)}$, then from the definition of $\bar{n}$, we have $f(x^{\bar{n}-1}) \le f(x)$, and the result follows from Theorem 1. Suppose $x \ne u$. We show there exists a specially structured feasible solution x' that is better than x. Indeed, let k be such that

$$U_k \le \mathbf{1}^\top x < U_{k+1}.$$

Define vector x' by

$$x'_i = \begin{cases} u_i, & i = 1, \dots, k, \\ \mathbf{1}^\top x - U_k, & i = k+1, \\ 0, & i = k+2, \dots, n. \end{cases}$$

Then, clearly x' is feasible for (4) and

$$\mathbf{1}^\top x' = \sum_{i=1}^{k} x'_i + x'_{k+1} + \sum_{i=k+2}^{n} x'_i = \sum_{i=1}^{k} u_i + \sum_{i=1}^{n} x_i - \sum_{i=1}^{k} u_i = \mathbf{1}^\top x.$$

Moreover, we obtain

$$\begin{aligned} c^\top x' &= \sum_{i=1}^{k} u_i c_i + c_{k+1} x'_{k+1} = \sum_{i=1}^{k} u_i c_i + c_{k+1} \sum_{i=1}^{n} x_i - c_{k+1} \sum_{i=1}^{k} u_i \\ &= \sum_{i=1}^{k} u_i c_i + c_{k+1} \sum_{i=1}^{k} x_i + c_{k+1} \sum_{i=k+1}^{n} x_i - c_{k+1} \sum_{i=1}^{k} u_i \\ &\geq \sum_{i=1}^{k} u_i c_i + \sum_{i=1}^{k} (x_i - u_i) c_i + \sum_{i=k+1}^{n} x_i c_i \quad \text{(by the monotonicity of } c_i\text{'s)} \\ &= c^\top x. \end{aligned}$$

Therefore, (15) implies that $f(x') - f(x) = -c^\top (x' - x) \leq 0$, that is, $f(x') \leq f(x)$.

(i) Now, we consider three cases for the index k introduced in the definition of x': $k \geq \bar{n}$, $k < \bar{n} - 2$, and $k = \bar{n} - 1, \bar{n} - 2$. In the latter case, we have $x^{(\bar{n}-2)} \leq x' \leq x^{(\bar{n})}$, so the assertion is true by Theorem 1, since

$$\min\{f(\bar{x}), f(\tilde{x})\} = \min\{f(x) \ : \ x \in [x^{(\bar{n}-2)}, x^{(\bar{n})}]\} \leq f(x') \leq f(x).$$

We show in both the other cases, there is a point in the set $\{x^{(i)}\}_{i=1,\dots,n}$ better than x', that is, $f(x^{(i)}) \leq f(x')$ for some $i = 1, \dots, n$. By Lemma 1, $f(x^{(\bar{n}-1)}) \leq f(x^{(i)})$ and the result follows by Theorem 1.

First, let $k \geq \bar{n}$. Then

$$\begin{aligned} f(x^{(k)}) - f(x') &= \frac{1}{2}(\mathbf{1}^\top x^{(k)} - \mathbf{1}^\top x')(\mathbf{1}^\top x^{(k)} + \mathbf{1}^\top x') - c^\top (x^{(k)} - x') \\ &= -\frac{1}{2} x'_{k+1}(2U_k + x'_{k+1}) + c_{k+1} x'_{k+1} \\ &= -x'_{k+1} \left(\frac{1}{2}(2U_k + x'_{k+1}) - c_{k+1} \right). \end{aligned}$$

On the other hand, we have

$$2U_k + x'_{k+1} = 2\sum_{i=1}^{\bar{n}-1} u_i + \sum_{i=\bar{n}}^{k} u_i + x'_{k+1} \geq U_{\bar{n}} + U_{\bar{n}-1}.$$

Therefore,

$$\frac{1}{2}(2U_k + x'_{k+1}) - c_{k+1} \geq \frac{1}{2}(U_{\bar{n}} + U_{\bar{n}-1}) - c_{\bar{n}} = G_{\bar{n}} \geq 0.$$

Thus $f(x^{(k)}) \leq f(x')$.

Now, let $k < \bar{n} - 2$. Then

$$\begin{aligned} f(x^{(k+1)}) - f(x') &= \frac{1}{2}(\mathbf{1}^\top x^{(k+1)} - \mathbf{1}^\top x')(\mathbf{1}^\top x^{(k+1)} + \mathbf{1}^\top x') - c^\top (x^{(k+1)} - x') \\ &= \frac{1}{2}(u_{k+1} - x'_{k+1})(U_{k+1} + U_k + x'_{k+1}) - c_{k+1}(u_{k+1} - x'_{k+1}) \\ &= (u_{k+1} - x'_{k+1}) \left(\frac{1}{2}(2U_k + x'_{k+1} + u_{k+1}) - c_{k+1} \right). \end{aligned}$$

On the other hand, we have

$$2U_k + x'_{k+1} + u_{k+1} \leq 2U_k + 2u_{k+1} \leq 2U_k + 2\sum_{i=k+1}^{\bar{n}-2} u_i + u_{\bar{n}-1} = U_{\bar{n}-2} + U_{\bar{n}-1}.$$

Hence,

$$\frac{1}{2}(2U_k + x'_{k+1} + u_{k+1}) - c_{k+1} \leq \frac{1}{2}(U_{\bar{n}-2} + U_{\bar{n}-1}) - c_{\bar{n}-1} = G_{\bar{n}-1} < 0.$$

That is, $f(x^{(k+1)}) < f(x')$. Thus in both cases, there exist a point, say $x^{(t)}$, such that $f(x^{(t)}) \leq f(x') \leq f(x)$. Now, by Lemma 1, $f(x^{(\bar{n}-1)}) \leq f(x^{(t)}) \leq f(x)$ and the result follows by Theorem 1.

Proof of (ii). Consider the possible values of k at the beginning of the proof of part (i). Here, we just have $k \geq \bar{n} = 1$. Now, similar argument for this case proves (ii).

Proof of (iii). Again consider the possible values of k at the beginning of the proof of part (i). Similar argument with case $k < \bar{n} - 2$ for $\bar{n} = n + 1$ proves part (iii).

□

We conclude the following result on the time needed to solve problem (4).

Theorem 3. There exists an $O(n \log n)$ time algorithm for problem (4).

Proof. When the index $\bar{n}$ is determined, the solution can be determined in $O(n)$ time. We need $O(n \log n)$ to sort the vector c, $O(n)$ to compute vector G, and $O(\log n)$ to find the index $\bar{n}$. That is, problem (4) can be solved in $O(n \log n)$. □

3 The algorithm

In this section, we propose our algorithm for solving problem (2). The algorithm consists of two phases: bounding the optimal Lagrangian multiplier and computing the optimal solution to the desired precision. The bounding phase is based on the Lagrangian dual of (2) and the solution structure of the relaxed version has been described in section 2.

3.1 Lagrangian dual

Let λ be the Lagrange multiplier of equality constraint in (2). Then, the Lagrangian function is given by

$$\begin{aligned}\phi(\lambda) &:= \min\left\{\frac{1}{2}(\mathbf{1}^\top x)^2 - c^\top x + \lambda(b - a^\top x) \ : \ 0 \le x \le u\right\} \\ &= \lambda b + \min\left\{\frac{1}{2}(\mathbf{1}^\top x)^2 - (c + \lambda a)^\top x \ : \ 0 \le x \le u\right\}.\end{aligned} \tag{16}$$

We have the following statement about the structure of the Lagrangian function ϕ.

Theorem 4. For a given Lagrange multiplier λ, define $\bar{n}$ as in Theorem 2. If $\bar{n} > 1$, then

$$\phi(\lambda) = \lambda b + f_\lambda(x^{(\bar{n}-1)}), \text{if } c_{\bar{n}}(\lambda) \le U_{\bar{n}-1} \le c_{\bar{n}-1}(\lambda), \qquad \text{(Type A)}$$
$$\phi(\lambda) = \lambda b + p_{\bar{n}}(\lambda), \text{if } U_{\bar{n}-1} < c_{\bar{n}}(\lambda), \qquad \text{(Type B)}$$
$$\phi(\lambda) = \lambda b + p_{\bar{n}-1}(\lambda), \text{if } U_{\bar{n}-1} > c_{\bar{n}-1}(\lambda), \qquad \text{(Type C)}$$

where f_λ is the objective function of the optimization part of (16), and

$$p_k(\lambda) = -\frac{1}{2}a_k^2\lambda^2 - a^\top d_k\lambda + \frac{1}{2}c_k^2 - c^\top d_k,$$
$$d_k = x^{(k-1)} + (c_k - U_{k-1})e_k.$$

Proof. The proof is based on the four possible cases for δ_1 and δ_2 in Theorem 2. We just prove (Type A) and, for the sake of brevity, we omit the remaining parts.

Suppose that $c_{\bar{n}}(\lambda) \le U_{\bar{n}-1} \le c_{\bar{n}-1}(\lambda)$. Then we have $c_{\bar{n}-1}(\lambda) - U_{\bar{n}-2} \ge u_{\bar{n}-1}$ and $c_{\bar{n}}(\lambda) - U_{\bar{n}-1} \le 0$. Therefore, the values of δ_1 and δ_2 in Theorem 2 can be determined as

$$\delta_1 = \min\{c_{\bar{n}-1}(\lambda) - U_{\bar{n}-2}, u_{\bar{n}-1}\} = u_{\bar{n}-1},$$
$$\delta_2 = \max\{c_{\bar{n}}(\lambda) - U_{\bar{n}-1}, 0\} = c_{\bar{n}}(\lambda) - U_{\bar{n}-1}.$$

Thus we have $\bar{x} = x^{(\bar{n}-2)} + \delta_1 e_{\bar{n}-1} = x^{(\bar{n}-1)}$. By some simplifications, we have $f_\lambda(\tilde{x}) - f_\lambda(\bar{x}) = \frac{1}{2}(c_{\bar{n}}(\lambda) - U_{\bar{n}-1})^2 \geq 0$. Now, Theorem 2 implies that $\min\{f_\lambda(x) \ : \ 0 \leq x \leq u\} = \min\{f(\tilde{x}), f(\bar{x})\} = f_\lambda(\bar{x}) = f_\lambda(x^{(\bar{n}-1)})$. □

Now, one may conclude that if $\bar{n}$ is fixed on an interval $[\lambda_a, \lambda_b]$, then $\phi(\lambda)$ is a piecewise function that contains exactly three pieces. However, the following simple example shows that this is not true.

Example 1. Consider problem (2) with the following parameters:

$$a^\top = \begin{bmatrix} -7 & -5 & 7 & -5 & 7 \end{bmatrix}, \quad c^\top = \begin{bmatrix} 54 & 44 & 15 & -8 & -70 \end{bmatrix},$$
$$u^\top = \begin{bmatrix} 62 & 48 & 36 & 84 & 59 \end{bmatrix}.$$

In Figure 1, we plot $\phi(\lambda)$ for $\lambda \in [-8.36, 7.00]$. We distinct three cases in (Type A), (Type B), and (Type C) in blue, red, and green, respectively. As it can be seen in Figure 1, $\phi(\lambda)$ consists of four pieces.

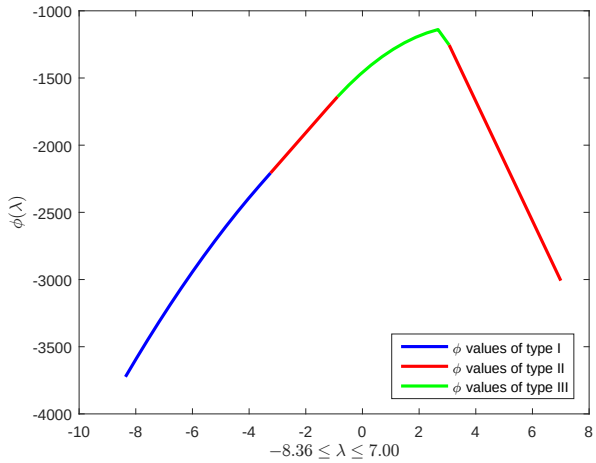

Figure 1: Plot of the Lagrangian function $\phi(\lambda)$ for Example 1.

The inner optimization problem in (16) is a special case of problem (4) that can be solved by Theorem 2. In Theorem 2, it is assumed that coefficients of the linear term in the objective function are sorted in decreasing order. In problem (16), the order of coefficients of the linear term depends on λ. From now on, we denote by $c_i(\lambda)$ the coefficient of x_i, that is, $c_i(\lambda) = c_i + \lambda a_i$. Moreover, we denote the line $\{c_i(\lambda) \ : \ \lambda \in \mathbb{R}\}$ by ℓ_i. It is easy to see that when λ becomes greater than the intersection of ℓ_i and ℓ_j, $c_i(\lambda)$ and $c_j(\lambda)$ change position in the ordered list of coefficients.

We use a modification of the well-known plane sweep algorithm to find the ordered intersection points of lines $\{\ell_i \ : \ i = 1, \ldots, n\}$. Now, let λ_a, λ', and

λ_b be three consecutive intersection points. Then, because the Lagrangian function is unimodal, the optimal Lagrange multiplier λ^* lies in the interval $[\lambda_a, \lambda_b]$ if $\phi(\lambda') > \phi(\lambda_a)$ and $\phi(\lambda') > \phi(\lambda_b)$.

We modify the implementation of the line-sweep algorithm proposed in [5]. In this algorithm, a vertical line ℓ sweeps the plane from left to right. The *status* of the sweep line is the ordered sequence of lines that intersect it. The status initially contains all lines in the order of decreasing slope, that is, the order of lines when they intersect with the sweep line at $\lambda = -\infty$. The status is updated when ℓ reaches an intersecting point. For example, suppose that the sequence of four lines ℓ_l, ℓ_i, ℓ_j, and ℓ_m appears in the status when ℓ reaches the intersection point of ℓ_i and ℓ_j. Then, ℓ_i and ℓ_j switch the position and intersection of lines ℓ_i and ℓ_m, and the intersection of ℓ_j and ℓ_l are to be checked. The new detected intersection points are stored to proceed. The order of cost coefficient of the linear term in $\phi(\lambda)$ is unchanged between two consecutive intersection points.

If $c_i(\lambda) < 0$ for some i, then $x_i = 0$ in the optimal solution to the $\phi(\lambda)$ subproblem. We introduce a set Z to store the non-vanished variables. To do so, we add a dummy line $\ell_0 : c_0(\lambda) = 0$. In each intersection of the dummy line and the other lines, the set Z should be updated. In fact, if ℓ_i intersect ℓ_0 and $i \notin Z$, then we add i to Z; otherwise, if $i \in Z$, then it should be removed from Z. In other words, since we sweep the plane from left to right, if ℓ_i intersect ℓ_0 and $a_i < 0$, then we add i to Z. If ℓ_i intersect ℓ_0 and $a_i > 0$, then it means that i should be removed from Z. Moreover, Z initially contains the set of all lines with a positive slope. With this modification, we guarantee that between two consecutive intersection points, the set of zero-valued variables is unchanged. It should be noted here that lines with equal slopes are sorted based on increasing order of c_i's. We summarize the approach in Algorithm 1. This algorithm is used as the first phase in the main algorithm.

Theorem 5. Algorithm 1 runs in $O(n^2 \log n)$ time.

Proof. Initializing state array ℓ, line indices array p and the queue Q in steps 3–7 needs $O(n \log n)$ time. In each iteration, we perform two main operations: computing the value of ϕ for a new intersect point λ^{new} and updating Q. The order of $c_i(\lambda^{\text{new}})$ and the vector G can be updated from the previous intersection point in $O(1)$ time. Finding $\bar{n}$ needs $O(\log n)$, using binary search. On the other hand, insertion and deletion on the priority queue Q takes $O(\log n)$ since one can implement the priority queue by a heap to store the intersection points. Therefore, each iteration of the main loop needs $O(\log n)$ time. Since there are $O(n^2)$ intersection points, the algorithm runs in $O(n^2 \log n)$. □

Let λ_{LB} and λ_{UB} be the smallest and greatest intersection points of lines $\{\ell_i \ : \ i = 1, \ldots, n\}$, respectively. The optimal solution to the Lagrangian problem may lie out of the interval $[\lambda_{LB}, \lambda_{UB}]$. In this case, Algorithm 1 fails to find the optimal interval. So, we explore the outside of $[\lambda_{LB}, \lambda_{UB}]$ in a separate phase.

Algorithm 1 A plane sweep algorithm for finding an interval containing the optimal solution to the Lagrangian dual problem.

Input: vectors c, a, and u and scaler b.
Output: interval $[\lambda_a, \lambda_b]$ that contains the optimal solution to the problem $\max_{\lambda\in\mathbb{R}} \phi(\lambda)$ or the smallest and largest intersection points.
Initialize a state array, $\ell = [1, \ldots, n]$, with lines $\ell[1], \ldots, \ell[n]$ sorted in decreasing order of their slope.
Initialize queue $Q = \emptyset$.
Initialize line indices array $p = [1, \ldots, n]$.
FAIL $\leftarrow$ `true`
Insert intersection points of all adjacent lines into Q.
Set $\lambda^{\text{prev}} \leftarrow -\infty$, $\lambda^{\text{prev prev}} \leftarrow -\infty$
while Q is not empty **do**
    Pop from Q the current intersection point λ^{new} and the corresponding two adjacent lines $\ell[i]$ and $\ell[j]$.
    Update state array: $\ell[p[i]] \leftrightarrow \ell[p[j]]$.
    Update the line indices array: $p[i] \leftrightarrow p[j]$.
    Insert the intersection point of $\ell[p[i]]$ and $\ell[p[i]+1]$ and the intersection point of $\ell[p[j]]$ and $\ell[p[j]-1]$ into Q, if there exists any.
    if $\phi(\lambda^{\text{prev}}) > \phi(\lambda^{\text{prev prev}})$ and $\phi(\lambda^{\text{prev}}) > \phi(\lambda^{\text{new}})$ **then**
        Set FAIL $\leftarrow$ `false`
        return $[\lambda^{\text{prev prev}}, \lambda^{\text{new}}]$ as the promising interval.
    end if
    Set $\lambda^{\text{prev prev}} \leftarrow \lambda^{\text{prev}}$.
    Set $\lambda^{\text{prev}} \leftarrow \lambda^{\text{new}}$.
end while
if FAIL **then**
    return the smallest λ_{LB} and the largest λ_{UB} intersection points.
end if

First, consider the exploration of $(-\infty, \lambda_{LB})$. Since the components of vector G in Theorem 2 are linear functions in term of λ, then there exists $\lambda'_{LB} < \lambda_{LB}$ such that the order of G_k's does not change for $\lambda < \lambda'_{LB}$. Indeed, a similar procedure for finding the smallest intersection of lines ℓ_i's can be used here to compute λ'_{LB}. Now, since $\phi(\lambda)$ is unimodal, one can conclude that

$$\max_{(-\infty,\lambda_{LB}]} \phi(\lambda) = \max_{[\lambda'_{LB},\lambda_{LB}]} \phi(\lambda). \tag{17}$$

Similarly, for the values of $\lambda > \lambda_{UB}$, one can find a threshold, say λ'_{UB}, such that

$$\max_{[\lambda_{UB},\infty)} \phi(\lambda) = \max_{[\lambda_{UB},\lambda'_{UB}]} \phi(\lambda). \tag{18}$$

We summarize the main algorithm in Algorithm 2.

Algorithm 2 A two-phase algorithm for solving rank-one QKP (2).

1: Run Algorithm 1 to find a promising interval that contains the optimal Lagrange multiplier.
2: **if** Algorithm 1 returns an interval $[\lambda_a, \lambda_b]$ **then**
3: Solve the optimization problem $\max_{[\lambda_a,\lambda_b]} \phi(\lambda)$ and return the optimal solution.
4: **else**
5: Solve optimization problems (17) and (18) and store the optimal values.
6: **end if**
7: **return** the best λ found as an optimal Lagrange multiplier.

It is clear that Algorithm 2 converges to the optimal solution since the output interval of Algorithm 1 contains the optimal solution and $\phi(\lambda)$ is unimodal. In fact, the single variable optimization problem in step 3 can be solved efficiently by a classical root-finding algorithm.

4 Computational experiments

In this section, we compare the running time of Algorithm 2 with the general convex quadratic programming solver, CPLEX. We implement Algorithm 2 with MATLAB R2019b. All runs are performed on a system with a Core i7 2.00 GHz CPU and 8.00 GB of RAM equipped with a 64bit Windows operating system. We solve single variables optimization problems (17), (18), and step 3 in Algorithm 2, using MATLAB built-in function fminbnd, which is based on the golden section search and parabolic interpolation.

Our testbed contains two types of randomly generated rank-one knapsack problems up to $n = 100,000$ variables. In the first type, the vectors a and c are integral and generated uniformly from the same interval. We denote this type by TypeI. In the second type (TypeII), the vectors a and c are positive

Table 1: Parameters for two types of problem instances.

Type	a	c	l	$u-l$
TypeI	$U(-50,50)$	$U(-50,50)$	$U(0,20)$	$U(1,100)$
TypeII	$U(-100,10)$	$U(10,100)$	$U(0,20)$	$U(1,100)$

and negative randomly generated integral vectors, respectively. In Table 1, we summarize the parameter values for problem instances.

As a well-known general convex quadratic programming solver, we chose CPLEX (ver. 12.9) to compare our results.

Based on our numerical results, we set the quadratic programming solver of CPLEX (qpmethod option) to the barrier. The barrier convergence tolerance, convergetol, is set to $1e-12$ (The default value is convergetol $= 1e-6$). It should be noted here that this setting is applied after we found that the default value leads to the optimal solutions that have components with a "meaningful" distance to their correct values. Another point is that for other optimizers such as primal and dual, CPLEX found the optimal solution in correct precision, but the running time is too long for large instances. For brevity, we do not report details related to these experiments.

After completing our experimental tests, we found in [10] that the sparsity of the Hessian matrix influences the performance of CPLEX. To increase the performance, we reformulate our problem as

$$\min\left\{\frac{1}{2}y^2 - c^\top x \ : \ \mathbf{1}^\top x - y = 0,\ a^\top x = b,\ 0 \le x \le u\right\}.$$

We denote the results corresponding to running CPLEX on the original problem and the aforementioned modification, respectively, by CPLEX_{org} and CPLEX_{ref}.

Table 2 shows the average running time for five runs of each algorithm/-solver for each problem size. Dash sign, "-", denoted the algorithm/solver encounters out-of-memory status.

In all cases, Algorithm 2 outperforms CPLEX_{org}. For instances up to $n = 5000$, our algorithm and CPLEX_{ref} have the same running time, whereas for larger instances, CPLEX_{ref} has smaller running time.

5 Conclusions

In this paper, we proposed a two-phase algorithm for rank-one QKPs. To this end, we studied the solution structure of the problem when it has no resource constraint. Indeed, we proposed an $O(n \log n)$ algorithm to solve this problem. We then used the solution structure to propose an $O(n^2 \log n)$ line-sweep algorithm that finds an interval that contains the optimal Lagrange multi-

Table 2: A comparison of running times (in seconds) between our algorithm and CPLEX$_{org}$ and CPLEX$_{ref}$.

n		Our algorithm	CPLEX$_{org}$	CPLEX$_{ref}$
1000	TypeI	0.06	0.09	0.01
	TypeII	0.01	0.06	0.02
1500	TypeI	0.04	0.15	0.02
	TypeII	0.02	0.13	0.02
2000	TypeI	0.04	0.27	0.02
	TypeII	0.02	0.27	0.02
5000	TypeI	0.09	2.21	0.02
	TypeII	0.06	2.12	0.03
10000	TypeI	0.26	16.26	0.04
	TypeII	0.23	16.95	0.05
15000	TypeI	0.62	61.20	0.10
	TypeII	0.63	65.88	0.10
20000	TypeI	1.16	-	1.20
	TypeII	0.88	-	1.02
50000	TypeI	3.22	-	0.11
	TypeII	3.19	-	0.11
100000	TypeI	12.19	-	0.14
	TypeII	11.31	-	0.17

plier. Then, the estimated optimal interval was explored for computing the optimal solution with the desired accuracy. Our computational tests showed that our algorithm has better running time than CPLEX when CPLEX is used to solve the original problem. After a reformulation of the problem, CPLEX outperforms our algorithm for instances with $n \geq 5000$.

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