



# The quadratic knapsack problem with setup

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## ABSTRACT

The Quadratic Knapsack Problem is a well-known generalization of the classical 0-1 knapsack problem, in which any pair of items produces a pairwise profit if both are selected. Another relevant generalization of the knapsack problem is the Knapsack Problem with Setup, in which the items are partitioned into classes, the items of a class can only be inserted into the knapsack if the corresponding class is activated, and activating a class involves a setup cost and a setup capacity reduction.

Despite a rich literature on these two problems, their obvious generalization, i.e., the Quadratic Knapsack Problem with Setup, was never investigated so far. We discuss applications, mathematical models, deterministic matheuristic algorithms, and computationally evaluate their performance.

## 1. Introduction

The *Quadratic Knapsack Problem* (QKP) has been intensively studied since its definition in 1980 (see Gallo et al. (1980)). As in the famous (0–1) *Knapsack Problem* (KP), we are given a knapsack with positive integer capacity  $c$ , a set of items  $N = \{1, \dots, n\}$  having a non-negative integer profit  $p_i$  and a positive integer weight  $w_i$  ( $i \in N$ ). In addition, in the QKP each unordered pair of distinct items  $\{i, j\}$  produces a non-negative integer pairwise profit  $p_{ij}$  if both items are inserted into the knapsack. Both the KP and the QKP consist of selecting a subset of items, whose overall weight does not exceed the capacity, that maximizes an appropriate profit function. While in the KP such function is just the sum of the profits of the selected items, in the QKP it also includes the sum of their pairwise profits. The KP is thus the special case of the QKP arising when  $p_{ij} = 0$  for all  $i < j$ . Several effective exact algorithms (see, e.g., Billionnet and Soutif (2004a,b), Caprara et al. (1999), Pisinger et al. (2007) and Fomeni et al. (2022)) and metaheuristics (see, e.g., Glover et al. (2002), Yang et al. (2013) and Chen and Hao (2017)) have been proposed for the QKP.

Another relevant generalization of the KP, which has been thoroughly investigated in the literature, is the *Knapsack Problem with Setup* (KPS), introduced in 1994 by Chajakis and Guignard (1994). In the KPS, the items are partitioned into  $r$  classes  $R_h \subseteq N$ ,  $h \in R = \{1, \dots, r\}$ , and the items of a class can only be inserted into the knapsack if the corresponding class is activated. Activating a class  $h$  involves a non-negative integer setup reduction  $d_h$  of the knapsack capacity and a non-negative activation setup cost  $f_h$ . (Slightly different definitions can be encountered in the literature.) The objective is to select a

subset of items maximizing the difference between item profits and class setup costs, such that their total weight does not exceed the difference between the capacity and the class setup reductions. Several effective exact algorithms (see, e.g., Chebil and Khemakhem (2015), della Croce et al. (2017) and Furini et al. (2018)) and heuristics (see, e.g., Khemakhem and Chebil (2016) and Amiri (2020)) have been proposed for the KPS.

As previously mentioned, there is a rich literature on both the QKP and the KPS. Quite surprisingly instead, the obvious generalization of both problems, i.e., the *Quadratic Knapsack Problem with Setup* (QKPS), to the best of our knowledge, was never investigated so far. The QKPS inherits all input parameters of the two problems above. The constraints are the same as the KPS, while the objective is to find a subset of items maximizing the difference between the total (individual and pairwise) item profit and the class setup cost.

The QKPS can be modeled as the following 0–1 Quadratic Program

$$(01QP) \quad \max \sum_{i \in N} p_i x_i + \sum_{i \in N} \sum_{j \in N: i < j} p_{ij} x_i x_j - \sum_{h \in R} f_h y_h \quad (1)$$

$$\text{s.t.} \quad \sum_{i \in N} w_i x_i + \sum_{h \in R} d_h y_h \leq c \quad (2)$$

$$x_i \leq y_h \quad (h \in R; i \in R_h) \quad (3)$$

$$x_i \in \{0, 1\} \quad (i \in N) \quad (4)$$

$$y_h \in \{0, 1\} \quad (h \in R), \quad (5)$$

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where  $x_i$  takes the value one iff item  $i$  is selected, and variable  $y_h$  takes the value one iff class  $h$  is activated. The objective function (1) is given by the sum of the individual and pairwise profits of the selected items, minus the setup costs of the classes they belong to. Inequality (2) imposes the capacity constraint on the total weight of the selected items, plus the setup reductions of their classes. Constraints (3) impose the activation of the necessary classes.

The QKP is the special case of (1)–(5) arising when  $r = 1$  and  $f_1 = d_1 = 0$ . (Note that in this case the auxiliary variable  $y_1$  and the corresponding linking constraints (3) are not needed.) It is known that the QKP is strongly  $\mathcal{NP}$ -hard (see, e.g., Gallo et al. (1980)), from which the same complexity applies to the QKPS.

Another special case is obtained when  $p_{ij} = 0$  for  $i, j = 1, \dots, n$  ( $i < j$ ), in which case (1)–(5) corresponds to the KPS. If, in addition,  $r = 1$  and  $f_1 = d_1 = 0$ , model (1), (2), (4) describes the KP. Both the KPS and the KP are weakly  $\mathcal{NP}$ -hard and can be solved in pseudo-polynomial time.

The QKP has a number of real-world applications, explored since the Seventies in different fields. Rhys (1970) modeled as a QKP the problem of selecting freight handling terminals to install, when the existence of a pair of terminals permits a service to be operated between them, and each service is associated with a revenue. Similar applications concerned electronic message handling stations, see Witzgall (1975). Typical applications of the KPS arise in machine scheduling, in particular when dealing with make-to-order production contexts in the management of different product categories (see, e.g., Chajakis and Guignard (1994)). The QKPS combines the QKP and the KPS, and can arise in applications like the one described in Page (2018), concerning the design of an auction to allocate the electromagnetic spectrum for cellular phones. The radio signal from a cell tower covers a geographic range, and the government sells licences for specific regions to different companies. The value of a licence clearly depends on the other licences acquired by the company, as the value of a licence for a certain region would be worth to a company that also acquires licences of neighboring regions. Indeed, holding neighboring licences implies, e.g., lower construction costs and common advertising media. The economists refer to these interdependent valuations as *externalities*. Let the classes correspond to regions (the setup costs being the licence prices), the items to infrastructures (e.g., cell towers), linear profits to the values of covering specific areas, and pairwise profits to their externalities. If the item weights measure the amount of resources (personnel, technological devices, etc.) needed by the cell towers, and the setup reductions and capacity represent, respectively, the amount of resources needed to open up the activities in a specific region and the overall resource budget available, the resulting optimization problem can be modeled as a QKPS.

The purpose of this paper is to provide a first study on the QKPS. The paper is structured as follows. Section 2 provides linear reformulations of the QKPS. Sections 3 and 4 present deterministic matheuristic methods, that proved to have a good computational performance, especially when the solutions they produce are refined through the local search procedures described in Section 5. Section 6 presents the results of extensive computational experiments. Finally, Section 7 provides some concluding remarks.

## 2. Reformulation linearization

The *Reformulation Linearization Technique* (RLT) was originally introduced by Adams and Sherali (1986) for 0–1 quadratic problems, and later extended by the same authors (Sherali and Adams, 1990) to general 0–1 problems. The basic underlying idea can however be found in earlier studies on linear formulations of the *quadratic assignment problem* dating back to the Sixties (see, e.g., the monograph by Burkard et al. (2012), Section 7.3, for a comprehensive treatment).

The RLT consists of a methodology to strengthen the continuous relaxation of 0–1 quadratic models through the addition of constraints

obtained by multiplying the original (linear) constraints by the model binary variables (and, possibly, by their complement). The resulting quadratic constraints and the original quadratic objective function are then linearized in a standard way, by introducing new binary variables and the corresponding linking constraints to replace the quadratic terms. The method was adapted to the QKP by Caprara et al. (1999), and later extended to constrained 0–1 quadratic problems and generalized quadratic assignment problems by Caprara (2008) and Guignard (2020), respectively.

An RLT model for the QKPS can be obtained as follows. Let  $h(i)$  denote the class index to which item  $i$  belongs ( $i \in R_{h(i)}$ ). We consider capacity constraint (2), and obtain two groups of new constraints by multiplying it by both variables  $x_j$  ( $j \in N$ ) and  $y_k$  ( $k \in R$ ):

- the former group,

$$\sum_{i \in N; i < j} w_i z_{ij} + \sum_{i \in N; j < i} w_i z_{ji} + \sum_{h \in R \setminus \{h(j)\}} d_h q_{hj} \leq (c - w_j - d_{h(j)}) x_j \quad (j \in N), \quad (6)$$

contains two families of quadratic terms, respectively represented by auxiliary binary variables

$$z_{ij} = x_i x_j \quad (i, j \in N; i < j)$$

and

$$q_{hj} = y_h x_j \quad (h \in R, j \in N \setminus R_h).$$

Note that, for a binary variable  $x_j$ , we have  $x_j^2 = x_j$ , while  $y_{h(j)} x_j = x_j$  follows from  $x_j \leq y_{h(j)}$ , see (3);

- similarly, in the latter group,

$$\sum_{i \in N \setminus R_k} w_i q_{ki} + \sum_{h \in R; h < k} d_h t_{hk} + \sum_{h \in R; k < h} d_h t_{kh} \leq (c - d_k) y_k - \sum_{i \in R_k} w_i x_i \quad (k \in R), \quad (7)$$

the quadratic terms are represented, respectively, by auxiliary binary variables  $q_{hj}$  and

$$t_{hk} = y_h y_k \quad (h, k \in R; h < k)$$

(as  $y_h^2 = y_h$ ).

By adding the linking constraints (9)–(11) we obtain the *Integer Linear Programming* (ILP) model

$$\text{(RLT) max} \quad \sum_{i \in N} p_i x_i + \sum_{i, j \in N; i < j} p_{ij} z_{ij} - \sum_{h \in R} f_h y_h \quad (8)$$

s.t. (2), (3), (4), (5), (6), (7)

$$z_{ij} \leq x_i, \quad z_{ij} \leq x_j, \quad z_{ij} \geq x_i + x_j - 1 \quad (i, j \in N; i < j) \quad (9)$$

$$q_{hj} \leq y_h, \quad q_{hj} \leq x_j, \quad q_{hj} \geq y_h + x_j - 1 \quad (h \in R; j \in N \setminus R_h) \quad (10)$$

$$t_{hk} \leq y_h, \quad t_{hk} \leq y_k, \quad t_{hk} \geq y_h + y_k - 1 \quad (h, k \in R; h < k) \quad (11)$$

$$z_{ij} \in \{0, 1\} \quad (i, j \in N; i < j) \quad (12)$$

$$q_{hj} \in \{0, 1\} \quad (h \in R; j \in N \setminus R_h) \quad (13)$$

$$t_{hk} \in \{0, 1\} \quad (h, k \in R; h < k) \quad (14)$$

We next present two ways to obtain alternative RLT models which computationally proved to be more effective for the QKPS.

## 2.1. Revised reformulation RLT1

First observe that, if  $p_{ij} = 0$ , then one can obtain an equivalent solution by setting  $z_{ij} = 0$ , and hence we can define variables  $z_{ij}$  only for those pairs  $\{i, j\}$  ( $i, j \in N$ ) for which  $i < j$  and  $p_{ij} > 0$ . The second observation is that the RLT-capacity constraints (6) and (7) are only introduced to strengthen the *Linear Programming* (LP) relaxation, but are redundant for the 01-LP RLT model, so they can be omitted in our analysis. Since variables  $z_{ij}$  appear with a strictly positive coefficient in objective function (8), in any optimal 01-LP solution  $(x^*, y^*, z^*)$  such variables will take the largest possible value allowed by (9), i.e.,  $z_{ij}^* = \min\{x_i^*, x_j^*\}$ . Since  $x_i^* \in \{0, 1\} \forall i \in N$ , then  $\min\{x_i^*, x_j^*\} \geq x_i^* + x_j^* - 1$ . This immediately proves that constraints  $z_{ij} \geq x_i + x_j - 1$  in (9) are redundant, while  $z_{ij} \in \{0, 1\}$  in (12) can be replaced with  $z_{ij} \geq 0$ . Note, however, that the above constraints may tighten the LP relaxation of the RLT model.

By adopting the notations

$$N^{<}(i) = \{j \in N : i < j \text{ and } p_{ij} > 0\},$$

$$N^{>}(i) = \{j \in N : i > j \text{ and } p_{ji} > 0\} \quad (i \in N),$$

we modify (6) as

$$\begin{aligned} & \sum_{i \in N; j \in N^{<}(i)} w_i z_{ij} + \sum_{i \in N; j \in N^{>}(i)} w_i z_{ji} \\ & + \sum_{h \in R \setminus \{h(j)\}} d_h q_{hj} \leq (c - w_j - d_{h(j)}) x_j \quad (j \in N) \end{aligned} \quad (15)$$

thus obtaining the revised model RLT1

$$(RLT1) \quad \max \quad \sum_{i \in N} p_i x_i + \sum_{i \in N; j \in N^{<}(i)} p_{ij} z_{ij} - \sum_{h \in R} f_h y_h \quad (16)$$

s.t. (2), (3), (4), (5), (7), (15)

$$z_{ij} \leq x_i, \quad z_{ij} \leq x_j, \quad (i \in N; j \in N^{<}(i)) \quad (17)$$

$$q_{hj} \leq y_h, \quad q_{hj} \leq x_j, \quad q_{hj} \geq y_h + x_j - 1 \quad (h \in R; j \in N \setminus R_h) \quad (10)$$

$$t_{hk} \leq y_h, \quad t_{hk} \leq y_k, \quad t_{hk} \geq y_h + y_k - 1 \quad (h, k \in R; h < k) \quad (11)$$

$$z_{ij} \geq 0 \quad (i \in N; j \in N^{<}(i)) \quad (18)$$

$$q_{hj} \in \{0, 1\} \quad (h \in R; j \in N \setminus R_h) \quad (13)$$

$$t_{hk} \in \{0, 1\} \quad (h, k \in R; h < k) \quad (14)$$

## 2.2. Revised reformulation RLT2

We next show that reformulation RLT1 of the previous section can be further modified by:

(i) eliminating the first two inequalities in constraints (10) and (11), and

(ii) relaxing constraints (13) and (14) by imposing that variables  $q_{hj}$  and  $t_{hk}$  take non-negative values without changing the optimal value of the LP relaxation. Indeed,

- variables  $q_{hj}$  and  $t_{hk}$  do not appear in the objective function (16) and can only affect its value by increasing the left-hand-side of the RLT capacity constraints (15) and (7), respectively. It follows that it is superfluous to impose an upper bound on them as their increase reduces the solution space thus possibly decreasing the solution value;
- the previous consideration also shows that the third inequality in constraints (10) (resp. (11)) forces  $q_{hj}$  (resp.  $t_{hk}$ ) to take at least the value one when  $y_h = x_j = 1$  (resp.  $y_h = y_k = 1$ ). It additionally

follows that constraints (13) and (14) can be further relaxed to only impose non-negativity of variables  $q_{hj}$  and  $t_{hk}$ .

The new reformulation follows:

$$\begin{aligned} (RLT2) \quad \max \quad & \sum_{i \in N} p_i x_i + \sum_{i \in N; j \in N^{<}(i)} p_{ij} z_{ij} - \sum_{h \in R} f_h y_h \quad (16) \\ \text{s.t.} \quad & (2), (3), (4), (5), (7), (15) \\ & z_{ij} \leq x_i, \quad z_{ij} \leq x_j \quad (i \in N; j \in N^{<}(i)) \quad (17) \\ & q_{hj} \geq y_h + x_j - 1 \quad (h \in R; j \in N \setminus R_h) \quad (19) \\ & t_{hk} \geq y_h + y_k - 1 \quad (h, k \in R; h < k) \quad (20) \\ & z_{ij} \geq 0 \quad (i \in N; j \in N^{<}(i)) \quad (18) \\ & q_{hj} \geq 0 \quad (h \in R; j \in N \setminus R_h) \quad (21) \\ & t_{hk} \geq 0 \quad (h, k \in R; h < k) \quad (22) \end{aligned}$$

It was pointed out in Section 2.1 that, due to the elimination of redundant constraints  $z_{ij} \geq x_i + x_j - 1$  in (9), the LP relaxation of RLT1 can be weaker than that provided by the original RLT. It is worth observing that the solutions produced by the LP relaxations of RLT1 and RLT2 have the same value.

## 3. Basic heuristic tools

Consider again model (1)–(5), and observe that, by fixing the value of the auxiliary variables  $y_h$ , the capacity is decreased by the setup reductions of the selected classes (i.e., those for which  $y_h = 1$ ) and hence the solution to the resulting QKP instance provides a feasible solution to the QKPS.

This idea is exploited in the solution methods presented in the following. The main engine within the proposed procedures is indeed an algorithm for the optimal solution to the QKP, for which, as already mentioned, a number of exact methods are available in the literature.

One of the most competitive QKP exact algorithms is that proposed by Caprara et al. (1999), for which an effective C implementation, *quadknap*, can be freely downloaded from *David Pisinger's optimization codes page*

<http://hjemmesider.diku.dk/~pisinger/quadknap.c>

In the following, we will invoke such code through the statement

$$([\bar{x}], \bar{z}) \leftarrow \text{quadknap}(\bar{I}, \bar{c})$$

where

- $\bar{I}$  denotes a subset of input items (including their profits and weights);
- $\bar{c}$  is a capacity value ( $\bar{c} \leq c$ );
- $[\bar{x}]$  provides the solution array computed by *quadknap* (where, for  $i \in \bar{I}$ ,  $\bar{x}_i = 1$  if item  $i$  is selected, and  $\bar{x}_i = 0$  otherwise), and  $\bar{z}$  the corresponding solution value.

The main procedure based on *quadknap* determines a feasible solution to a QKPS instance by only considering a subset of classes and a capacity defined by the original capacity  $c$  minus the setup reductions of such classes. Let  $Q$  denote a QKPS instance (defined by all parameters introduced in Section 1). For a given  $S \subseteq R$ , procedure *QKnap*, shown in Algorithm 1, defines a QKP instance consisting of the items belonging to the classes in  $S$  and the corresponding reduced capacity, solves it through *quadknap* (i.e., by disregarding the setup

costs), and reconstructs a QKPS solution by defining the solution arrays  $([x], [y])$  and the solution value  $z$  induced by  $[\bar{x}]$ .

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**Algorithm 1:** Procedure QKnaP
 

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**input** : A QKPS instance  $Q$ , a set  $S \subseteq R$   
**output**:  $([x], [y], z) \equiv$  A feasible solution  $[x], [y]$  to  $Q$ , and its value  $z$

- 1  $\bar{I} := \cup_{h \in S} R_h, \bar{c} := c - \sum_{h \in S} d_h;$
- 2 **if**  $\min\{w_i : i \in \bar{I}\} > \bar{c}$  **then**  $([\bar{x}] := 0, \bar{z} := 0)$  **else**  
 $([\bar{x}], \bar{z}) \leftarrow \text{quadknap}(\bar{I}, \bar{c});$
- 3 **define** the QKPS solution  $([x], [y])$  corresponding to  $([\bar{x}]);$
- 4  $z := \bar{z} - \sum_{h \in S} f_h y_h.$

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Besides being used in the greedy algorithms presented in Section 4, and in the local search procedures described in Section 5, procedure QKnap will be used to construct an initial feasible solution, as shown in the next section.

The time complexity of QKnaP is in general non polynomial, as it invokes quadknap to solve a QKP instance. It is however possible to execute quadknap with a prefixed (constant) limit on the CPU time (as we did in all our implementations). In our analysis of the time required by the presented procedures, we will thus evaluate the number of calls to quadknap.

### 3.1. Initialization

First observe that any instance of the QKPS can be initially reduced by eliminating (useless) classes  $h$ , if any, for which  $\min\{w_i : i \in R_h\} > c - d_h$ . A feasible solution to the reduced instance can then be obtained by invoking QKnaP for each individual class, and retaining the best solution found. Procedure Initialize, shown in Algorithm 2, computes in addition, for each class  $h$ , a profit-to-weight score value.

$$V_h = \frac{P_h}{\sum_{i \in R_h} w_i x_i^* + d_h} \quad (23)$$

given by the ratio between the profit  $P_h$  determined by QKnaP and the total weight (in the solution  $[x^*]$  returned by QKnaP) of the selected items, increased by the corresponding setup reduction of class  $h$ . Initialize invokes quadknap  $O(r)$  times.

In order to reduce the number of executions of quadknap, which is the most time consuming component of our algorithms, a globally defined family  $\Sigma$  stores all class sets for which QKnaP was invoked. Since the QKPS solution produced by QKnaP( $Q, S$ ) only depends on the composition of class set  $S$ , QKnaP is not executed if  $S$  belongs to family  $\Sigma$ , which is initialized in Algorithm 2 with all single classes and used/updated by all procedures presented in the following.

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**Algorithm 2:** Procedure Initialize
 

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**input** : A QKPS instance  $Q$   
**output**:  $([x], [y], z, [V], [P]) \equiv$  A feasible solution  $[x], [y]$  to  $Q$ , and its value  $z$ ,  
 an array  $[V]$  of profit-to-weight score values for each class  
 an array  $[P]$  of solution values for each single class

- 1  $z := 0, [x] := \mathbf{0}, [y] := \mathbf{0};$
- 2 **for**  $h := 1$  **to**  $r$  **do**
- 3  $([x^*], [y^*], P_h) \leftarrow \text{QKnaP}(Q, \{h\});$
- 4 **if**  $P_h > z$  **then**  $z := P_h, [x] := [x^*], [y] := [y^*];$
- 5  $V_h := P_h / (\sum_{i \in R_h} w_i x_i^* + d_h)$
- 6 **end**
- 7  $\Sigma := \{\{1\}, \{2\}, \dots, \{r\}\}.$

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## 4. Greedy algorithms

Once an instance has been initialized, an improved solution can be computed by procedure Greedy, shown in Algorithm 3. The classes are ordered by non-increasing value of their score  $V_h$ , and a set  $S$  of solution classes is

- (i) initialized with the class having the highest score value, and
- (ii) iteratively augmented by adding a class at a time and invoking QKnaP: classes which improve the incumbent solution value  $z$  are permanently added to  $S$ .

Procedure Greedy invokes Initialize once, and then, for  $r - 1$  times, it invokes quadknap, i.e., the overall number of calls to quadknap is  $O(r)$ .

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**Algorithm 3:** Procedure Greedy
 

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**input** : A QKPS instance  $Q$   
**output**:  $([x], [y], z) \equiv$  A feasible solution  $[x], [y]$  to  $Q$ , and its value  $z$

- 1  $([x], [y], z, [V], [P]) \leftarrow \text{Initialize}(Q);$
- 2 **sort** the classes by non-increasing  $V_h$  value and update the indices;
- 3  $S := \{1\};$
- 4 **for**  $h := 2$  **to**  $r$  **do**
- 5  $S^* := S \cup \{h\}, \Sigma := \Sigma \cup S^*;$
- 6  $([x^*], [y^*], z^*) \leftarrow \text{QKnaP}(Q, S^*);$
- 7 **if**  $z^* > z$  **then**  $S := S^*, z := z^*, [x] := [x^*], [y] := [y^*]$
- 8 **end**

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Preliminary computational experiments proved that ordering the classes by non-increasing value of scores  $V_h$  provides better solutions than those obtained by ordering the classes by non-increasing value of profit  $P_h$ .

Note that, for the case of two classes ( $r = 2$ ), procedure Greedy evaluates all possible subsets of classes, and hence it produces the optimal solution, provided the time limit assigned to the QKP code quadknap allows it to complete the three executions.

A refined, although more time consuming, algorithm, which can provide better solutions, is shown in Algorithm 4. Procedure Refined Greedy, determines the class  $h^*$  with maximum score value  $V_{h^*}$  and initializes a local incumbent solution value  $\bar{z}$  to  $P_{h^*}$  and a set of “candidate” classes  $S$  to  $h^*$ . It then iteratively checks the effect of adding one additional class  $h$  at a time, by invoking QKnaP for the resulting family  $S^*$ . If the value  $\Pi_h$  of the corresponding solution improves the local incumbent solution value  $\bar{z}$ , a relative score value is computed as

$$W_h := \frac{\Pi_h}{\sum_{i \in S^*} (\sum_{i \in R_i} w_i x_i^* + d_i)} \quad (24)$$

and set to zero otherwise. (The overall incumbent solution, of value  $z$ , is also possibly updated.)

Once all classes have been checked, the one with maximum relative score value is permanently added to  $S$ , and the process is iterated for the remaining candidate classes  $R \setminus S$ . The procedure terminates when none of the candidate classes improves the local incumbent solution.

At each **while** iteration, the cardinality of  $R \setminus S$  decreases by one (if not, a **return** occurs). Therefore, at most  $O(r)$  iterations are performed, each requiring  $O(r)$  calls to quadknap, for a total of  $O(r^2)$  quadknap executions.

## 5. Local search procedures

The solutions provided by the greedy algorithms can be improved through local search. Traditional local search methods to knapsack-like problems rely on removals, insertions, and exchanges of items. The algorithms we propose in the present section consider instead



**Algorithm 4:** Procedure Refined Greedy

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input : A QKPS instance  $\mathcal{Q}$ 
output:  $([x], [y], z) \equiv A$  feasible solution  $[x], [y]$  to  $\mathcal{Q}$ , and its value  $z$ 

1  $([x], [y], z, [V], [P]) \leftarrow \text{Initialize}(\mathcal{Q});$ 
2  $h^* := \arg \max_{h \in R} \{V_h\}, S := \{h^*\};$ 
3 if  $P_{h^*} > 0$  then  $\bar{z} := P_{h^*}$  else  $\bar{z} := 0;$ 
4 while  $R \setminus S \neq \emptyset$  do
5   foreach  $h \in R \setminus S$  do
6      $S^* := S \cup \{h\};$ 
7      $\Sigma := \Sigma \cup S^*;$ 
8      $([x^*], [y^*], \Pi_h) \leftarrow \text{QKnaP}(\mathcal{Q}, S^*);$ 
9     if  $\Pi_h > \bar{z}$  then
10       $W_h := \Pi_h / \sum_{l \in S^*} (\sum_{i \in R_l} w_i x_i^* + d_l);$ 
11      if  $\Pi_h > z$  then  $z := \Pi_h, [x] := [x^*], [y] := [y^*];$ 
12    else
13       $W_h := 0;$ 
14    end
15  end
16   $\bar{h} := \arg \max_{h \in R \setminus S} \{W_h\};$ 
17  if  $\Pi_{\bar{h}} > \bar{z}$  then  $\bar{z} := \Pi_{\bar{h}}, S := S \cup \{\bar{h}\}$  else return
18 end

```

---

removals and exchanges of *classes*. For each move, a series of calls to procedure QKnaP (and hence to code quadknap) looks for a QKPS solution improving the incumbent one: each execution of quadknap is halted whenever an upper bound computation excludes the possibility of improving on the incumbent solution.

### 5.1. Removals

Procedure Remove, shown in Algorithm 5, receives a feasible solution  $[x], [y], z$  (*global incumbent*) and initializes to it a *local incumbent*  $[\hat{x}], [\hat{y}], \hat{z}$ . It then iteratively excludes one class,  $\bar{h}$ , from the set of classes which are selected in the current solution, and computes a (possibly improved) solution by invoking QKnaP for the remaining selected classes. The local incumbent is updated whenever an improved solution is obtained. While the final local incumbent improves on the global incumbent, the process is iterated.

The **foreach** loop invokes procedure QKnaP at most  $r$  times, each requiring a single call to quadknap. After every **foreach** execution, either the stop condition of the **while** loop becomes true or the number of classes  $h$  with  $y_h = 1$  decreases by one. It follows that the **foreach** loop is executed  $O(r)$  times, yielding an overall  $O(r^2)$  calls to quadknap.

### 5.2. Exchanges

The general structure of procedure Exchange (shown in Algorithm 6), is similar to that of Remove. The input solution  $[x], [y], z$  (global incumbent) is used to initialize a local incumbent  $[\hat{x}], [\hat{y}], \hat{z}$ . For each different pair of classes such that one is currently selected and one not, the former ( $h^1$ ) is excluded and replaced with the latter ( $h^0$ ): QKnaP is then invoked to determine the corresponding QKPS solution, possibly updating the local incumbent. On exit from the nested **foreach** loop: if the global incumbent can be updated, the **while** loop iterates the process; otherwise, the procedure terminates.

The nested **foreach** loop invokes QKnaP  $O(r^2)$  times. Whenever the value of the global incumbent is increased, the **while** loop is iterated, and hence, in the worst case, Exchange can require a pseudo-polynomial number of quadknap executions (in which case, however, one should expect a very good solution, due to a large number of improvements).

**Algorithm 5:** Procedure Remove

---

```

input : A QKPS instance  $\mathcal{Q}$ , a feasible solution  $([x], [y])$  to  $\mathcal{Q}$ , and its value  $z$ 
output: A possibly improved QKPS solution  $([x], [y])$ , and its value  $z$ 

1  $\hat{z} := z, [\hat{x}] := [x], [\hat{y}] := [y];$ 
2  $Stop := \text{false};$ 
3 while  $Stop = \text{false}$  do
4   foreach  $\bar{h} \in R : y_{\bar{h}} = 1$  do
5      $S := \{h \in R : y_h = 1\} \setminus \{\bar{h}\};$ 
6     if  $S \notin \Sigma$  then  $\Sigma := \Sigma \cup S$  else continue;
7      $([\bar{x}], [\bar{y}], \bar{z}) \leftarrow \text{QKnaP}(\mathcal{Q}, S);$ 
8     if  $\bar{z} > \hat{z}$  then  $\hat{z} := \bar{z}, [\hat{x}] := [\bar{x}], [\hat{y}] := [\bar{y}];$ 
9   end
10  if  $\hat{z} > z$  then  $z := \hat{z}, [x] := [\hat{x}], [y] := [\hat{y}]$  else  $Stop := \text{true}$ 
11 end

```

---

**Algorithm 6:** Procedure Exchange

---

```

input : A QKPS instance  $\mathcal{Q}$ , a feasible solution  $([x], [y])$  to  $\mathcal{Q}$  and its value  $z$ 
output: A possibly improved QKPS solution  $([x], [y])$  and its value  $z$ 

1  $Stop := \text{false};$ 
2  $\hat{z} := z, [\hat{x}] := [x], [\hat{y}] := [y];$ 
3 while  $Stop = \text{false}$  do
4   foreach  $h^1 \in R : y_{h^1} = 1$  do
5     foreach  $h^0 \in R : y_{h^0} = 0$  do
6        $S := \{h \in R : y_h = 1\} \setminus \{h^1\} \cup \{h^0\};$ 
7       if  $S \notin \Sigma$  then  $\Sigma := \Sigma \cup S$  else continue;
8        $([\bar{x}], [\bar{y}], \bar{z}) \leftarrow \text{QKnaP}(\mathcal{Q}, S);$ 
9       if  $\bar{z} > \hat{z}$  then  $\hat{z} := \bar{z}, [\hat{x}] := [\bar{x}], [\hat{y}] := [\bar{y}];$ 
10    end
11  end
12  if  $\hat{z} > z$  then  $z := \hat{z}, [x] := [\hat{x}], [y] := [\hat{y}]$  else  $Stop := \text{true}$ 
13 end

```

---

## 6. Computational experiments

All algorithms presented in the previous sections were implemented in C++ language and compiled with g++, but the quadknap solver, which was compiled with the GNU Compiler GCC. All experiments were executed on a single thread of a 13th Gen Intel Core i9-13900KF 64 GB Processor running at 3.00 GHz, and operating under Ubuntu 22.04 LTS. The models were solved using solvers CPLEX 22.11 and Gurobi 10.02.

### 6.1. Benchmarks

As the QKPS is a novel problem, we derived benchmarks instances by combining the main generation schemes adopted for its underlying combinatorial problems (the QKP and the KPS).

Following the classical scheme originally proposed by Gallo et al. (1980) for the QKP, we used four values  $d \in (0, 1]$  for the density of the non-zero quadratic terms:  $d \in \{0.25, 0.50, 0.75, 1.00\}$ . Linear profits  $p_i$  ( $i = 1, \dots, n$ ) and pairwise profits  $p_{ij}$  ( $i = 1, \dots, n-1; j = i+1, n$ ) were generated with probability  $d$  as random integer values uniformly drawn from  $[1, 100]$ , and set to 0 with probability  $1-d$ . Weights  $w_i$  ( $i = 1, \dots, n$ ) were generated as uniformly random integers from  $[10, 100]$ , while the capacity  $c$  was set to  $[0.5 \sum_{i=1}^n w_i]$ .

Since the KPS is a weakly  $\mathcal{NP}$ -hard problem, “easy” to solve in practice even for very large-size instances, the number of items and the number of classes commonly used in the literature (with order of









### 6.3. Results for large size instances

Table 3 evaluates the winners of Table 1 (RLT1(Gurobi) and RLT2(CPLEX)) and Table 2 (Greedy + Local and Refined Greedy + Local) on instances with  $n \in \{300, 400, 500\}$ . In this case, both solvers CPLEX and Gurobi had a time limit of 2 h per instance, while each matheuristic had a time limit of (i) 20 s for each execution of the QKP code Quadknap within the greedy algorithms, and (ii) 10 s for each execution of the same code within the local search procedures.

Each line refers to a triplet  $(r, n, d)$ , reported in the first three columns. For all methods, the first four entries provide (over the corresponding 5 instances)

- %Bgap = average percentage gap (see above);
- Time = average CPU time expressed in seconds;
- Value = average solution value (rounded to the nearest integer);
- #B = number of instances for which the method produced the best solution value.

In addition, for the two models, the last two entries give

- %Ogap = average percentage optimality gap (see above);
- #opt = number of instances solved to proven optimality.

For each group of 20 instances corresponding to a pair  $\{r, n\}$ , the average values of %Bgap, Time, Value and %Ogap, and the total values of #B and #opt, are reported in lines “Avg/Sum”. Lines “r-Avg/Sum” provide the same values over the 60 instances generated for each value of  $r$ , while the last line, “Over-Avg/Sum”, gives the overall statistics over all the 180 large instances.

Contrary to what happens for smaller instances, the performance of RLT1(Gurobi) is globally better than that of RLT2(Cplex). Both models are however clearly worse than the matheuristics, as they produce globally much worse results with CPU times one or two orders of magnitude larger. (The only partial exception occurs for  $d = 0.25$ , for which RLT1(Gurobi) finds a larger number of best solutions, although almost always hitting the time limit.)

Concerning the matheuristic methods, the results obtained by Refined Greedy + Local are slightly better than those obtained by Greedy + Local, at the expense of a moderate CPU time increase. The overall winner appears to be Refined Greedy + Local, which finds about 90% of best solution values, with an overall average CPU time around 5 min.

## 7. Conclusions

We have studied a relevant variant of the quadratic knapsack problem, never investigated before in the literature. We have provided a traditional quadratic model and different linear reformulations of the problem. We have developed deterministic matheuristic methods and local search procedures to improve the solutions they obtain. Extensive computational experiments indicate that these methods are able to produce good quality solutions within reasonable computing times.

### CRedit authorship contribution statement

**Laura Galli:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Silvano Martello:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Carlos Rey:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Paolo Toth:** Writing – review & editing, Writing – original draft, Visualization,

Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

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### Data availability

Data will be made available on request.

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