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## An iterated "hyperplane exploration" approach for the Quadratic Knapsack Problem

Yuning Chen<sup>a</sup> and Jin-Kao Hao<sup>a,b,\*</sup>

<sup>a</sup>LERIA, Université d'Angers, 2 Bd Lavoisier, 49045 Angers, France <sup>b</sup>Institut Universitaire de France, Paris, France Computers & Operations Research 77: 226-239, 2017

#### Abstract

The quadratic knapsack problem (QKP) is a well-known combinatorial optimization problem with numerous applications. Given its NP-hard nature, finding optimal solutions or even high quality suboptimal solutions to QKP in the general case is a highly challenging task. In this paper, we propose an iterated "hyperplane exploration" approach (IHEA) to solve QKP approximately. Instead of considering the whole solution space, the proposed approach adopts the idea of searching over a set of hyperplanes defined by a cardinality constraint to delimit the search to promising areas of the solution space. To explore these hyperplanes efficiently, IHEA employs a variable fixing strategy to reduce each hyperplane-constrained sub-problem and then applies a dedicated tabu search procedure to locate high quality solutions within the reduced solution space. Extensive experimental studies over three sets of 220 QKP instances indicate that IHEA competes very favorably with the stateof-the-art algorithms both in terms of solution quality and computing efficiency. We provide additional information to gain insight into the key components of the proposed approach.

*Keywords*: Quadratic Knapsack problem; Hyperplane exploration; Tabu search; Variable fixing; Heuristics.

\* Corresponding author. Email addresses: yuning@info.univ-angers.fr (Yuning Chen), hao@info.univ-angers.fr (Jin-Kao Hao).

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#### 1 **1** Introduction

The quadratic knapsack problem (QKP) [14] can be informally described as follows. We are given a capacity-constrained knapsack and a set of candidate objects (or items). Each object has a positive weight, and if selected, generates an object profit and a pairwise profit with any other selected object. The purpose of QKP is to select a subset of objects to fill the knapsack so as to maximize the overall profit while the total weight of the selected objects does not exceed the knapsack capacity.

<sup>9</sup> Formally, let c be the knapsack capacity and  $N = \{1, 2, ..., n\}$  the set of <sup>10</sup> objects. Let  $p_{ii}$  be the profit of object  $i \ (i \in N)$ ,  $w_i$  be its weight. For each <sup>11</sup> pair of objects i and  $j \ (1 \le i \ne j \le n)$ ,  $p_{ij}$  denotes the pairwise profit <sup>12</sup> which is added to the total profit only when both objects are selected. Let  $x_i$ <sup>13</sup>  $(1 \le i \le n)$  be the decision variables such that  $x_i = 1$  if object i is selected, <sup>14</sup>  $x_i = 0$  otherwise. Then QKP can be formulated as follows:

Maximize 
$$f(x) = \sum_{i=1}^{n} \sum_{j=i}^{n} p_{ij} x_i x_j$$
 (1)

subject to:

$$\sum_{j=1}^{n} w_j x_j \le c \tag{2}$$

$$x \in \{0,1\}^n \tag{3}$$

QKP can be reduced to the classical knapsack problem (KP) by restricting the 15 pairwise profit  $p_{ij}$  to 0 for all  $1 \le i \ne j \le n$  and thus generalizes KP. From 16 a graph-theoretic view of point, QKP is also a generalization of the Clique 17 problem [6, 28]. From the perspective of computational complexity, QKP is 18 NP-hard in the strong sense [6]. It is also tightly related to other challenging 19 problems (e.g., edge-weighted maximum clique [9] and weighted maximum b-20 clique [27]), and appears as a column generation sub-problem when solving 21 the graph partitioning problem [22]. In addition to its theoretical importance, 22 QKP is capable of formulating a number of practical applications [28] like 23 satellite site selection in telecommunications, locations of airports and railway 24 stations in logistics and compiler design. 25

QKP is well studied in the literature. Over the last decades, much effort has been devoted to developing exact algorithms. Most of these algorithms are based on the general branch-and-bound (B&B) framework. In this context, many useful techniques were introduced including upper planes [14], Lagrangian relaxation [2,6], linearization [1,22], semidefinite programming [21]. The progress made on exact methods continually enlarged the class of QKP instances that can be solved optimally. Among state-of-the-art exact approaches, the B&B algorithm introduced in [29] is probably one of the most successful 1 methods which uses aggressive problem reduction techniques. Today's stateof-the-art exact methods are able to solve instances with up to 1500 variables. 3

On the other hand, to handle problems whose optimal solutions cannot be 4 reached by an exact algorithm, heuristics constitute a useful and complemen-5 tary approach which aims to find sub-optimal solutions as good as possible to 6 large problems within a reasonable time. Existing QKP heuristic methods can 7 be classified into two categories, namely the randomized or stochastic heuris-8 tics (which use random choices in their search components) and deterministic 9 heuristics (which, given a particular input, always produce the same output). 10 Representative randomized heuristic approaches for QKP include three greedy, 11 genetic and greedy genetic algorithms [23], a Mini-Swarm algorithm [35], and a 12 GRASP-tabu search algorithm [37]. Typical deterministic heuristic approaches 13 include an upper plane based heuristic [14], a greedy constructive heuristic [5], 14 a hybrid method [1] combining the greedy heuristic of [5] and the "fill-up and 15 exchange" procedure of [14], a linearization and exchange heuristic [20] and 16 a dynamic programming heuristic [12]. Different from the methods dealing 17 directly with QKP, the approach of [18] reformulates it as an unconstrained 18 binary quadratic problem (UBQP) and applies a tabu search algorithm de-19 signed for UBQP to solve the reformulated model. Among the aforementioned 20 heuristics, the Mini-Swarm algorithm [35], the GRASP-tabu search algorithm 21 of [37] and the very recent dynamic programming heuristic of [12] are the 22 state-of-the-art approaches which are used as our references for performance 23 assessment and comparisons. Finally, several approximation algorithms can 24 be found in [24, 36]. For a comprehensive survey of different solution methods 25 prior to 2007, the reader is referred to [28]. 26

One observes that, compared to the research effort on exact algorithms which 27 has taken place for a long time, studies on heuristics for QKP are more recent 28 and less abundant. In this work, we are interested in solving large scale QKP 29 instances approximately and present an effective heuristic approach which 30 explores the idea of searching over promising hyperplanes. The proposed ap-31 proach basically introduces an additional cardinality constraint to the original 32 model to prune regions of the search space where no optimal solution exists. 33 Such an idea proved to be very useful for designing effective heuristics for the 34 multidimensional knapsack problem [4,11,32]. Similar ideas were also explored 35 as a type of "generalized branching" [30] or "constraint branching" [13] within 36 the general B&B framework. In this work, we adapt for the first time the idea 37 of hyperplane exploration in the context of QKP. For this purpose, we address 38 two relevant issues which are critical to make our approach successful. First, 39 we need to identify the promising hyperplanes which are likely to contain high 40 quality solutions. Second, we want to search efficiently inside the identified hy-41 perplanes since each hyperplane, though already much reduced relative to the 42 original model, may still contain a very large number of candidate solutions. 43 <sup>1</sup> Based on the above considerations, our proposed iterated "hyperplane explo-

<sup>2</sup> ration" algorithm (IHEA) for QKP makes two original contributions.

• From the algorithmic perspectives, we present for the first time a decom-3 position approach for solving QKP. By introducing the cardinality con-Δ straint, IHEA divides the initial problem into several disjoint hyperplane-5 constrained sub-problems and focuses its exploration within the most promis-6 ing hyperplanes while discarding unpromising sub-problems. To further re-7 duce the search space of each hyperplane-constrained problem, IHEA uses 8 specific rules to fix a large number of variables. To seek high quality so-9 lutions within each reduced sub-problem, IHEA employs a dedicated tabu 10 search procedure which is able to tunnel through infeasible regions to facili-11 tate transition between structurally different feasible solutions. An informed 12 perturbation strategy is also applied to establish a global form of diversifi-13 cation and thereby to allow examining additional unexplored hyperplanes. 14 From the perspective of computational results, the proposed IHEA approach 15 • displays very competitive performances on three groups of 220 benchmark 16 instances. Particularly, it is able to attain easily all the optimal solutions 17 with a 100% success rate for the first group of 100 instances with up to 18 300 objects. For the second group of 80 larger instances with 1000 to 2000 19 objects, IHEA provides improved best results for 6 instances (new lower 20 bounds) and attains the best known results for the remaining cases. We 21 also report results for a third group of very large instances with up to 6000 22 variables for which our approach achieves an average gap of less than 1.359% 23

between the best lower bound and the well-known upper bound  $\hat{U}_{CPT}^2$  [6].

The rest of the paper is organized as follows. Section 2 describes the proposed approach. Section 3 presents an extensive computational assessment in comparison with the state-of-the-art approaches and reports new results for a set of very large-sized instances. Section 4 studies some key ingredients of the proposed approach. Conclusions are drawn in Section 5.

## <sup>30</sup> 2 Iterated "hyperplane exploration" algorithm for QKP

- <sup>31</sup> In this section, we present our iterated "hyperplane exploration" algorithm for
- $_{\rm 32}~$  QKP. We begin with some useful notations and definitions, and then present
- <sup>33</sup> the main components of the proposed approach.

For a precise presentation of the IHEA algorithm, the following notations and definitions are first introduced.

- Given a solution  $x \in \{0,1\}^n$  of a QKP instance P,  $I_1(x)$  and  $I_0(x)$  denote respectively the index set of variables receiving the value of 1 and 0 in x;
- Given a solution  $x \in \{0,1\}^n$  of a QKP instance  $P, \sigma(x)$  denotes the sum of the values of all variables in x (i.e.,  $\sigma(x) = |I_1(x)|$ ).
- Given two solutions  $x \in \{0,1\}^n$  and  $x' \in \{0,1\}^n$ ,  $|x,x'| = \sum_{j=1}^n |x_j x'_j|$ 8 9

denotes the Hamming distance between x and x'.

- Function  $f_r(x)$  calculates a raw objective value of solution  $x \in \{0,1\}^n$  which 10 could be either feasible or infeasible with respect to the capacity constraint. 11

**Definition 1** Given a solution  $x \in \{0, 1\}^n$ , the contribution of object  $i \ (i \in \mathbb{R})$ 12 N) to the objective value with respect to x is given by: 13

$$C(i,x) = p_{ii} + \sum_{j \in I_1(x), j \neq i} p_{ij}$$
(4)

**Definition 2** Given a solution  $x \in \{0,1\}^n$ , the density of object  $i \ (i \in N)$ 14 with respect to x is given by: 15

$$D(i,x) = C(i,x)/w_i \tag{5}$$

**Definition 3** A constrained QKP with a k dimensional hyperplane constraint 16 is defined as: 17

$$CQKP[k] = \begin{cases} \max \sum_{i=1}^{n} \sum_{j=i}^{n} p_{ij} x_i x_j \\ s.t. \\ \sum_{j=1}^{n} w_j x_j \le c \\ \sum_{j=1}^{n} x_j = k \\ x \in \{0,1\}^n \end{cases}$$
(6)

where  $\sum_{j=1}^{n} x_j = k$  is a hyperplane constraint which restricts the solution space 18 of QKP in the k dimensional hyperplane. Each feasible solution of problem 19 CQKP[k] has exactly k selected objects. 20

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Note that the notion of contribution C(i, x) (Definition 1) is related to the 1 upper planes of [14] with two notable differences. First, C(i, x) involves both 2 a problem instance and a solution x while an upper plane only depends on 3 the problem instance (and is independent of any solution). Second, an upper 4 plane can be used to produce an upper bound for QKP while C(i, x) does not have such a utility. In our work, C(i, x) is used as an indicator to evaluate the contribution of a particular item i to the total profit with respect to the 7 given solution x. This indicator allows us to dynamically identify the most profitable item (according to the search state) to be included into the current 9 solution in order to maximize the total profit. 10

## 11 2.2 General idea of the "hyperplane exploration" algorithm

<sup>12</sup> Let CQKP[k]  $(1 \le k \le n)$  be a constrained QKP (see Definition 3), it is <sup>13</sup> obvious that its solution space is a subspace of the original QKP. Therefore, <sup>14</sup> any feasible solution of the CQKP[k]  $(1 \le k \le n)$  is also a feasible solution <sup>15</sup> of the original QKP. Let  $\Omega^F$  be the feasible solution space of a QKP instance <sup>16</sup> such that:

17 
$$\Omega^F = \{x \in \{0,1\}^n : \sum_{j=1}^n w_j x_j \le c\},\$$

Then the feasible solution space of the constrained QKP with a k dimensional hyperplane constraint (CQKP[k]) is given by:

20 
$$\Omega_{[k]} = \{ x \in \Omega^F : \sigma(x) = k \}$$

<sup>21</sup> QKP can be decomposed into *n* independent sub-problems (constrained QKPs): <sup>22</sup> CQKP[1], CQKP[2], ..., CQKP[n]. These *n* sub-problems represent *n* disjoint <sup>23</sup> subspaces and the feasible solution space of QKP is the union of the solution <sup>24</sup> space of all its sub-problems, i.e.,  $\Omega^F = \bigcup_{k=1}^n \Omega_{[k]}$ .

For QKP, if items are sorted in non-decreasing order according to their weight 25  $w_j \ (j \in N)$ , there must exist only one positive integer  $k_{UB}$  simultaneously ver-26 ifying the following two constraints: 1)  $\sum_{j=1}^{k_{UB}} w_j \le c, 2$ )  $\sum_{j=1}^{k_{UB}+1} w_j > c$ ; similarly, if 27 items are sorted in non-increasing order according to their weight  $w_i$   $(j \in N)$ , 28 there must be only one positive integer  $k_{LB}$  simultaneously verifying the fol-29 lowing two constraints: 1)  $\sum_{j=1}^{k_{LB}} w_j \le c, 2$ )  $\sum_{j=1}^{k_{LB}+1} w_j > c$ . Following the literature 30 like [1, 2, 6, 14, 28, 29], we assume non-negative entries in the profit matrix. 31 Notice that the existing QKP benchmark instances follow this assumption. 32 This leads to the following proposition. 33

<sup>34</sup> **Proposition 1.** There must exist optimal solutions of QKP in hyperplanes

whose dimensions satisfy:  $k_{LB} \leq k \leq k_{UB}$ .

**Proof.** Given a feasible solution  $x^1 \in \Omega_{[k_1]}$   $(0 < k_1 < k_{LB})$ , and a feasible 2 solution  $x^2 \in \Omega_{[k_2]}$   $(k_{LB} \leq k_2 \leq k_{UB}, k_1 < k_2)$  which is obtained by including another  $(k_2 - k_1)$  unselected items to  $x^1$ . Then  $x^2$  and  $x^1$  have  $k_1$  selected items 3 4 in common. Since  $(k_2 - k_1) \geq 1$ , and the contribution of any selected item in  $x^2$ 5 is greater than or equal to 0, we have:  $f(x^2) \ge f(x^1)$ . Consequently, there must 6 exist solutions in  $\bigcup_{k=k_{LB}}^{k_{UB}} \Omega_{[k]}$  whose objective value is greater than or equal to 7 the objective value of the best solution in  $\bigcup_{k=1}^{k_{LB}-1} \Omega_{[k]}$ . On the other hand, 8  $k_{UB}$  is the maximum number of items that can be contained in the knapsack 9 which means any solution in hyperplanes with a dimension greater than  $k_{UB}$ 10 is infeasible. Therefore, no feasible solution in  $\cup_{k=k_{UB}+1}^{n}\Omega_{[k]}$  has an objective 11 value better than the objective value of the best solution in  $\bigcup_{k=k_{IB}}^{k_{UB}} \Omega_{[k]}$ .  $\Box$ 12

To make an effective search, we can focus on hyperplanes with a dimension <sup>13</sup> k within the interval  $[k_{LB}, k_{UB}]$  and definitely discard other subspaces<sup>1</sup>. This <sup>14</sup> leads to a first (and large) reduction of the solution space from  $\bigcup_{k=1}^{n} \Omega_{[k]}$  to <sup>15</sup>  $\bigcup_{k=k_{LB}}^{k_{UB}} \Omega_{[k]}$ . <sup>16</sup>

However, the remaining search space  $\bigcup_{k=k_{LB}}^{k_{UB}} \Omega_{[k]}$  could still be too large to be explored efficiently, especially when the gap between  $k_{LB}$  and  $k_{UB}$  is large which is typically the general case (see Section 4.1). In order to further prune some less-promising solution spaces, we explore the hypothesis that high quality solutions are located in a set of "promising" hyperplanes whose dimensions are close to  $k_{UB}$ . This hypothesis is confirmed by the experimental results presented in Section 3 and Section 4.1.

Based on the above hypothesis, the general idea of our IHEA approach is to 24 progressively and intensively explore a small number of "interesting" hyper-25 planes whose dimensions are close to  $k_{UB}$  so that a large subspace is effectively 26 pruned and the search effort is more focused. We carry out the hyperplane ex-27 ploration in increasing order of their dimensions aiming to identify solutions 28 of increasing quality, and restart this process with a perturbation when no 29 improvement can be found. When the search seems to stagnate in one hyper-30 plane, we seek better solutions in a higher dimensional hyperplane. To explore 31 a given hyperplane, additional variable fixing techniques are applied to fix a 32 number of variables so as to further shrink the subspace to be examined. 33

<sup>&</sup>lt;sup>1</sup> In case an optimal solution exists in a hyperplane with a dimension  $k < k_{LB}$ , an optimal solution  $x^*$  identified in  $k \in [k_{LB}, k_{UB}]$  must include items with zero contribution. In a practical situation where the (positive) weight of an item represents a cost, an additional step is required to remove from  $x^*$  the zero contribution items.

#### <sup>1</sup> 2.3 General procedure of the "hyperplane exploration" algorithm

<sup>2</sup> Our iterated "hyperplane exploration" approach is composed of three steps:

(1) Construct an initial high quality solution  $x^0$  and use  $\sigma(x^0)$  to determine the starting dimension of the "promising" hyperplanes; ( $\sigma(x^0) \in [k_{LB}, k_{UB}]$  and  $\sigma(x^0)$  is close to  $k_{UB}$ )

- 6 (2) For each hyperplane dimension  $k = \sigma(x^0), \sigma(x^0) + 1, \sigma(x^0) + 2...$ , execute 7 the following three steps:
  - a. Construct a constrained problem CQKP[k];

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- b. Identify some variables that are very likely to be part of the optimal solution, fix these variables to 1 and remove them from CQKP[k], leading to a reduced constrained problem CQKP'[k];
- c. Run a hyperplane exploration algorithm to solve CQKP'[k]. In our case, we employ a search procedure based on tabu search [16] to find a high quality solution within the current search space  $\Omega_{[k]}$ . If this solution improves on the best feasible solution found in previous hyperplanes, we move to the next hyperplane; otherwise we skip to step (3).

(3) Apply a perturbation to restart the search from a new starting point. This perturbation (removing some specifically selected items) typically displaces the search from the current hyperplane to a lower dimensional hyperplane which introduces a possibility to visit more not-explored-yet search spaces (e.g., hyperplanes with a dimension lower than  $\sigma(x^0)$ ) where high quality solutions might exist (though with a small probability).

Algorithm 1 shows the pseudo-code of the IHEA algorithm for QKP, whose 23 components are detailed in the following sections. At the very beginning, an 24 initial solution is generated by a greedy randomized construction procedure 25 (Section 2.4.1) and is further improved by a descent procedure (Section 2.4.2). 26 Then, the initial dimension of the hyperplane as well as the first constrained 27 problem are determined from the initial solution. From this point, the al-28 gorithm enters the "hyperplane exploration" phase which examines a series 29 of hyperplane constrained QKP problems. At each iteration of the 'while' 30 loop, IHEA first applies specific variable fixing rules to construct a reduced 31 constrained problem  $RCP(V_{fixed}, CQKP[k], x')$  where  $V_{fixed}$  contains a set of fixed variables (Section 2.5).  $RCP(V_{fixed}, CQKP[k], x')$  is then solved by 32 33 the tabu search procedure (Section 2.6). Each time a better solution  $x_{[k]}^*$  is 34 discovered (i.e.,  $f(x_{[k])}^* > f(x^b)$ ) by tabu search, IHEA updates the best solu-35 tion found  $x^{b}$  and moves on to solve another constrained problem in a higher 36 dimensional hyperplane. To do this, the algorithm increments k by one and 37 reinitializes x' by randomly adding one unselected item to  $x^b$ . The 'while' loop 38 terminates when no improving solution can be found. The global best solution 39 is updated at the end of the 'while' loop. IHEA then makes some dedicated 40 changes (perturbations) to  $x^b$ , improves the perturbed solution (with the de-41

scent procedure) to a local optimum, and use the local optimum to start a new round of the "hyperplane exploration" procedure. The above whole procedure continues until a maximum number of allowed iterations is reached.

Algorithm 1 Pseudo-code of the IHEA algorithm for QKP.

1: Input: P: an instance of the QKP; L: size of running list; rcl: max allowed size of restricted candidate list; MaxIter: max number of iterations; **Output**: the best solution  $x^*$  found so far 2: 3:  $x^0 \leftarrow Greedy\_Randomized\_Construction(rcl)$ 4:  $x^0 \leftarrow Descent(x^0)$ 5:  $x' \leftarrow x^0 / * x'$  represents the current solution \*/ 6:  $Iter \leftarrow 0' / *$  Iteration counter \*/ 7:  $x^b \leftarrow x'$  /\*  $x^b$  records the best solution found in current iteration \*/ 8:  $x^* \leftarrow x^{b'}/{}^* x^*$  records the global best solution \*/ 9: repeat  $SolutionImproved \leftarrow true$ 10:  $k \leftarrow \sigma(x')$ 11: 12: Construct constrained problem CQKP[k]13: /\* "hyperplane exploration" phase \*/ while SolutionImproved do 14:  $V_{fixed} \leftarrow Determine\_Fixed\_Variables(k, x')$ 15: Construct reduced constrained problem  $RCP(V_{fixed}, CQKP[k], x')$ 16: Run  $TabuSearch\_Engine(L, x', x^b)$  to solve  $RCP(V_{fixed}, CQKP[k], x')$  and 17: keep a best solution  $x_{[k]}^*$ if  $f(x_{[k]}^*) > f(x^b)$  then 18:  $x^b \leftarrow x^*_{[k]}$ 19:  $k \leftarrow k + 1$ 20:  $x' \leftarrow \mathsf{Randomly} \ \mathsf{add} \ \mathsf{one} \ \mathsf{item} \ \mathsf{to} \ x^b$ 21: 22: Construct constrained problem CQKP[k]23: else 24:  $SolutionImproved \leftarrow false$ 25: 26: end if end while if  $f(x^b) > f(x^*)$  then 27:  $x^* \leftarrow x^b$ 28: 29: end if 30: /\* Perturbation phase \*/  $x' \leftarrow Perturbation(x^b, Iter)$ 31:  $x' \leftarrow Descent(x')$ 32:  $x^{b} \leftarrow x'$ 33:  $\tilde{I}ter \leftarrow Iter + 1$ 34: 35: until Iter > MaxIter

### 2.4 Initial solution

IHEA constructs an initial solution according to a greedy randomized constructive heuristic. In order to place the initial solution in a "good" hyperplane, we additionally improve the constructed solution with a descent procedure. In this section, we explain these two procedures.

#### 1 2.4.1 Greedy randomized construction procedure

Our greedy randomized construction procedure follows the spirit of the GRASP approach [10] which has been investigated in [37] to solve QKP. Different from [37] where the construction procedure is used as the main search algorithm, our IHEA algorithm uses this construction procedure to obtain an initial solution.

<sup>7</sup> Starting from a partial solution x where all items are set unselected initially, <sup>8</sup> the construction procedure iteratively and adaptively selects some items to be <sup>9</sup> included in x (i.e., the corresponding variables receive the value of 1) while <sup>10</sup> maintaining the solution feasibility. At each iteration, we randomly select one <sup>11</sup> unselected item from a restricted candidate list *RCL* and add the item to the <sup>12</sup> partial solution.

Let  $R(x) = \{i \in I_0(x) : w_i + \sum_{j \in I_1(x)} w_j \leq c\}$  be the set of unselected items that can fit into the knapsack with respect to x. Let rcl be the maximum size of the restricted candidate list. Then RCL contains  $min\{rcl, |R(x)|\}$  unselected items which have the largest *density* values (Section 2.1) and do not violate the capacity constraint when any of them is included to the current partial solution x. Formally,  $\forall i \in RCL$ , the following two conditions hold: 1)  $i \in R(x)$ , 2)  $D(i, x) \geq D(j, x)$  ( $\forall j \in I_0(x) \setminus RCL$ ).

The items in RCL are ranked according to their *density* values and the  $r^{th}$ ( $1 \leq r \leq |RCL|$ ) ranked item is associated with a bias  $b_r = 1/e^r$ . Thus, the  $r^{th}$  item is selected with a probability p(r) which is calculated as:  $p(r) = b_r / \sum_{j=1}^{|RCL|} b_j$ . Once an item is selected and added to the partial solution x, RCL is updated as well as the objective value of the partial solution. This procedure repeats until RCL becomes empty.

One notices that the initial solution constructed by this greedy randomized procedure must be in a hyperplane whose dimension is not smaller than  $k_{LB}$ since it is a tight packing plan that cannot include any more unselected item, and not greater than  $k_{UB}$  since it is a feasible solution. Also, this dimension is experimentally proved to be close to  $k_{UB}$  (see Section 4.1). The underlying reason is that items with a small weight are biased towards being selected to join the knapsack.

#### 33 2.4.2 Descent procedure

Starting from a solution generated through the greedy randomized construction procedure, IHEA uses a descent procedure to reach a local optimum (The descent procedure is also applied after a perturbation, see Section 2.7). This
descent procedure helps: 1) to generate a promising hyperplane which may contain high quality solutions; 2) to improve the quality of the initial solution

which allows the hyperplane exploration to start from a high platform.

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Our descent procedure jointly employs two different neighborhoods defined by two basic move operators: *ADD* and *SWAP*.

- ADD(i): This move operator adds an unselected item  $i \ (i \in I_0(x))$  to a given solution x. It can be considered as a special case of *FLIP* used in [37] by restricting the flipped variables to those having the value of 0 in the given solution.  $N_A$  denotes the neighborhood induced by the ADD operator, and  $N_A^F$  is a subset of  $N_A$  that contains only feasible neighbor solutions.
- SWAP(i, j): Given a solution x, SWAP(i, j) exchanges an unselected item  $i \ (i \in I_0(x))$  with a selected item j of  $x \ (j \in I_1(x))$ . This operator is commonly used in the existing QKP approaches [1,37]. A SWAP operation can be realized as two consecutive FLIP operations where one is to flip a variable from 0 to 1 and the other is to flip another variable from 1 to 0.  $N_S$  denotes the neighborhood induced by the SWAP operator, and  $N_S^F$  is a subset of  $N_S$  that contains only feasible neighbor solutions.

The aim of the descent procedure is to attain a local optimum (as good as possible) in both neighborhoods  $N_A^F$  and  $N_S^F$  starting from a solution x (either possible) in both neighborhoods  $N_A^F$  and  $N_S^F$  starting from a solution x (either procedure). To this end, the algorithm iteratively explores  $N_A^F$  and  $N_S^F$  in a token-ring way  $N_A^F \to N_S^F \to N_A^F \to N_S^F$ .... For each iteration, a feasible neighbor solution x' is picked at random from the neighborhood under consideration and replaces the incumbent solution x if x' is better than x (i.e., f(x') > f(x)).

It should be noted that our descent procedure is different from the "fill-up and exchange" procedure of [14] which also relies on ADD and SWAP. Our descent procedure examines neighbor solutions in random order and accepts the first encountered improving neighbor while the "fill-up and exchange" procedure checks neighbor solutions in a deterministic way. Moreover, our descent procedure explores  $N_A^F$  and  $N_S^F$  in a token-ring way while the "fill-up and exchange" process explores these neighborhoods in a sequential way.

#### 2.5 Variable fixing and problem reduction

By adding a hyperplane constraint  $\sigma(x) = k$  to QKP, the induced con-31 strained problem CQKP[k] removes a large part of the solution space (of 32 order  $O(2^n - C_n^k)$  from the original QKP. However, the solution space of 33 the constrained problem CQKP[k] might still be too large to be efficiently 34 searched by an algorithm. Indeed, as we employ a search algorithm which ex-35 plores both feasible and infeasible solutions (see Section 2.6), CQKP[k] has 36 a search space of  $2^k$  where k, though smaller than n, could still be large. To 37 further reduce the search space to explore, we fix some variables in CQKP[k]. 38

Recall that in Algorithm 1, the starting solution x' of  $TabuSearch\_Engine$  for solving each constrained problem CQKP[k] is modified from the best solution  $x^b$  such that x' and  $x^b$  are either the same in the first hyperplane (see Line of Algorithm 1) or different only in one variable (see Line 21 of Algorithm 1). For each CQKP[k], based on x', our variable fixing step tries to identify a set of variables  $V_{fixed}$  that are highly likely to be part of the optimal solution and fixes them to the value of 1. We then remove these variables (these variables are said fixed) from CQKP[k], leading to a reduced constrained problem  $RCP(V_{fixed}, CQKP[k], x')$ .

In order to limit the risk of fixing wrong variables, we follow the general idea 10 of identifying a set of "strongly determined" variables [15]. For this purpose, 11 we make use of information from the *density* value associated with each item. 12 According to the definition presented in Section 2.1, for those selected items 13 in a given solution, the *density* of an item represents its contribution (profit) 14 per weight unit. Thus, the *density* value is a good indicator of the importance 15 of a selected item. Given a QKP solution  $x' \in \{0,1\}^n$ , our variable fixing rules 16 can be summarized as a three-step method: 17

(1) For each variable  $x'_i$  such that  $i \in I_1(x')$ , calculate its *density* value D(i, x');

20 (2) Sort all variables in  $I_1(x')$  in non-increasing order according to their 21 density values D(i, x')  $(i \in I_1(x'))$ , leading to a sorted index set  $SI_1(x')$ ; 22 (3) Extract the first  $n_f$  variables in  $SI_1(x')$  to form the fixed variable set 23  $V_{fixed}$   $(n_f$  is the number of fixed variables, i.e.,  $n_f = |V_{fixed}|)$ . Fix the 24 variables in  $V_{fixed}$  with the value of 1, leading to a reduced constrained 25 problem  $RCP(V_{fixed}, CQKP[k], x')$  whose variable set is  $(I_1(x') \setminus V_{fixed}) \cup$ 26  $I_0(x')$ .

<sup>27</sup> In the last step,  $n_f$  is determined using the following empirical formula:

$$n_f = k_{LB} + max\{(|I_1(x')| - k_{LB}) * (1 - 1/(0.008 * n)), 0\}$$
(7)

where  $k_{LB}$  is the minimum number of items that can be contained in the knapsack. Typically,  $|I_1(x')|$  is larger than  $k_{LB}$ . It is easy to understand that a solution with only  $k_{LB}$  selected items is unlikely to be a good solution since the packing plan is not tight enough. The number of items that can be fixed  $(n_f)$  is specified by formula (7).

Formula (7) was identified in the following manner. We first obtained optimal solutions for a set of instances of different sizes (ranging from n = 100 to 500) with the exact solver of [6]. We also obtained a set of near-optimal solutions provided by our solution initialization procedure of Section 2.4. We sorted the selected items of the near-optimal solutions according to their density values, and then compared them to the optimal solutions. Finally, we arrived 1 at the following observations: 1) the number of items that can be fixed  $(n_f)$  2 is somewhere between  $k_{LB}$  and  $|I_1(x')|$ ; 2) the number of items that can be 3 fixed enlarges as the size of the instance increases. The design of formula (7) 4 basically integrates these observations. 5

Note that different strategies for temporary or definitive variable fixing were 6 explored in [2] for QKP and studied in other contexts like 0-1 mixed integer 7 programming, integer linear programming and binary quadratic programming 8 [7, 33, 34]. Moreover, the notion of item density was previously used in other 9 construction procedures [5,37]. For instance, from the set of given items, the 10 greedy construction procedure in [5] drops iteratively the "lightest" items one 11 by one until the remaining items form a feasible solution (i.e., the knapsack 12 constraint becomes satisfied). Furthermore, unlike our procedure where the 13 density of each item is calculated only once, the procedure of [5] updates, 14 after each iteration, the density value of each remaining item. 15

## 2.6 Hyperplane exploration with tabu search

The tabu search procedure  $(TabuSearch\_Engine)$  described in this section is designed to solve the reduced constrained problem  $RCP(V_{fixed}, CQKP[k], x')$ , i.e., identify feasible solutions that are better than  $x^b$  which is the current best solution found in the current course of the "hyperplane exploration" procedure. The key ingredients of  $TabuSearch\_Engine$  are described as follows. 21

- Neighborhood: It is known that allowing a controlled exploration of in-22 feasible solutions may enhance the performance of a heuristic search al-23 gorithm, by facilitating transitions between structurally different feasible 24 solutions [17]. Following this idea, we employ the  $N_S$  neighborhood (de-25 fined in Section 2.4.2) which contains both feasible and infeasible neighbor 26 solutions. In order to explore effectively the search space of a given hy-27 perplane, we restrict our tabu search procedure to visit solutions that are 28 considered better than the best feasible solution found so far, leading to 29 a restricted SWAP neighborhood  $N_S^R$ . Precisely, given the objective value 30 of the current best feasible solution with objective value  $f_{min}$ , the neigh-31 borhood  $N_S^R(x)$  of a solution x (either feasible or infeasible) is defined as: 32  $N_S^R(x) = \{x' \in N_S(x) : f_r(x') > f_{min}\}$  where  $f_r$  is the raw objective value. 33
- Tabu list management: We use the reverse elimination method (*REM*) <sup>34</sup> introduced in [16] for our tabu list management. *REM* defines an exact tabu <sup>35</sup> mechanism which prevents any visited solution from being revisited. *REM* <sup>36</sup> uses a *running list* to store the attributes of all implemented moves. One can <sup>37</sup> trace back the *running list* to identify the tabu status of a move by making <sup>38</sup> use of another list called residual cancellation sequence (*RCS*) where an <sup>39</sup>

- attribute is either added if it is not yet in the RCS or removed from RCSotherwise. Interested readers are referred to [8,16,32] for more details on this
- <sup>3</sup> method. For the *SWAP* operator used by *TabuSearch\_Engine*, when there
- are only two attributes left in RCS (i.e., |RCS| = 2), the move composed
- <sup>5</sup> of these two attributes is declared tabu in the next iteration. The procedure
- <sup>6</sup> of updating the tabu status is described in Algorithm 2.
- Evaluation function: The evaluation function used by *TabuSearch\_Engine*
- s considers two factors to assess a solution x: 1) raw objective value  $f_r(x)$ , 2)
- <sup>9</sup> capacity violation  $v_c(x) = c \sum_{j=1}^n w_j x_j$ . A transition is made from the current
- solution x to a neighbor solution  $x' \in N_S^R(x)$  if  $\forall x'' \in (N_S^R(x) \setminus \{x'\}), x'$  veri-
- fies one of the following two conditions: 1)  $v_c(x') < v_c(x''), 2$   $v_c(x') = v_c(x'')$ and  $f_r(x') \ge f_r(x'')$ .

Algorithm 2 presents the pseudo-code of *TabuSearch\_Engine* which takes 13 three elements as its input: 1) the max size of the running list which serves as 14 the termination condition; 2) an initial solution (feasible or unfeasible) which 15 serves as its starting point; 3) a reference feasible solution  $x^{ref}$  which restricts 16 the search to visit solutions whose objective value is better than that of  $x^{ref}$ . 17 At each iteration, the algorithm identifies the best non-tabu SWAP move 18 relative to the above evaluation function, and applies the move to obtain a 19 new solution. Each time a feasible solution is discovered (i.e.,  $v_{min} = 0$ ), the 20 running list is reset and  $f_{min}$  is updated. TabuSearch\_Engine terminates if 21 one of the following two conditions is verified: 1) all moves are tabu, i.e., 22  $v_{min} = \infty$ ; 2) the running list is full, i.e.,  $erl \ge L$ . 23

<sup>24</sup> Note that tabu search was also used in [37] to enhance a GRASP procedure.

- <sup>25</sup> However, these two studies are quite different. First, our general IHEA ap-
- <sup>26</sup> proach focuses on decomposing the initial solution space into a set of hyperplane-
- <sup>27</sup> constrained and reduced solution spaces while GRASP+tabu of [37] explores
- <sup>28</sup> the original solution space. Second, our tabu search procedure is dedicated to
- <sup>29</sup> effectively explore the solution space of a hyperplane-constrained sub-problem.
- As such, its design (in terms of neighborhood, tabu list management and evaluation function) is different from GRASP+tabu. Third, our tabu search ex-
- <sup>32</sup> plores both feasible and infeasible solutions while GRASP+tabu only visits
- <sup>1</sup><sup>33</sup> feasible solutions. Compared to the approach of [18], their tabu search al-
- <sup>34</sup> gorithm was dedicated to the unconstrained binary quadratic problem and
- <sup>35</sup> operates with the "one-flip" move operator (called "shift" in [37]) which adds
- <sup>36</sup> or removes an item (SWAP was not used).

Algorithm 2 Pseudo-code of TabuSearch\_Engine

```
1: Input: L: max size of running list; x^{in}: an initial solution; x^{ref}: a reference
      feasible solution
 2: Output: the best feasible solution found so far x^*
 3: |RL| \leftarrow L /* Initialize the size of running list to L * /
 4: f_{min} \leftarrow f(x^{ref}) / * f_{min} records the objective value of the current best feasible
     solution */
 5: x^* \leftarrow x^{ref} / x^* records the best feasible solution found so far */
 \begin{array}{ccc} 6: \ erl \leftarrow 0 \\ 7: \ x \leftarrow x^{in} \end{array}
 8: while v_{min} \neq \infty \lor erl < L do
 9:
         (v_{min}, f_{max}) \leftarrow (\infty, -\infty)
10:
         for each i \in I_0(x) do
11:
            for each j \in I_1(x) do
                if tabu[i][j] \neq iter then
12:
13:
                    (x_i, x_j) \leftarrow (1, 0)
14:
                   if (f_r(x) > f_{min}) \land ((v_c(x) < v_{min}) \lor ((v_c(x) = v_{min}) \land (f_r(x) \ge f_{max})))
                   \mathbf{then}
                       (i^*, j^*) \leftarrow (i, j); (v_{min}, f_{max}) \leftarrow (v_c(x), f_r(x))
15:
16:
                    end if
                    (x_i, x_j) \leftarrow (0, 1)
17:
                end if
18:
19:
            end for
20:
         end for
         if v_{min} \neq \infty then
\bar{2}1:
22:
             (x_{i^*}, x_{j^*}) \leftarrow (1, 0)
23:
            if v_{min} = 0 then
24:
                erl \leftarrow 0; f_{min} \leftarrow f_r(x); x^* \leftarrow x
25:
26:
            else
                iter \leftarrow iter + 1; RL \leftarrow RL \cup \{i^*\} \cup \{j^*\}; erl \leftarrow erl + 2
                /* UPDATE TABU STATUS*/
27:
                i \leftarrow (erl - 1)
                while i \ge 0 do
28:
                    j \leftarrow R\overline{L}[i]
29:
30:
                   if j \in RCS then
31:
                       RCS \leftarrow RCS \setminus \{j\}
32:
                   else
                       \widetilde{R}CS \leftarrow RCS \cup \{j\}
33:
34:
                    end if
35:
                   if |RCS| = 2 then
36:
                       tabu[RCS[0]][RCS[1]] \leftarrow iter; tabu[RCS[1]][RCS[0]] \leftarrow iter
37:
                   end if
38: 39:
                i \leftarrow i - 1
end while
40:
            end if
41:
         end if
42: end while
```

2.7 Perturbation

To establish a global form of diversification and reinforce the capacity of the algorithm to visit unexplored "promising" hyperplanes, we employ a perturbation strategy to restart the search from a new starting point (usually in a lower dimensional hyperplane w.r.t. the current hyperplane). A perturbation is applied when the hyperplane-based search stagnates, i.e., the local optimum  $x_{[k]}^*$  6

of the current constrained problem CQKP[k] does not improve the best solution found in the current hyperplane exploration phase  $x^b$ . This best solution  $x^b$  could be either the local optimum obtained by the initializing construction procedure (or perturbation procedure) followed by the descent procedure, or the local optimum of the last constrained problem CQKP[k-1]  $(x^*_{[k-1]})$ .

Given a feasible solution x, the general idea of our perturbation strategy is to 6 remove a small number (say s, s > 0) of items which are chosen from t (s  $\leq$  $t \leq (I_1(x) - n_f)$  selected items with the lowest densities and then replace the removed items with some other unselected items. To do this, we first sort all the 9 selected items in x according to the ascending order of their densities D(x,i)10  $(i \in I_1(x))$ . We then remove s items which are selected from the first t sorted 11 items and re-construct the solution using the greedy randomized construction 12 procedure of Section 2.4.1, leading to a perturbed solution. This perturbed 13 solution is further improved by using the descent procedure of Section 2.4.2. 14 The calibration of the parameters t and s is discussed in Section 3.2. 15

<sup>16</sup> To improve the diversification effect of the perturbation, we employ a short-<sup>17</sup> term memory to prevent recently removed items from being added back to <sup>18</sup> the solution in subsequent iterations. Each time an item is removed from the <sup>19</sup> solution, it is not allowed to be inserted to the solution in next rand(1, s)<sup>20</sup> iterations where rand(1, s) takes a random value between 1 and s.

#### 21 2.8 Implementation improvement

A fast incremental evaluation technique was introduced in [14] to determine rapidly the effect of the *ADD* and *SWAP* moves for their "fill-up and exchange" procedure which explores only feasible regions. We slightly extend this technique to make it applicable to evaluate the raw objective values of the new solutions encountered in either feasible or infeasible solution spaces. In addition, we also introduce a fast feasibility checking technique.

Given a solution x, which may be either feasible or infeasible, flipping a vari-28 able  $x_i$  produces a new solution x' whose raw objective value can be con-29 veniently calculated in O(1) time as:  $f_r(x') = f_r(x) + (1 - 2 * x_i) * C(i, x)$ , 30 where C(i, x) is the contribution of variable  $x_i$ . Therefore, any solution gen-31 erated by a move operator which can be realized with constant times of flip 32 operations can be evaluated in O(1) time as well. This is the case for the 33 ADD and SWAP operators which can be realized with one and two flip oper-34 ations respectively. Using this fast evaluation technique leads to a significant 35 acceleration compared to a complete evaluation which requires  $O(n^2)$  time. 36

To achieve this saving, we maintain a memory structure  $\Delta$  to store the current contribution value of each variable  $\Delta_i$  (corresponding to C(i, x) for a given solution x) which is updated each time a flip operation is performed. Given an empty solution where all variables are assigned the value of 0, the contribution of flipping any variable is initialized to its profit value, i.e.,  $\Delta_i \leftarrow p_i, i \in N$ . Thereafter, once a move is performed, the contribution value of each variable after flipping a variable  $x_i$  can be efficiently updated as follows:

$$\Delta_{j} = \begin{cases} \Delta_{j}, & if \quad j = i \\ \Delta_{j} + q_{ij}, & if \quad x_{i} = 1 \quad and \quad j \in N \setminus \{i\} \\ \Delta_{j} - q_{ij}, & if \quad x_{i} = 0 \quad and \quad j \in N \setminus \{i\} \end{cases}$$

$$\tag{8}$$

The total time of updating the structure  $\Delta$  is bounded by O(n). Using this memory structure, a new solution x' transitioned from the current solution  $x_{7}$  by adding an unselected item  $x_i$  can be evaluated using the following equation:

$$f_r(x') = f_r(x) + \Delta_i \tag{9}$$

Similarly, a new solution x' produced by swapping items  $x_i$  ( $x_i = 1$ ) and  $x_j$  ( $x_j = 0$ ) of the current solution x can be evaluated by the following equation:

$$f_r(x') = f_r(x) - \Delta_i + \Delta_j - p_{ij} \tag{10}$$

In addition to  $\Delta$ , we maintain another memory structure which stores the sum of weights of all the selected items in the current solution, which is updated accordingly after an operation is performed. This memory structure allows the capacity constraint checking to be achieved with a time complexity of O(1). 14

#### 3 Computational Experiments

This section is dedicated to a computational assessment of the proposed algorithm and comparisons with the state-of-the-art QKP approaches.

#### 3.1 Experimental protocol

To evaluate the efficiency of the proposed algorithm, we carry out extensive <sup>19</sup> experiments on a set of 220 instances ranging from small to very large sizes. <sup>20</sup> These instances can be divided into three groups: <sup>21</sup>

15

Group I. This group is composed of 100 small and medium sized benchmark 1 instances generated by Billionnet and Soutif [2]. These instances, generated 2 in the same way as in [5, 6, 14, 20], are very popular and used to test many 3 QKP algorithms. These instances are characterized by their number of ob-4 jects  $n \in \{100, 200, 300\}$ , density  $d \in \{25\%, 50\%, 75\%, 100\%\}$  (i.e., number 5 of non-zero coefficients of the objective function divided by n(n+1)/2). Each 6 (n, d) combination involves 10 different instances distinguished by their la-7 bels except for (300,75%) and (300,100%) where instances are missing. Op-8 timal solutions are known for these instances. The instance data files can 9 be downloaded at http://cedric.cnam.fr/~soutif/QKP/QKP.html. 10 Group II. The second group includes 80 large-sized benchmark instances 11

<sup>11</sup> • Group 11. The second group includes do large-sized benchmark instances
<sup>12</sup> which are recently generated by Yang et al. [37]. These instances have a num<sup>13</sup> ber of objects from 1000 to 2000, a value of density from 25% to 100%. Due
<sup>14</sup> to their large size, optimal solutions are still unknown for these instances.
<sup>15</sup> The instance data files are available at http://www.info.univ-angers.
<sup>16</sup> fr/pub/hao/QKP.html

• Group III. This group is composed of 40 new instances of very large sizes that we propose for this study. They are characterized by their number of objects  $n \in \{5000, 6000\}$  and density  $d \in \{25\%, 50\%, 75\%, 100\%\}$ . For each (n, d) combination, 5 instances were proposed. These instances are available from the authors of this work (they are too large to be put on our web).

The above three groups of instances were all generated using the same gener-22 ator that was very popular and commonly used in QKP literature [1, 6, 14, 20]. 23 The parameter settings for the generator are the same as well: the coefficients 24  $p_{ii}$  of the objective function are integers that are uniformly distributed in the 25 interval [0,100]; each weight  $w_i$  is uniformly distributed in [1,50]; the capacity c 26 is randomly selected from  $[50, \sum_{j=1}^{n} w_j]$ . However, to ensure the hardness of the 27 new instances of Group III, we have performed the following selection process. 28 For each instance, we attained the best objective value of ten feasible solu-29 tions, each of which was built by randomly filling the knapsack. A gap between 30 the objective value of the random solution and the best objective value from 31 our IHEA algorithm was then calculated. We denote this gap as randGap. 32 For each (n, d) combination, we generated 10 instances, 5 of which having 33 the largest randGaps were selected to join Group III. The average randGap34 (in percentage) of all instances in Group III is 69.36% which indicates that a 35 randomly generated solution is rather poor. From this perspective, finding a 36 high quality solution for these instances is a non-trivial task. 37

<sup>38</sup> Our IHEA algorithm was coded in C++  $^2$  and compiled by GNU gcc 4.1.2 <sup>39</sup> with the '-O3' option. The experiments were conducted on a computer with <sup>40</sup> an AMD Opteron 4184 processor (2.8GHz and 2GB RAM) running Ubuntu

<sup>&</sup>lt;sup>2</sup> Our best solution certificates are available at: http://www.info.univ-angers.fr/pub/hao/QKPResults.zip.

Para.	Description	Value	Section
rcl	max allowed size of restricted candidate list	20	2.4.1
L	size of the running list	300	2.6
t	size of the least-density items for perturbation	$min\{10, (I_1(x) - n_f)\}$	2.7
s	number of items to be perturbed	$min\{3,t\}$	2.7
MaxIter	max number of iterations	$\sqrt{n}$ +65	2.3

Table 1Parameter settings of the IHEA algorithm

12.04. When running the DIMACS machine benchmark program dfmax.c on graphs r300.5, r400.5 and r500.5 (available at ftp://dimacs.rutgers.edu/ 2 pub/dsj/clique/) (compliled without optimization flag), the run time on our machine is 0.40, 2.50 and 9.55 seconds respectively for these graphs. 4

#### 3.2 Parameter calibration

Our IHEA algorithm relies on five parameters (see Table 1). To calibrate these 6 parameters, we employed an automatic configuration method called Iterated 7 F-race (IFR) [3] which was implemented in the irace package [25]. For each 8 parameter to be tuned, IFR requires a range of values as input. Based on 9 preliminary experiments, we used the range of values as follows:  $rcl \in [10, 30]$ , 10  $L \in [100, 400], p_1 \in [5, 20], \text{ and } p_2 \in [1, 7]. p_1 \text{ and } p_2 \text{ are two parameters}$ 11 associated with t and s, i.e.,  $t = min\{p_1, (I_1(x) - n_f)\}$  and  $s = min\{p_2, t\}$ . 12 We restricted the training set to 26 representative instances: one instance from 13 each (n, d) combination. To run IFR, we used the tuning budget of 3000 IHEA 14 runs, each run being given 50 iterations. Once the previous four parameters 15 are determined, the termination condition parameter MaxIter can be easily 16 tuned by taking into account the balance between quality and efficiency of 17 the IHEA algorithm. The parameter values shown in Table 1 were used in all 18 experiments in the following sections unless otherwise mentioned. 19

#### 3.3 Comparative results on small and medium instances of Group I

Our first experiment was performed on the benchmark instances of Group <sup>21</sup> I. These instances were first solved to optimality by the exact algorithm of <sup>22</sup> [2], with hundreds or thousands of CPU seconds on a 300 MHz Pentium II <sup>23</sup> Processor. Several recent heuristic approaches are able to attain these optimal <sup>24</sup> solutions with much less computing efforts (typically a few seconds) [35, 37]. <sup>25</sup> To evaluate the performance of our IHEA algorithm, three leading heuristic <sup>26</sup> methods were considered for our comparison: <sup>27</sup>

- A Mini-Swarm approach [35]. The experiments reported in [35] were per-

20

Table 2

Scaling factors for the computers used in the reference algorithms. Our computer (AMD Opteron 4184) serves as the basis.

Algorithm	Reference	Processor type	Frequency (GHz)	Factor
IHEA	-	AMD Opteron 4184	2.8	1.0
Min-Swarm	[35]	Pentium IV	3.06	1.09
GRASP+tabu	[37]	Pentium	1.73	0.62

<sup>1</sup> formed on a computer with a 3.06 GHz P4 processor.

A recent Dynamic Programming heuristic approach [12]. Among all algo-2 \_ rithm variants studied in [12], the best performance was achieved by the 3 version using  $\tilde{\pi}_i^3/w_i$  as the item ordering rule coupled with the "fill-up and 4 exchange" procedure proposed in [14]. This algorithm version, denoted as 5 DP+FE, was included for our comparative study. The results of DP+FE 6 in this study were obtained by running the source code (which was kindly 7 given to us by the authors of [12]) on our machine. Since DP+FE is a 8 deterministic heuristic algorithm, it was executed for a single run. 9

A GRASP-tabu approach [37]. This approach includes two algorithm variants (GRASP and GRASP+tabu). We used the results of GRASP+tabu
 for our comparative study since it dominates GRASP alone. The reported results were obtained on a Pentium 1.73 GHz processor with 2 GB RAM.

It is not a straightforward task to make a fully fair comparative analysis 14 with the reference approaches due to the differences in computing hardware, 15 termination criterion, etc. This is particularly true for the computing times. 16 For this reason, we focus our study on the quality criterion of the solutions 17 found. Nevertheless, we include information on computing time for indicative 18 purposes. Following [26, 31], we used the CPU frequency of our computer 19 (AMD Opteron 4184 2.8 GHz) as a basis to scale the times of the reference 20 algorithms reported in [35, 37] (see Table 2 for the scaling factors). 21

Like the two reference randomized algorithms (Min-Swarm and GRASP+tabu), 22 we ran our IHEA algorithm 100 times to solve each problem instance. To show 23 a general picture and simplify the presentation, we divide the whole instance 24 set into 8 classes according to the (n, d) combination. Table 3 displays for each 25 instance class and for each randomized algorithm, the average value of three 26 indicators: 1) success rate (SR), i.e., the number of the trials over 100 runs 27 hitting the known optimal solution; 2) relative percentage deviation (RPD), 28 the average gap between the best lower bound  $(f_{LB})$  and the best solution 29 value  $(f_{best})$  in percentage over 100 trials where the gap is calculated by  $((f_{LB}))$ 30 -  $f_{best}/f_{LB} \times 100$ ; 3) the average CPU time in seconds for one trial (t(s)). 31 Note that for the single-run deterministic algorithm (DP+FE), the average 32 values over multiple runs are not needed. For our IHEA algorithm, we also 33 report the average time when the algorithm first encounters the best solution 34  $(t_b(s))$  over 100 trials. Since our proposed algorithm as well as the reference 35 algorithms can easily attain the optimal results for all the benchmark in-36

Table 3 Comparative results of IHEA with 3 state-of-the-art algorithms on the 100 benchmark instances of Group I [2]. The values in bold indicate the improved results of IHEA.

-														
	INST.	Min-Swarm [35]		5]	DP+FE [12]			GRASP+tabu [37]				IHEA		
	-	SR(%)	RPD	t(s)	SR(%)	RPD	t(s)	SR(%)	RPD	t(s)	SR(%)	RPD	t(s)	$t_b(s)$
	$100_{-}25$	93.900	0.012	0.482	40.000	0.319	0.697	100.000	0.000	0.060	100.000	0.000	0.325	0.004
	$100_{-}50$	94.200	0.004	0.442	80.000	0.018	0.708	100.000	0.000	0.057	100.000	0.000	0.253	0.002
	$100_{-}75$	97.500	0.001	0.396	80.000	0.008	0.704	100.000	0.000	0.052	100.000	0.000	0.334	0.003
	$100_{-}100^{1}$	100.000	0.000	0.224	77.777	0.005	0.657	100.000	0.000	0.048	100.000	0.000	0.248	0.002
	$200_{-}25$	90.300	0.009	1.559	60.000	0.056	7.341	100.000	0.000	0.286	100.000	0.000	0.714	0.029
	$200_{-}50$	92.400	0.001	1.967	50.000	0.009	8.239	99.900	9.4E-6	0.301	100.000	0.000	0.827	0.035
	$200_{-}75$	90.900	0.003	2.361	60.000	0.010	7.055	100.000	0.000	0.318	100.000	0.000	0.946	0.010
	$200_{-}100$	100.000	0.000	1.305	60.000	0.004	6.683	100.000	0.000	0.251	100.000	0.000	0.722	0.005
	$300_{-}25^{2}$	-	-	-	33.333	0.061	28.341	99.667	0.001	0.735	100.000	0.000	1.122	0.018
	$300_{-}50$	-	-	-	50.000	0.003	31.324	100.000	0.000	0.763	100.000	0.000	1.156	0.015
-														

<sup>1</sup> Instance 100\_100\_4 is not available and is not considered when we calculate the average value for the instance class 100\_100. <sup>2</sup> Instance 300\_25\_3 is not available and is not considered when we calculate the average value for the instance class 300\_25.

stances under consideration, these optimal results are not listed in the table (see [2,35,37] for these optimal results). The results of the reference algorithms are extracted from the corresponding papers [35,37] (the code of the reference algorithms are not available).

From Table 3, we observe that our IHEA algorithm attains the known optimal 5 values with a successful rate of 100% for all these instances with an average computing time of no more than 1.156 seconds. The average best solution 7 time  $t_b(s)$  of IHEA is even more interesting since the maximum time is only 8 0.035 seconds (for 200\_50). IHEA outperforms the Min-Swarm approach in a the success rate and the relative percentage deviation by consuming typically 10 less CPU seconds. Meanwhile, IHEA dominates the deterministic DP+FE 11 algorithm in terms of both solution quality and computational efficiency for 12 all instance classes. Compared to GRASP+tabu which is one of the current 13 best performing heuristic algorithms, IHEA remains very competitive since it 14 solves all these instances to optimality with a 100% success rate while there 15 are 2 instances for which GRASP+tabu is not able to achieve a success rate 16 of 100%. Another interesting feature of IHEA is that its average computing 17 time is approximately linear relative to the size of the instance which was not 18 observed for the reference algorithms. 19

#### 3.4 Comparative results on large instances of Group II

In this section, we investigate the behavior of our algorithm on the second  $_{21}$  group of 80 large instances (n = 1000 or 2000) with unknown optima. Like  $_{22}$  GRASP+tabu of [37], our IHEA algorithm was executed 100 times for each instance. As reference algorithms, we again used GRASP+tabu (which reported the current best known lower bounds for these instances) and DP+FE. The results of DP+FE were obtained by executing a single run of its source code  $_{26}$ 

20

1

2

3

on our machine while the results of GRASP+tabu were extracted from [37]. 1 Table 4 (for instances with 1000 objects) and Table 5 (for instances with 2000 2 objects) summarize the comparative results. The listed indicators include the 3 best lower bound discovered (column Best), the success rate (column SR) to 4 attain the best lower bound, the relative percentage deviation (column RPD) 5 and the average computing time for one trial (t(s)). We also report the av-6 erage best time over 100 trials for our IHEA algorithm (column  $t_b(s)$ ). The 7 best known results are indicated in italic and the new improved results are 8 highlighted in bold. In the last two rows, #Bests indicates the number of 9 italic and bold values, and Avg. denotes the average value for each column. 10

Table 4 and 5 disclose that our IHEA algorithm outperforms both GRASP+tabu 11 and DP+FE in terms of all indicators. Firstly, IHEA attains the best known 12 lower bounds or improves these lower bounds for all 80 instances. Specifically, 13 it discovers improved best lower bounds for 6 instances and attains the previ-14 ous best known lower bounds for the remaining 74 instances. Secondly, the suc-15 cess rate and relative percentage deviation achieved by IHEA are consistently 16 better than or equal to those achieved by the randomized GRASP+tabu. In 17 particular, IHEA performs better in these two indicators for 24 out of 80 cases 18 and is equal for the remaining 56 cases. GRASP+tabu has 24 cases for which 19 the success rate is under 100% while IHEA has only 3 such cases. Moreover, 20 IHEA is better both in its lowest success rate (95% vs. 6%) and in its aver-21 age success rate (99.9% vs. 91.63%) compared to GRASP+tabu. Notice that 22 the success rate of IHEA can be further improved by simply extending the 23 max iteration parameter (MaxIter). For example, when we set the MaxIter 24 to  $(\sqrt{n+130})$ , IHEA achieves a 100% success rate for all these instances but 25 at the expense of more computing time. Thirdly, IHEA always needs much 26 less computing effort to achieve a similar or better performance compared to 27 GRASP+tabu and DP+FE. 28

To solve instances with 1000 variables and 2000 variables respectively, IHEA 29 consumes an average computing time of 6.0 seconds and 22.73 seconds while 30 these values are 27.96 seconds and 329.65 seconds for GRASP+tabu, 2917.70 31 seconds and 51695.75 seconds for DP+FE. This implies that IHEA scales very 32 well with a weak increasing ratio of its average computing time (i.e., 22.73/6.033  $\approx 3.79$ ) when the problem size grows from 1000 to 2000 objects while this 34 ratio is much higher for GRASP+tabu (329.65/27.96  $\approx$  11.79) and DP+FE 35  $(51695.75/2917.70 \approx 17.72)$ . Notice also that compared to the average time 36 which is proportional to the *MaxIter* parameter, the average best solution 37 time (column  $t_b(s)$ ) is even much shorter (i.e., 0.47 seconds) across the whole 38 instance set. Given this fact, it is easy to see that the large gap between the 39 average  $t_b(s)$  and t(s) is consumed by the algorithm only to complete its run, 40 but useless for improving the best solution. Finally, comparing GRASP+tabu 41 with DP+FE, the former outperforms the latter by achieving significantly 42 more best known lower bounds (74 vs. 11) with much less average computing 43

Table 4 Comparative results of IHEA with two state-of-the-art algorithms on the 40 instances with 1000 objects of Group II. The best known results are in italic and the new best known results are in boldface.

INST	DP+FE [12] GRASP+tabu [37]						IHEA				
111,51.	Best	t(s)	Best	SR(%)	RPD	t(s)	Best	SR(%)	RPD	t(s)	tb(s)
1000_25_1	6172407	1682.280	6172407	100.000	0.000	18.234	6172407	100.000	0.000	2.765	0.094
$1000_{25_{2}}$	229833	2103.290	229941	66.000	0.008	20.448	229941	100.000	0.000	5.390	0.091
1000_25_3	172418	1919.350	172418	100.000	0.000	13.429	172418	100.000	0.000	5.892	0.050
$1000_{25}_{4}$	367365	2537.720	367426	100.000	0.000	16.188	367426	100.000	0.000	7.293	0.068
$1000_{25}_{5}$	4885569	2626.970	4885611	100.000	0.000	23.368	4885611	100.000	0.000	5.543	0.144
1000_25_6	15528	608.550	15689	100.000	0.000	5.072	15689	100.000	0.000	1.635	0.020
$1000_{25}7$	4945741	2725.220	4945810	100.000	0.000	22.636	4945810	100.000	0.000	4.804	0.306
1000_25_8	1709954	3762.890	1710198	100.000	0.000	44.150	1710198	100.000	0.000	7.104	0.416
1000_25_9	496315	2839.990	496315	100.000	0.000	18.619	496315	100.000	0.000	6.891	0.060
1000_25_10	1173686	3607.270	1173792	100.000	0.000	36.537	1173792	100.000	0.000	7.573	0.148
$1000_{50_{1}}$	5663517	3722.470	5663590	100.000	0.000	31.459	5663590	100.000	0.000	6.870	0.108
$1000_{50_{2}}$	180831	1450.870	180831	100.000	0.000	0.893	180831	100.000	0.000	3.692	0.045
1000_50_3	11384139	2071.250	11384283	100.000	0.000	19.753	11384283	100.000	0.000	3.338	0.088
$1000_{50}_{4}$	322184	1868.860	322226	100.000	0.000	13.677	322226	100.000	0.000	5.433	0.059
1000_50_5	9983477	2570.760	9984247	86.000	1.5E-4	25.315	9984247	98.000	6.0E-6	3.662	0.541
1000_50_6	4106186	3801.720	4106261	100.000	0.000	36.010	4106261	100.000	0.000	7.691	0.113
$1000_{50}7$	10498135	2322.160	10498370	84.000	1.3E-4	20.727	10498370	100.000	0.000	3.584	0.271
1000_50_8	4981017	3826.980	4981146	20.000	0.012	72.100	4981146	99.000	1.0E-6	9.155	1.648
1000_50_9	1727727	3382.020	1727861	100.000	0.000	32.717	1727861	100.000	0.000	9.381	0.847
1000_50_10	2340590	3605.070	2340724	94.000	2.3E-4	59.074	2340724	100.000	0.000	7.416	0.163
$1000_{75_{1}}$	11569498	3334.210	11570056	65.000	7.6E-5	39.680	11570056	100.000	0.000	4.892	0.514
$1000_{75_{2}}$	1901119	3094.560	1901389	100.000	0.000	20.131	1901389	100.000	0.000	6.492	0.129
1000_75_3	2096415	3208.980	2096485	100.000	0.000	24.713	2096485	100.000	0.000	8.742	0.107
$1000_{-}75_{-}4$	7305195	3821.020	7305321	100.000	0.000	34.156	7305321	100.000	0.000	6.846	0.119
1000_75_5	13969705	2887.190	13970240	93.000	4.0E-4	23.182	13970842	100.000	0.000	6.022	0.130
1000_75_6	12288299	3178.950	12288738	100.000	0.000	20.733	12288738	100.000	0.000	4.463	0.161
1000_75_7	1095837	2580.270	1095837	100.000	0.000	14.359	1095837	100.000	0.000	7.119	0.099
1000_75_8	5575592	3804.420	5575813	100.000	0.000	42.451	5575813	100.000	0.000	7.833	0.142
1000_75_9	695595	2171.330	695774	100.000	0.000	14.062	695774	100.000	0.000	4.624	0.126
1000_75_10	2507627	3349.440	2507677	100.000	0.000	29.338	2507677	100.000	0.000	6.863	0.074
1000_100_1	6243330	3849.500	6243494	100.000	0.000	44.646	6243494	100.000	0.000	7.018	0.116
1000_100_2	4853927	3627.050	4854086	61.000	0.001	52.601	4854086	100.000	0.000	7.092	0.193
1000_100_3	3171955	3320.520	3172022	100.000	0.000	29.177	3172022	100.000	0.000	6.391	0.096
1000_100_4	754542	1990.800	754727	100.000	0.000	14.651	754727	100.000	0.000	5.207	0.075
$1000_{-}100_{-}5$	18646607	2829.350	18646620	99.000	6.9E-7	24.273	18646620	100.000	0.000	4.070	0.289
1000_100_6	16019697	3247.810	16018298	96.000	4.2E-6	25.780	16020232	100.000	0.000	5.204	0.117
1000_100_7	12936205	3587.160	12936205	100.000	0.000	27.590	12936205	100.000	0.000	5.533	0.129
1000_100_8	6927342	3850.890	6927738	100.000	0.000	59.551	6927738	100.000	0.000	7.298	0.113
1000_100_9	3874959	3463.920	3874959	100.000	0.000	32.414	3874959	100.000	0.000	7.085	0.067
1000_100_10	1334389	2474.890	1334494	100.000	0.000	14.651	1334494	100.000	0.000	6.270	0.094
#Bests	7	-	38	30	30	-	40	40	40	-	-
Avg.	5128111	2917.699	5128228	94.100	6E-4	27.964	5128291	99.925	0.000	6.005	0.204

time (178.87 seconds vs. 27306.73 seconds) across 80 instances of Group II. <sup>1</sup> This observation confirms a safe ranking of the three compared algorithms in <sup>2</sup> decreasing order of their performance: IHEA, GRASP+tabu and DP+FE. <sup>3</sup>

Table 5 Comparative results of IHEA with two state-of-the-art algorithms on the 40 instances with 2000 objects of Group II. The best known results are in italic and the new best known results are in boldface.

INST	DP+F	'E [12]	GRASP+tabu [37]				IHEA				
	Best	t(s)	Best	$\mathrm{SR}(\%)$	RPD	t(s)	Best	$\mathrm{SR}(\%)$	RPD	t(s)	tb(s)
2000_25_1	5268004	57726.920	5268188	100.000	0.000	320.273	5268188	100.000	0.000	22.264	0.479
$2000_{25_{2}}$	13293940	51050.130	13294030	100.000	0.000	205.053	13294030	100.000	0.000	24.917	2.191
2000_25_3	5500323	57419.270	5500433	56.000	4.5E-4	496.081	5500433	100.000	0.000	28.933	0.780
2000_25_4	14624769	46620.160	14625118	100.000	0.000	215.072	14625118	100.000	0.000	17.050	0.766
2000_25_5	5975645	57416.960	5975751	100.000	0.000	457.765	5975751	100.000	0.000	28.102	0.502
2000_25_6	4491533	56155.800	4491691	100.000	0.000	294.252	4491691	100.000	0.000	23.442	0.767
$2000_{25}7$	6388475	57116.940	6388756	100.000	0.000	346.090	6388756	100.000	0.000	25.178	0.671
2000_25_8	11769395	52832.060	11769873	100.000	0.000	277.109	11769873	100.000	0.000	22.584	0.718
2000_25_9	10959388	54258.650	10960328	100.000	0.000	278.882	10960328	100.000	0.000	22.420	0.564
2000_25_10	139233	14686.960	139236	100.000	0.000	68.070	139236	100.000	0.000	7.551	0.087
2000_50_1	7070736	52860.690	7070736	39.000	0.027	294.078	7070736	100.000	0.000	28.016	0.441
2000_50_2	12586693	57518.440	12587545	100.000	0.000	331.619	12587545	100.000	0.000	23.943	1.349
2000_50_3	27266846	48397.300	27268336	100.000	0.000	191.506	27268336	100.000	0.000	22.691	0.359
2000_50_4	17754391	57376.090	17754434	100.000	0.000	485.249	17754434	100.000	0.000	24.506	0.447
2000_50_5	16804699	57563.580	16805490	90.000	9.3E-4	923.936	16806059	100.000	0.000	32.057	0.538
2000_50_6	23075693	52613.210	23076155	50.000	5.1E-4	285.256	23076155	100.000	0.000	21.579	0.631
2000_50_7	28757657	46437.960	28759759	6.000	0.008	442.792	28759759	100.000	0.000	25.365	0.525
2000_50_8	1580242	32416.870	1580242	100.000	0.000	102.412	1580242	100.000	0.000	13.937	0.169
2000_50_9	26523637	48529.930	26523791	100.000	0.000	212.114	26523791	100.000	0.000	19.695	0.438
2000_50_10	24746249	50565.420	24747047	100.000	0.000	253.202	24747047	100.000	0.000	20.613	0.377
2000_75_1	25121327	57579.990	25121998	100.000	0.000	500.371	25121998	100.000	0.000	22.721	0.529
2000_75_2	12663927	54629.120	12664670	89.000	4.7E-4	316.231	12664670	100.000	0.000	21.584	0.401
2000_75_3	43943294	45151.420	43943994	100.000	0.000	171.362	43943994	100.000	0.000	18.723	0.763
$2000_{-}75_{-}4$	37496414	50255.520	37496613	100.000	0.000	219.561	37496613	100.000	0.000	19.901	0.434
2000_75_5	24835254	56840.030	24834948	73.000	2.1E-4	424.285	24835349	100.000	0.000	27.439	0.533
2000_75_6	45137702	44437.730	45137758	100.000	0.000	190.011	45137758	100.000	0.000	20.862	0.345
2000_75_7	25502503	57480.680	25502608	100.000	0.000	303.887	25502608	100.000	0.000	21.848	0.402
2000_75_8	10067752	52566.820	10067892	100.000	0.000	213.795	10067892	100.000	0.000	21.560	0.333
2000_75_9	14177079	55684.210	14171994	97.000	1.6E-5	329.877	14177079	100.000	0.000	32.008	0.482
2000_75_10	7815419	48717.480	7815755	78.000	8.7E-5	201.636	7815755	100.000	0.000	20.537	1.730
2000_100_1	37929562	57195.970	37929909	100.000	0.000	270.140	37929909	100.000	0.000	21.622	0.418
2000_100_2	33665281	57844.250	33647322	95.000	8.2E-5	490.736	33665281	100.000	0.000	34.322	0.548
2000_100_3	29951509	57198.420	29952019	34.000	0.003	923.360	29952019	100.000	0.000	23.249	0.436
2000_100_4	26948234	57484.560	26949268	100.000	0.000	440.690	26949268	100.000	0.000	23.800	0.542
$2000_{-}100_{-}5$	22040523	58316.780	22041715	70.000	3.0E-4	466.252	22041715	95.000	1.1E-5	23.346	6.286
2000_100_6	18868630	56282.860	18868887	100.000	0.000	339.878	18868887	100.000	0.000	22.315	0.387
2000_100_7	15850198	54333.570	15850597	100.000	0.000	358.472	15850597	100.000	0.000	22.555	0.399
2000_100_8	13628210	52206.350	13628967	100.000	0.000	231.923	13628967	100.000	0.000	22.250	0.356
2000_100_9	8394440	45817.310	8394562	97.000	2.2E-4	188.672	8394562	100.000	0.000	18.686	0.361
2000_100_10	4923413	38243.750	4923559	92.000	1.4E-4	124.031	4923559	100.000	0.000	15.041	0.913
#Bests	4	-	36	26	26	-	40	40	40	-	-
Avg.	18088455	51695.754	18088299	89.150	0.001	329.650	18088900	99.875	0.000	22.730	0.735

<sup>1</sup> 3.5 Computational results on very large instances of Group III

<sup>2</sup> We now present the last experiment on the 40 very large instances of Group III

<sup>3</sup> with 5000 to 6000 variables with unknown optima. In addition to their size, the

<sup>4</sup> hardness of these instances is also ensured through the selection process when

<sup>5</sup> they were created (see Section 3.1). To measure the solution quality obtained

by our IHEA algorithm, we used the method proposed in [6] to calculate upper 1 bounds  $\hat{U}_{CPT}^2$  (the current tightest bounds), which was previously used in [37] 2 to evaluate their algorithms. The results of DP+PE [12] on these instances 3 are not reported since DP+PE requires intolerable amount of computing time 4 (indeed, we did not obtain any result with a time limit of one week). 5

Our IHEA algorithm was executed 100 times for each instance. Table 6 sum-6 marizes the results: the best lower bound (column Best), the gap between the 7 upper bound  $\hat{U}_{CPT}^2$  and the best lower bound in percentage (column GAP, 8 calculated by  $(U_{CPT}^2 - \text{Best})/\text{Best} \times 100)$ , success rate (column SR), relative 9 percentage deviation (column RPD), the average computational time for one 10 trial (column t(s)) and the average best solution time aver 100 trials (column 11  $t_b(s)$ ). The last row (Avq.) indicates the average value of each column. From 12 Table 6, we observe that IHEA is able to attain high quality lower bounds for 13 all these large and difficult instances. These lower bounds are typically very 14 close to the corresponding upper bounds. Indeed, the average gap between the 15 best lower bound and the upper bound  $\hat{U}_{CPT}^2$  is 1.359% for the whole instance 16 set. Moreover, IHEA achieves a success rate of 100% for 30 out of 40 instances 17 (75%). The average success rate across all instances is 87.675%. When we ex-18 amine the computing time, the results are quite acceptable. Specifically, the 19 average run time for one trial is 174.075 seconds. The best solution time is 20 much shorter with an average value of 14.456 seconds. 21

#### 4 Discussion

The computational outcomes and comparisons with state-of-the-art algorithms 23 presented in Section 3 demonstrated the effectiveness of the proposed IHEA 24 approach. In this section, we provide additional information to gain more in-25 sights into the "hyperplane exploration" component (Section 4.1), and further 26 investigate two other important ingredients of the IHEA algorithm: the vari-27 able fixing strategy (Section 4.2) and the perturbation strategy (Section 4.3). 28 To simplify the presentation of Sections 4.1 and 4.2, we used a subset of 8 rep-29 resentative instances (see Table 7-8) from the 80 benchmarks of Group II [37]. 30 These instances cover all sizes and all densities of Group II. We denote this 31 subset of instances as Group ii. 32

### 4.1 Insight into the "hyperplane exploration" phase

To show the influence of the "hyperplane exploration" component on the efficiency of IHEA, we provide additional information on the 8 representative instances of Group ii in Table 7 (complementary to Tables 4 and 5) includ-<sup>36</sup>

22

Table 6
Computational

 $6000_{25}4$ 

 $6000_{25}5$ 

6000\_50\_1

 $6000_{50_{2}}$ 

 $6000_{50_{3}}$ 

6000\_50\_4

6000\_50\_5

6000\_75\_1

6000\_75\_2

6000\_75\_3

6000\_75\_4

 $6000_{75}5$ 

6000\_100\_1

6000\_100\_2

6000\_100\_3

6000\_100\_4

6000\_100\_5

Avg.

191531304

36121510

194344567

323753804

31913824

225556641

40931924

204512250

42422207

524508156

197004931

74350712

292257056

219791358

376967122

355609720

686364195

Computa	tional resu	lts of IHEA	A on the	40 very	large ir	nstances	of Group III
-	INST.	Best	$\operatorname{Gap}(\%)$	$\mathrm{SR}(\%)$	RPD	t(s)	$t_b(s)$
-	5000_25_1	23667450	2.729	100.000	0.000	130.664	1.973
	5000_25_2	37914560	3.323	100.000	0.000	143.679	2.843
	5000_25_3	68295820	1.718	100.000	0.000	126.904	2.668
	$5000_{25}4$	33866053	2.292	100.000	0.000	139.453	3.374
	5000_25_5	9533115	5.409	100.000	0.000	111.366	3.227
	$5000_{-}50_{-}1$	45194685	2.432	100.000	0.000	144.125	2.503
	5000_50_2	88355678	0.830	100.000	0.000	143.188	2.488
	5000_50_3	152447303	0.376	100.000	0.000	143.813	2.960
	$5000_{-}50_{-}4$	171000228	0.915	100.000	0.000	148.015	3.392
	5000_50_5	1187339	6.570	100.000	0.000	61.106	0.326
	$5000_{75_{1}}$	28170819	1.230	100.000	0.000	105.745	1.674
	$5000_{75_{2}}$	195434758	0.406	100.000	0.000	149.977	2.834
	5000_75_3	64324704	0.970	76.000	3.9E-5	141.571	36.113
	$5000_{75_{4}}$	247348595	0.796	100.000	0.000	144.213	2.942
	5000_75_5	46462750	0.478	4.000	1.0E-4	136.119	45.054
	$5000_{-}100_{-}1$	214425886	0.083	100.000	0.000	150.076	2.974
	$5000_{-}100_{-}2$	18783132	0.367	100.000	0.000	76.661	1.164
	$5000_{-}100_{-}3$	10784650	0.203	100.000	0.000	61.450	0.648
	$5000_{-}100_{-}4$	160539947	0.065	100.000	0.000	153.082	2.780
	5000_100_5	33166524	0.552	67.000	$9.0\mathrm{E}\text{-}5$	105.708	38.976
	$6000_{25_{1}}$	69832542	1.788	100.000	0.000	204.230	5.621
	$6000_25_2$	3697236	5.232	100.000	0.000	123.770	2.797
	6000_25_3	79300092	1.964	100.000	0.000	246.285	3.490

0.276

1.423

1.622

0.376

2.502

0.999

1.885

0.999

1.187

0.477

1.083

0.344

0.069

0.149

0.087

0.058

0.100

1.359

87.000

100.000

100.000

66.000

100.000

100.000

100.000

12.000

100.000

60.000

100.000

100.000

100.000

1.000

96.000

100.000

38.000

87.675

1.2E-5

0.000

0.000

9.6E-5

0.000

0.000

0.000

5.2E-5

0.000

3.4E-3

0.000

0.000

0.000

9.7E-4

1.0E-6

0.000

4.2E-5

1.2E-4

238.917

208.762

214.187

272.235

220.343

198.893

186.351

267.433

182.990

177.873

220.513

282.668

219.599

257.679

266.202

245.857

211.295

174.075

9.093

3.447

4.060

4.864

3.015

5.776

6.849

86.722

2.754

4.100

3.822

4.054

122.758

46.105

3.710

69.904

14.456

24.377

ing the best hyperplane where IHEA locates the best solution (column  $k^*$ ), 1 the average dimension of the initial hyperplane  $(Avg.k_0)$ , the hyperplane di-2 mension lower bound  $(k_{LB})$ , the hyperplane dimension upper bound  $(k_{UB})$ 3 and the average number of hyperplanes explored (Avq.k). Table 7 shows that 4 the average number of hyperplanes that IHEA explores is always less than 3 5 for these instances. There is one case where Avg.k is exactly 2 which means 6 TabuSearch\_Engine finds improved solutions in the first hyperplane but not 7 in the second. For the other 7 cases, TabuSearch\_Engine sometimes discov-8 ers improved solutions in the second hyperplane, which explains why their g

Table 7 Additional information of IHEA on the 8 representative instances of Group ii

INST.	$k^*$	$Avg.k_0$	$k_{LB}$	$k_{UB}$	Avg.k
1000_25_5	880	879.010	520	881	2.904
$1000_{50}8$	627	626.000	242	627	2.928
$1000_{-}75_{-}5$	858	857.000	490	858	2.924
1000_100_6	796	796.000	397	796	2.000
$2000_25_3$	929	928.010	236	931	2.896
$2000_{-}50_{-}5$	1153	1152.000	378	1153	2.969
$2000_{-}75_{-}9$	864	863.000	207	864	2.967
$2000_{-}100_{-}2$	1154	1153.000	387	1154	2.970
Avg.	907.63	906.75	357.13	908.00	2.82

Avq.k value is more than 2 but less than 3. Based on this observation, we 1 conclude that each iteration of the "hyperplane exploration" phase of IHEA 2 typically explores a very limited number of hyperplanes which contributes to 3 its performance. To understand why such a small number of hyperplanes is 4 explored, we examine the initial hyperplane  $(Avq.k_0)$ . It can be seen that the 5 initial hyperplane is always equal or very close to the best hyperplane (see 6 column  $k^*$ ). Indeed, there is 1 out of 8 cases where the initial hyperplane 7 is exactly the best hyperplane where the best solution is found, and 7 cases 8 where the initial hyperplane is only one dimension away from the best hyper-9 plane. Moreover, Table 7 indicates that the dimension of the initial hyperplane 10 (column  $Avg.k_0$ ), which is always within the interval  $[k_{LB}, k_{UB}]$ , is very close 11 to  $k_{UB}$ . The difference between the average values of  $Avg.k_0$  and  $k_{UB}$  is only 12 908.00-906.75.00=1.25. Similar observations can be made for other instances 13 of Group II. 14

## 4.2 Impact of the variable fixing strategy

As shown in Section 2.5, for a given hyperplane, IHEA has a "high quality" 16 solution as its input. Before exploring the hyperplane with tabu search, we 17 use the density criterion to fix a number of selected items (to the value of 18 1) and thus generate a reduced problem for tabu search. This variable fixing 19 strategy is motivated by the idea that selected items with high density in a 20 high quality solution are strongly determined and should not be destroyed 21 during tabu search. To verify the usefulness of this variable fixing strategy, 22 we conducted an experiment to compare IHEA with a variant IHEA<sub>NoVF</sub> 23 where the variable fixing strategy is disabled (i.e., removing lines 15-17 from 24 Algorithm 1). As such *TabuSearch\_Engine* explores directly the search space 25 of CQKP[k] instead of  $RCP(V_{fixed}, CQKP[k], x')$  (see Section 2.3). 26

We ran IHEA and IHEA<sub>NoVF</sub> 100 times to solve all instances of Group II under the same condition as before. We divide the whole instance set into 8 classes according to the (n, d) combination. Table 8 summarizes the results. In addition of the average best solution value (Avg.Best), average success rate (Avg.SR) 30

Compara	Somparative results of mEA and mEA <sub>NoVF</sub> on the benchmarks of Group m									
INST.		IHE	А			$IHEA_{NoVF}$				
	Avg.Best	Avg.SR	t(s)	Avg.%	$_{FV} \operatorname{Avg.}{\%}_W$	$F_{FV}$ Avg.Best	Avg.SR	t(s)	-	
1000_25	2016960.700	100.000	5.489	0.928	0.000	2016960.700	99.400	101.332		
$1000_{-}50$	5118953.900	99.700	6.022	0.938	0.000	5118953.900	90.900	114.268		
$1000_{-}75$	5900793.200	100.000	6.390	0.932	0.000	5900793.200	83.100	120.730		
1000_100	7476457.700	100.000	6.117	0.932	0.000	7476457.700	99.400	102.621		
$2000_{-}25$	7841340.400	100.000	22.244	0.964	0.000	7841340.400	99.400	591.328		
$2000_{-}50$	18617410.400	100.000	23.240	0.967	0.000	18617410.400	99.900	617.926		
$2000_{-}75$	<b>24676371.600</b>	100.000	22.718	0.967	0.000	24676368.000	88.600	546.975		
2000_100	21220476.400	99.500	22.719	0.963	0.000	21220453.500	80.000	466.538		
Avg.	11608595.538	99.900	14.367	0.949	0	11608592.225	92.587	332.715		

Table 8 Comparative results of IHEA and IHEA<sub>NoVF</sub> on the benchmarks of Group II

and average total computing time (Avg.t(s)), we also list for IHEA the aver-

<sup>2</sup> age percentage of fixed variable (Avg.  $%_{FV}$ ) and average percentage of wrongly

<sup>3</sup> fixed variable (Avg. $\%_{WFV}$ ), where the percentage of the fixed variables is

 $_4~$  calculated by: #fixed\_variable/k  $\times~100$  and the percentage of wrongly fixed

s variable is calculated by: #wrongly\_fixed\_variable/#fixed\_variable  $\times$  100. The

<sup>6</sup> wrongly fixed variables are identified by comparing the fixed variables to the

 $_{7}$  best known solution reported in Tables 4 and 5. The last row (Avg.) indicates

<sup>8</sup> the average value of some columns.

Table 8 shows that IHEA performs better than IHEA<sub>NoVF</sub> in terms of both average best solution value (Avg.Best) and average success rate (Avg.SR) 10 for 2 out of 8 instance classes. For the remaining 6 instance classes where 11 both algorithms achieve the same best results, IHEA always attains a higher 12 average success rate than IHEA<sub>NoVF</sub>. A Wilcoxon signed rank test with a 13 significance factor of 0.05 was applied to these two groups of success rates 14 and the resulting p-value of 0.001602 clearly shows that IHEA is significantly 15 better than IHEA<sub>NoVF</sub>. Moreover, when we examine the average computing 16 time, we find that IHEA is 23 times faster than IHEA<sub>NoVF</sub> (14.376 vs 332.715) 17 seconds). Such a drastic speed-up is achieved thanks to the fact that a large 18 number of variables are fixed and few of them are wrongly fixed. Indeed, 19 the average value of the average number of fixed variables in percentage (see 20 column Avg. $\%_{FV}$ ) is 94.9% which means that 94.9% of the search space is 21 eliminated on average, and the average number of wrongly fixed variables (see 22 column Avg. $\mathcal{N}_{WFV}$  is always 0 which means no variable is wrongly fixed for 23 these instances. 24

## 25 4.3 Impact of the perturbation strategy

<sup>26</sup> IHEA uses a density based perturbation strategy to introduce a form of global <sup>27</sup> diversification for a better exploration of the solution space (Section 2.7). To

27 diversification for a better exploration of the solution space (Section 2.7). To

assess the impact of the adopted perturbation strategy, we conducted an ex-

<sup>29</sup> periment to compare the performance of IHEA with two variants  $IHEA_{RDPT}$ 

Table 9			
Comparative results of IHEA with	th IHEA <sub>RDPT</sub> and	l IHEA <sub>NOPT</sub> on	the 80 large
instances of Group II [37]. The val	lues in bold denote	e the best results	of row Sum.

INST.	IHE	A		IHEA <sub>R</sub>	DPT		IHEA <sub>NOPT</sub>		
	Avg.Best	Avg.SR	Avg.t(s)	Avg.Best	$\operatorname{Avg.SR}$	Avg.t(s)	Avg.Best	Avg.SR	Avg.t(s
1000_25	2016960.700	100.000	5.489	2016960.700	96.200	7.649	2016958.100	78.300	0.134
$1000_{-}50$	5118953.900	99.700	6.022	5118953.900	78.200	8.327	5118885.300	61.100	0.144
$1000_{-}75$	5900793.200	100.000	6.390	5900793.200	98.400	9.218	5900733.000	75.700	0.149
$1000_{-}100$	7476457.700	100.000	6.117	7476457.700	93.600	9.010	7476457.700	79.900	0.146
$2000_25$	7841340.400	100.000	22.244	7841340.400	89.900	31.684	7841340.400	57.900	0.569
$2000_{-}50$	18617410.400	100.000	23.240	18617410.400	97.600	32.179	18617161.000	88.300	0.576
$2000_{-}75$	24676371.600	100.000	22.718	24676371.600	97.500	31.554	24675823.000	81.100	0.563
$2000_{-}100$	21220476.400	99.500	22.719	21220476.400	100.000	31.750	21218753.400	77.800	0.533
Avg.	11608595.538	99.900	14.367	11608595.538	93.925	20.171	11608263.988	75.012	0.352

and IHEA<sub>NOPT</sub>. IHEA<sub>RDPT</sub> randomly removes s selected items without considering their densities while IHEA<sub>NOPT</sub> eliminates the perturbation phase <sup>1</sup> from IHEA. This experiment was also performed on the 80 instances of Group <sup>3</sup> II. As usual, each algorithm was executed 100 times on each instance. <sup>4</sup>

Table 9 summarizes the results based on three indicators: 1) average best solu-5 tion value (Avg.Best); 2) average success rate (Avg.SR); 3) average computing 6 time for one trial (Avg.t(s)). The last row of the table (Avq.) indicates the 7 average of the listed values of each column. From Table 9, we observe that 8 eliminating the perturbation phase from the IHEA algorithm causes a great 9 deterioration of its performance in terms of both best solution value and suc-10 cess rate. Indeed, compared to IHEA and IHEA<sub>RDPT</sub>, IHEA<sub>NOPT</sub> achieved a 11 smaller average best solution (Avg.Best) value for 6 out of 8 instance classes 12 and even a smaller average success rate (Avg.SR) for all 8 classes. When com-13 paring IHEA<sub>RDPT</sub> with IHEA, one observes that, although IHEA<sub>RDPT</sub> does 14 not deteriorate the best solution value, it is less stable than IHEA by achieving 15 a smaller average success rate for 7 out of 8 instance classes. A Wilcoxon signed 16 rank test with a significance factor of 0.05 was applied to compare the success 17 rates of  $IHEA_{RDPT}$  and IHEA, and the resulting p-value of 0.001602 discloses 18 that IHEA<sub>RDPT</sub> is significantly worse than IHEA. Moreover, IHEA<sub>RDPT</sub> re-19 quired on average more computing time than IHEA (20.171 seconds v.s. 14.367 20 seconds). This experiment confirms that the perturbation phase of IHEA is 21 useful and the adopted density based strategy is effective. 22

### 5 Conclusions

23

This paper deals with the NP-hard Quadratic Knapsack Problem which is <sup>24</sup> a highly useful model in practice. To approximate this hard combinatorial <sup>25</sup> problem, we developed an iterated "hyperplane exploration" approach mixing <sup>26</sup> problem reduction techniques and local optimization with tabu search. The <sup>27</sup> proposed approach introduces a hyperplane constraint to the original QKP <sup>28</sup> model to generate a series of "interesting" hyperplane-constrained problems
whose solution space represents a small subset of the original solution space
of QKP. To further reduce the hyperplane-constrained problem, we employ
specific variable fixing rules based on item density information to fix "strongly
determined" variables. The dedicated tabu search procedure is then used to
explore the reduced hyperplane-constrained problem. Finally a perturbation
strategy is applied to help the search to escape from deep local optima.

We assessed the performance of the proposed approach and presented com-8 parisons with three best performing methods on two sets of 180 well-known 9 benchmark instances (up to 2000 items) and a set of 40 new instances (with 10 5000 and 6000 items). The computational experiments showed that the pro-11 posed approach competes very favorably with the state-of-the-art algorithms. 12 Specifically, IHEA consistently attained the known optimal solution with a 13 100% success rate for all 100 small-sized benchmarks (with 100 to 300 ob-14 jects). For the set of 80 large benchmarks with 1000 and 2000 objects, IHEA 15 discovered 6 improved results (new best lower bounds) and attained the re-16 maining 74 best known results. Encouraging results on 40 new very large in-17 stances (with 5000 and 6000 objects) additionally confirmed the effectiveness 18 of our approach where the average gap between the best lower bound and the 19 well known upper bound  $\hat{U}_{CPT}^2$  is bounded by 1.359%. The experiments also 20 showed that the proposed approach is more computationally effective than 21 the existing heuristics. Furthermore, we performed additional experiments to 22 gain insight into the "hyperplane exploration" component of the proposed ap-23 proach, and investigate the beneficial role of two key strategies of the proposed 24 approach: the variable fixing strategy and the perturbation strategy. 25

We comment that even if IHEA follows the common assumption of non-26 negative profits (see Section 2.2, Proposition 1), this is not a necessary condi-27 tion to apply it. Indeed, in the case of negative profits, Proposition 1 does not 28 hold necessarily and as such the hyperplanes containing the optimal solutions 29 can no more be bounded correctly. Nevertheless, IHEA can still be applied to 30 locate high quality solutions within a set of promising hyperplanes which can 31 be identified by any specific means. In this sense, the proposed IHEA approach 32 is general and applicable to any QKP instance even though its performance 33 may decrease for instances with negative profits. 34

For future work, there are several interesting directions that could be inves-35 tigated. First, given the current IHEA algorithm, we can improve the hyper-36 plane exploration (tabu search) by introducing adaptive memory techniques 37 based on recency and/or frequency information projection [19]. Some advanced 38 search frameworks like path relinking and scatter search [16] could also be 39 integrated to reinforce the tabu search engine. Generally, under the IHEA ap-40 proach, the task of hyperplane exploration can be performed by any effective 41 search algorithm which can be either a heuristic or an exact solver. Second, 42

it would be useful to investigate additional methods able to identify the most <sup>1</sup> "promising" hyperplanes and thus reduce the number of hyperplanes to be <sup>2</sup> explored. Finally, given that the idea of hyperplane decomposition is quite <sup>3</sup> general, it would be interesting to investigate its merit for solving other knapsack and related problems. <sup>5</sup>

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