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

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#### 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 state-of-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.


[^0]
## 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.

Formally, let $c$ be the knapsack capacity and $N=\{1,2, \ldots, n\}$ the set of objects. Let $p_{i i}$ be the profit of object $i(i \in N), w_{i}$ be its weight. For each pair of objects $i$ and $j(1 \leq i \neq j \leq n), p_{i j}$ denotes the pairwise profit which is added to the total profit only when both objects are selected. Let $x_{i}$ $(1 \leq i \leq n)$ be the decision variables such that $x_{i}=1$ if object $i$ is selected, $x_{i}=0$ otherwise. Then QKP can be formulated as follows:

$$
\begin{equation*}
\text { Maximize } \quad f(x)=\sum_{i=1}^{n} \sum_{j=i}^{n} p_{i j} x_{i} x_{j} \tag{1}
\end{equation*}
$$

subject to:

$$
\begin{gather*}
\sum_{j=1}^{n} w_{j} x_{j} \leq c  \tag{2}\\
x \in\{0,1\}^{n} \tag{3}
\end{gather*}
$$

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

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 ( $\mathrm{B} \& \mathrm{~B}$ ) 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 $\mathrm{B} \& \mathrm{~B}$ algorithm introduced in [29] is probably one of the most successful methods which uses aggressive problem reduction techniques. Today's state-of-the-art exact methods are able to solve instances with up to 1500 variables.

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

One observes that, compared to the research effort on exact algorithms which has taken place for a long time, studies on heuristics for QKP are more recent and less abundant. In this work, we are interested in solving large scale QKP instances approximately and present an effective heuristic approach which explores the idea of searching over promising hyperplanes. The proposed approach basically introduces an additional cardinality constraint to the original model to prune regions of the search space where no optimal solution exists. Such an idea proved to be very useful for designing effective heuristics for the multidimensional knapsack problem [4,11,32]. Similar ideas were also explored as a type of "generalized branching" [30] or "constraint branching" [13] within the general $\mathrm{B} \& \mathrm{~B}$ framework. In this work, we adapt for the first time the idea of hyperplane exploration in the context of QKP. For this purpose, we address two relevant issues which are critical to make our approach successful. First, we need to identify the promising hyperplanes which are likely to contain high quality solutions. Second, we want to search efficiently inside the identified hyperplanes since each hyperplane, though already much reduced relative to the original model, may still contain a very large number of candidate solutions.

Based on the above considerations, our proposed iterated "hyperplane exploration" algorithm (IHEA) for QKP makes two original contributions.

- From the algorithmic perspectives, we present for the first time a decomposition approach for solving QKP. By introducing the cardinality constraint, IHEA divides the initial problem into several disjoint hyperplaneconstrained sub-problems and focuses its exploration within the most promising hyperplanes while discarding unpromising sub-problems. To further reduce the search space of each hyperplane-constrained problem, IHEA uses specific rules to fix a large number of variables. To seek high quality solutions within each reduced sub-problem, IHEA employs a dedicated tabu search procedure which is able to tunnel through infeasible regions to facilitate transition between structurally different feasible solutions. An informed perturbation strategy is also applied to establish a global form of diversification and thereby to allow examining additional unexplored hyperplanes.
- From the perspective of computational results, the proposed IHEA approach displays very competitive performances on three groups of 220 benchmark instances. Particularly, it is able to attain easily all the optimal solutions with a $100 \%$ success rate for the first group of 100 instances with up to 300 objects. For the second group of 80 larger instances with 1000 to 2000 objects, IHEA provides improved best results for 6 instances (new lower bounds) and attains the best known results for the remaining cases. We also report results for a third group of very large instances with up to 6000 variables for which our approach achieves an average gap of less than $1.359 \%$ between the best lower bound and the well-known upper bound $\hat{U}_{C P T}^{2}[6]$.

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.

## 2 Iterated "hyperplane exploration" algorithm for QKP

In this section, we present our iterated "hyperplane exploration" algorithm for QKP. We begin with some useful notations and definitions, and then present the main components of the proposed approach.

### 2.1 Basic notations and definitions

1

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., $\left.\sigma(x)=\left|I_{1}(x)\right|\right)$.
- Given two solutions $x \in\{0,1\}^{n}$ and $x^{\prime} \in\{0,1\}^{n},\left|x, x^{\prime}\right|=\sum_{j=1}^{n}\left|x_{j}-x_{j}^{\prime}\right| \quad$ 。 denotes the Hamming distance between $x$ and $x^{\prime}$.
- Function $f_{r}(x)$ calculates a raw objective value of solution $x \in\{0,1\}^{n}$ which could be either feasible or infeasible with respect to the capacity constraint.

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

$$
\begin{equation*}
C(i, x)=p_{i i}+\sum_{j \in I_{1}(x), j \neq i} p_{i j} \tag{4}
\end{equation*}
$$

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

$$
\begin{equation*}
D(i, x)=C(i, x) / w_{i} \tag{5}
\end{equation*}
$$

Definition 3 A constrained QKP with a $k$ dimensional hyperplane constraint is defined as:

$$
C Q K P[k]=\left\{\begin{array}{l}
\max \sum_{i=1}^{n} \sum_{j=i}^{n} p_{i j} x_{i} x_{j}  \tag{6}\\
\text { s.t. } \\
\sum_{j=1}^{n} w_{j} x_{j} \leq c \\
\sum_{j=1}^{n} x_{j}=k \\
x \in\{0,1\}^{n}
\end{array}\right.
$$

where $\sum_{j=1}^{n} x_{j}=k$ is a hyperplane constraint which restricts the solution space of QKP in the $k$ dimensional hyperplane. Each feasible solution of problem $C Q K P[k]$ has exactly $k$ selected objects.

Note that the notion of contribution $C(i, x)$ (Definition 1) is related to the upper planes of [14] with two notable differences. First, $C(i, x)$ involves both a problem instance and a solution $x$ while an upper plane only depends on the problem instance (and is independent of any solution). Second, an upper 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 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 solution in order to maximize the total profit.

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

Let $C Q K P[k](1 \leq k \leq n)$ be a constrained QKP (see Definition 3), it is obvious that its solution space is a subspace of the original QKP. Therefore, any feasible solution of the $\operatorname{CQKP}[k](1 \leq k \leq n)$ is also a feasible solution of the original QKP. Let $\Omega^{F}$ be the feasible solution space of a QKP instance such that:
$\Omega^{F}=\left\{x \in\{0,1\}^{n}: \sum_{j=1}^{n} w_{j} x_{j} \leq c\right\}$,
Then the feasible solution space of the constrained QKP with a $k$ dimensional hyperplane constraint ( $C Q K P[k]$ ) is given by:
$\Omega_{[k]}=\left\{x \in \Omega^{F}: \sigma(x)=k\right\}$.
QKP can be decomposed into $n$ independent sub-problems (constrained QKPs): $C Q K P[1], C Q K P[2], \ldots, C Q K P[n]$. These $n$ sub-problems represent $n$ disjoint subspaces and the feasible solution space of QKP is the union of the solution space of all its sub-problems, i.e., $\Omega^{F}=\cup_{k=1}^{n} \Omega_{[k]}$.

For QKP, if items are sorted in non-decreasing order according to their weight $w_{j}(j \in N)$, there must exist only one positive integer $k_{U B}$ simultaneously verifying the following two constraints: 1) $\left.\sum_{j=1}^{k_{U B}} w_{j} \leq c, 2\right) \sum_{j=1}^{k_{U B}+1} w_{j}>c$; similarly, if items are sorted in non-increasing order according to their weight $w_{j}(j \in N)$, there must be only one positive integer $k_{L B}$ simultaneously verifying the following two constraints: 1) $\left.\sum_{j=1}^{k_{L B}} w_{j} \leq c, 2\right) \sum_{j=1}^{k_{L B}+1} w_{j}>c$. Following the literature like $[1,2,6,14,28,29]$, we assume non-negative entries in the profit matrix. Notice that the existing QKP benchmark instances follow this assumption. This leads to the following proposition.

Proposition 1. There must exist optimal solutions of QKP in hyperplanes
whose dimensions satisfy: $k_{L B} \leq k \leq k_{U B}$.
Proof. Given a feasible solution $x^{1} \in \Omega_{\left[k_{1}\right]}\left(0<k_{1}<k_{L B}\right)$, and a feasible solution $x^{2} \in \Omega_{\left[k_{2}\right]}\left(k_{L B} \leq k_{2} \leq k_{U B}, k_{1}<k_{2}\right)$ 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 in common. Since $\left(k_{2}-k_{1}\right) \geq 1$, and the contribution of any selected item in $x^{2}$ is greater than or equal to 0 , we have: $f\left(x^{2}\right) \geq f\left(x^{1}\right)$. Consequently, there must exist solutions in $\cup_{k=k_{L B}}^{k_{U B}} \Omega_{[k]}$ whose objective value is greater than or equal to the objective value of the best solution in $\cup_{k=1}^{k_{L B}-1} \Omega_{[k]}$. On the other hand, $k_{U B}$ is the maximum number of items that can be contained in the knapsack which means any solution in hyperplanes with a dimension greater than $k_{U B}$ is infeasible. Therefore, no feasible solution in $\cup_{k=k_{U B}+1}^{n} \Omega_{[k]}$ has an objective value better than the objective value of the best solution in $\cup_{k=k_{L B}}^{k_{U B}} \Omega_{[k]}$.

To make an effective search, we can focus on hyperplanes with a dimension $k$ within the interval $\left[k_{L B}, k_{U B}\right]$ and definitely discard other subspaces ${ }^{1}$. This leads to a first (and large) reduction of the solution space from $\cup_{k=1}^{n} \Omega_{[k]}$ to $\cup_{k=k_{L B}}^{k_{U B}} \Omega_{[k]}$.

However, the remaining search space $\cup_{k=k_{L B}}^{k_{U B}} \Omega_{[k]}$ could still be too large to be explored efficiently, especially when the gap between $k_{L B}$ and $k_{U B}$ 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 $k_{U B}$. 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 progressively and intensively explore a small number of "interesting" hyperplanes whose dimensions are close to $k_{U B}$ so that a large subspace is effectively pruned and the search effort is more focused. We carry out the hyperplane exploration in increasing order of their dimensions aiming to identify solutions of increasing quality, and restart this process with a perturbation when no improvement can be found. When the search seems to stagnate in one hyperplane, we seek better solutions in a higher dimensional hyperplane. To explore a given hyperplane, additional variable fixing techniques are applied to fix a number of variables so as to further shrink the subspace to be examined.
$\overline{1}$ In case an optimal solution exists in a hyperplane with a dimension $k<k_{L B}$, an optimal solution $x^{*}$ identified in $k \in\left[k_{L B}, k_{U B}\right]$ 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.

### 2.3 General procedure of the "hyperplane exploration" algorithm

Our iterated "hyperplane exploration" approach is composed of three steps:
(1) Construct an initial high quality solution $x^{0}$ and use $\sigma\left(x^{0}\right)$ to determine the starting dimension of the "promising" hyperplanes; $\left(\sigma\left(x^{0}\right) \in\right.$ [ $k_{L B}, k_{U B}$ ] and $\sigma\left(x^{0}\right)$ is close to $k_{U B}$ )
(2) For each hyperplane dimension $k=\sigma\left(x^{0}\right), \sigma\left(x^{0}\right)+1, \sigma\left(x^{0}\right)+2 \ldots$, execute the following three steps:
a. Construct a constrained problem $C Q K P[k]$;
b. Identify some variables that are very likely to be part of the optimal solution, fix these variables to 1 and remove them from $C Q K P[k]$, leading to a reduced constrained problem $C Q K P^{\prime}[k]$;
c. Run a hyperplane exploration algorithm to solve $C Q K P^{\prime}[k]$. 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 $\sigma\left(x^{0}\right)$ ) where high quality solutions might exist (though with a small probability).

Algorithm 1 shows the pseudo-code of the IHEA algorithm for QKP, whose components are detailed in the following sections. At the very beginning, an initial solution is generated by a greedy randomized construction procedure (Section 2.4.1) and is further improved by a descent procedure (Section 2.4.2). Then, the initial dimension of the hyperplane as well as the first constrained problem are determined from the initial solution. From this point, the algorithm enters the "hyperplane exploration" phase which examines a series of hyperplane constrained QKP problems. At each iteration of the 'while' loop, IHEA first applies specific variable fixing rules to construct a reduced constrained problem $R C P\left(V_{\text {fixed }}, C Q K P[k], x^{\prime}\right)$ where $V_{\text {fixed }}$ contains a set of fixed variables (Section 2.5). $R C P\left(V_{\text {fixed }}, C Q K P[k], x^{\prime}\right)$ is then solved by the tabu search procedure (Section 2.6). Each time a better solution $x_{[k]}^{*}$ is discovered (i.e., $f\left(x_{[k])}^{*}>f\left(x^{b}\right)\right)$ by tabu search, IHEA updates the best solution found $x^{b}$ and moves on to solve another constrained problem in a higher dimensional hyperplane. To do this, the algorithm increments $k$ by one and reinitializes $x^{\prime}$ by randomly adding one unselected item to $x^{b}$. The 'while' loop terminates when no improving solution can be found. The global best solution is updated at the end of the 'while' loop. IHEA then makes some dedicated changes (perturbations) to $x^{b}$, improves the perturbed solution (with the de-
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.
    Input: \(P\) : an instance of the \(Q K P ; L\) : size of running list; \(r c l\) : max allowed size of
    restricted candidate list; MaxIter: max number of iterations;
    Output: the best solution \(x^{*}\) found so far
    \(x^{0} \leftarrow\) Greedy_Randomized_Construction(rcl)
    \(x^{0} \leftarrow \operatorname{Descent}\left(x^{0}\right)\)
    \(x^{\prime} \leftarrow x^{0} / * x^{\prime}\) represents the current solution */
    Iter \(\leftarrow 0 / *\) Iteration counter */
    \(x^{b} \leftarrow x^{\prime} / * x^{b}\) records the best solution found in current iteration */
    \(x^{*} \leftarrow x^{b} / * x^{*}\) records the global best solution */
    repeat
        SolutionImproved \(\leftarrow\) true
        \(k \leftarrow \sigma\left(x^{\prime}\right)\)
        Construct constrained problem CQKP[k]
        /* "hyperplane exploration" phase */
        while SolutionImproved do
            \(V_{\text {fixed }} \leftarrow\) Determine_Fixed_Variables \(\left(k, x^{\prime}\right)\)
            Construct reduced constrained problem \(R C P\left(V_{\text {fixed }}, C Q K P[k], x^{\prime}\right)\)
                Run TabuSearch_Engine \(\left(L, x^{\prime}, x^{b}\right)\) to solve \(R C P\left(V_{\text {fixed }}, C Q K P[k], x^{\prime}\right)\) and
                keep a best solution \(x_{[k]}^{*}\)
                if \(f\left(x_{[k]}^{*}\right)>f\left(x^{b}\right)\) then
                \(x^{b} \leftarrow x_{[k]}^{*}\)
                \(k \leftarrow k+1\)
                \(x^{\prime} \leftarrow\) Randomly add one item to \(x^{b}\)
                Construct constrained problem CQKP[k]
                else
                    SolutionImproved \(\leftarrow\) false
                end if
        end while
        if \(f\left(x^{b}\right)>f\left(x^{*}\right)\) then
            \(x^{*} \leftarrow x^{b}\)
        end if
        /* Perturbation phase */
        \(x^{\prime} \leftarrow \operatorname{Perturbation}\left(x^{b}\right.\), Iter \()\)
        \(x^{\prime} \leftarrow \operatorname{Descent}\left(x^{\prime}\right)\)
        \(x^{b} \leftarrow x^{\prime}\)
        Iter \(\leftarrow\) Iter +1
    until Iter \(\geq\) 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.

### 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.

Starting from a partial solution $x$ where all items are set unselected initially, the construction procedure iteratively and adaptively selects some items to be included in $x$ (i.e., the corresponding variables receive the value of 1 ) while maintaining the solution feasibility. At each iteration, we randomly select one unselected item from a restricted candidate list $R C L$ and add the item to the partial solution.

Let $R(x)=\left\{i \in I_{0}(x): w_{i}+\sum_{j \in I_{1}(x)} w_{j} \leq c\right\}$ be the set of unselected items that can fit into the knapsack with respect to $x$. Let $r c l$ be the maximum size of the restricted candidate list. Then $R C L$ contains $\min \{r c l,|R(x)|\}$ 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, $\forall i \in R C L$, the following two conditions hold: 1) $i \in R(x)$, 2) $D(i, x) \geq D(j, x)\left(\forall j \in I_{0}(x) \backslash R C L\right)$.

The items in $R C L$ are ranked according to their density values and the $r^{t h}$ $(1 \leq r \leq|R C L|)$ ranked item is associated with a bias $b_{r}=1 / e^{r}$. Thus, the $r^{t h}$ item is selected with a probability $p(r)$ which is calculated as: $p(r)=$ $b_{r} / \sum_{j=1}^{|R C L|} b_{j}$. Once an item is selected and added to the partial solution $x$, $R C L$ is updated as well as the objective value of the partial solution. This procedure repeats until $R C L$ 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 $k_{L B}$ since it is a tight packing plan that cannot include any more unselected item, and not greater than $k_{U B}$ since it is a feasible solution. Also, this dimension is experimentally proved to be close to $k_{U B}$ (see Section 4.1). The underlying reason is that items with a small weight are biased towards being selected to join the knapsack.

### 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

Our descent procedure jointly employs two different neighborhoods defined by two basic move operators: $A D D$ and $S W A P$.

- $A D D(i)$ : This move operator adds an unselected item $i\left(i \in I_{0}(x)\right)$ 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 $A D D$ operator, and $N_{A}^{F}$ is a subset of $N_{A}$ that contains only feasible neighbor solutions.
- $\operatorname{SWAP}(i, j)$ : Given a solution $x, \operatorname{SWAP}(i, j)$ exchanges an unselected item $i\left(i \in I_{0}(x)\right)$ with a selected item $j$ of $x\left(j \in I_{1}(x)\right)$. 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 $S W A P$ 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 obtained by the construction procedure or the perturbation procedure). To this end, the algorithm iteratively explores $N_{A}^{F}$ and $N_{S}^{F}$ in a token-ring way $N_{A}^{F} \rightarrow N_{S}^{F} \rightarrow N_{A}^{F} \rightarrow N_{S}^{F} \ldots$. For each iteration, a feasible neighbor solution $x^{\prime}$ is picked at random from the neighborhood under consideration and replaces the incumbent solution $x$ if $x^{\prime}$ is better than $x$ (i.e., $f\left(x^{\prime}\right)>f(x)$ ).

It should be noted that our descent procedure is different from the "fill-up and exchange" procedure of [14] which also relies on $A D D$ and $S W A P$. 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 constrained problem $C Q K P[k]$ removes a large part of the solution space (of order $\left.O\left(2^{n}-C_{n}^{k}\right)\right)$ from the original QKP. However, the solution space of the constrained problem $C Q K P[k]$ might still be too large to be efficiently searched by an algorithm. Indeed, as we employ a search algorithm which explores both feasible and infeasible solutions (see Section 2.6), CQKP[k] has a search space of $2^{k}$ where $k$, though smaller than $n$, could still be large. To further reduce the search space to explore, we fix some variables in $C Q K P[k]$.

Recall that in Algorithm 1, the starting solution $x^{\prime}$ of TabuSearch_Engine for solving each constrained problem $C Q K P[k]$ is modified from the best solution $x^{b}$ such that $x^{\prime}$ and $x^{b}$ are either the same in the first hyperplane (see Line 7 of Algorithm 1) or different only in one variable (see Line 21 of Algorithm 1). For each $C Q K P[k]$, based on $x^{\prime}$, our variable fixing step tries to identify a set of variables $V_{\text {fixed }}$ 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 $C Q K P[k]$, leading to a reduced constrained problem $R C P\left(V_{\text {fixed }}, C Q K P[k], x^{\prime}\right)$.

In order to limit the risk of fixing wrong variables, we follow the general idea of identifying a set of "strongly determined" variables [15]. For this purpose, we make use of information from the density value associated with each item. According to the definition presented in Section 2.1, for those selected items in a given solution, the density of an item represents its contribution (profit) per weight unit. Thus, the density value is a good indicator of the importance of a selected item. Given a QKP solution $x^{\prime} \in\{0,1\}^{n}$, our variable fixing rules can be summarized as a three-step method:
(1) For each variable $x_{i}^{\prime}$ such that $i \in I_{1}\left(x^{\prime}\right)$, calculate its density value $D\left(i, x^{\prime}\right)$;
(2) Sort all variables in $I_{1}\left(x^{\prime}\right)$ in non-increasing order according to their density values $D\left(i, x^{\prime}\right)\left(i \in I_{1}\left(x^{\prime}\right)\right)$, leading to a sorted index set $S I_{1}\left(x^{\prime}\right)$;
(3) Extract the first $n_{f}$ variables in $S I_{1}\left(x^{\prime}\right)$ to form the fixed variable set $V_{\text {fixed }}\left(n_{f}\right.$ is the number of fixed variables, i.e., $\left.n_{f}=\left|V_{\text {fixed }}\right|\right)$. Fix the variables in $V_{\text {fixed }}$ with the value of 1 , leading to a reduced constrained problem $R C P\left(V_{\text {fixed }}, C Q K P[k], x^{\prime}\right)$ whose variable set is $\left(I_{1}\left(x^{\prime}\right) \backslash V_{\text {fixed }}\right) \cup$ $I_{0}\left(x^{\prime}\right)$.

In the last step, $n_{f}$ is determined using the following empirical formula:

$$
\begin{equation*}
n_{f}=k_{L B}+\max \left\{\left(\left|I_{1}\left(x^{\prime}\right)\right|-k_{L B}\right) *(1-1 /(0.008 * n)), 0\right\} \tag{7}
\end{equation*}
$$

where $k_{L B}$ is the minimum number of items that can be contained in the knapsack. Typically, $\left|I_{1}\left(x^{\prime}\right)\right|$ is larger than $k_{L B}$. It is easy to understand that a solution with only $k_{L B}$ 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 $\left(n_{f}\right)$ 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 at the following observations: 1) the number of items that can be fixed $\left(n_{f}\right)$ is somewhere between $k_{L B}$ and $\left.\left|I_{1}\left(x^{\prime}\right)\right| ; 2\right)$ the number of items that can be fixed enlarges as the size of the instance increases. The design of formula (7) basically integrates these observations.

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

### 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 $R C P\left(V_{\text {fixed }}, C Q K P[k], x^{\prime}\right)$, 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.

- Neighborhood: It is known that allowing a controlled exploration of infeasible solutions may enhance the performance of a heuristic search algorithm, by facilitating transitions between structurally different feasible solutions [17]. Following this idea, we employ the $N_{S}$ neighborhood (defined in Section 2.4.2) which contains both feasible and infeasible neighbor solutions. In order to explore effectively the search space of a given hyperplane, we restrict our tabu search procedure to visit solutions that are considered better than the best feasible solution found so far, leading to a restricted $S W A P$ neighborhood $N_{S}^{R}$. Precisely, given the objective value of the current best feasible solution with objective value $f_{\text {min }}$, the neighborhood $N_{S}^{R}(x)$ of a solution $x$ (either feasible or infeasible) is defined as: $N_{S}^{R}(x)=\left\{x^{\prime} \in N_{S}(x): f_{r}\left(x^{\prime}\right)>f_{\text {min }}\right\}$ where $f_{r}$ is the raw objective value.
- Tabu list management: We use the reverse elimination method (REM) introduced in [16] for our tabu list management. REM defines an exact tabu mechanism which prevents any visited solution from being revisited. REM uses a running list to store the attributes of all implemented moves. One can trace back the running list to identify the tabu status of a move by making use of another list called residual cancellation sequence ( $R C S$ ) where an
attribute is either added if it is not yet in the $R C S$ or removed from $R C S$ otherwise. Interested readers are referred to $[8,16,32]$ for more details on this method. For the SWAP operator used by TabuSearch_Engine, when there are only two attributes left in $R C S$ (i.e., $|R C S|=2$ ), the move composed of these two attributes is declared tabu in the next iteration. The procedure of updating the tabu status is described in Algorithm 2.
- Evaluation function: The evaluation function used by TabuSearch_Engine considers two factors to assess a solution $x: 1$ ) raw objective value $f_{r}(x), 2$ ) 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 $x^{\prime} \in N_{S}^{R}(x)$ if $\forall x^{\prime \prime} \in\left(N_{S}^{R}(x) \backslash\left\{x^{\prime}\right\}\right), x^{\prime}$ verifies one of the following two conditions: 1) $\left.v_{c}\left(x^{\prime}\right)<v_{c}\left(x^{\prime \prime}\right), 2\right) v_{c}\left(x^{\prime}\right)=v_{c}\left(x^{\prime \prime}\right)$ and $f_{r}\left(x^{\prime}\right) \geq f_{r}\left(x^{\prime \prime}\right)$.

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

Note that tabu search was also used in [37] to enhance a GRASP procedure. However, these two studies are quite different. First, our general IHEA approach focuses on decomposing the initial solution space into a set of hyperplaneconstrained and reduced solution spaces while GRASP+tabu of [37] explores the original solution space. Second, our tabu search procedure is dedicated to 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 explores both feasible and infeasible solutions while GRASP+tabu only visits feasible solutions. Compared to the approach of [18], their tabu search algorithm was dedicated to the unconstrained binary quadratic problem and operates with the "one-flip" move operator (called "shift" in [37]) which adds or removes an item (SWAP was not used).

```
Algorithm 2 Pseudo-code of TabuSearch_Engine
    Input: \(L\) : max size of running list; \(x^{i n}\) : an initial solution; \(x^{r e f}\) : a reference
    feasible solution
    Output: the best feasible solution found so far \(x^{*}\)
    \(|R L| \leftarrow L / *\) Initialize the size of running list to \(L^{*} /\)
    \(f_{\min } \leftarrow f\left(x^{r e f}\right) / * f_{\text {min }}\) records the objective value of the current best feasible
    solution */
    \(x^{*} \leftarrow x^{r e f} / * x^{*}\) records the best feasible solution found so far */
    \(e r l \leftarrow 0\)
    while \(v_{\text {min }} \neq \infty \vee\) erl \(<L\) do
        \(\left(v_{\min }, f_{\max }\right) \leftarrow(\infty,-\infty)\)
        for each \(i \in I_{0}(x)\) do
            for each \(j \in I_{1}(x)\) do
                if tabu \([i][j] \neq\) iter then
                    \(\left(x_{i}, x_{j}\right) \leftarrow(1,0)\)
                    if \(\left(f_{r}(x)>f_{\text {min }}\right) \wedge\left(\left(v_{c}(x)<v_{\text {min }}\right) \vee\left(\left(v_{c}(x)=v_{\text {min }}\right) \wedge\left(f_{r}(x) \geq f_{\text {max }}\right)\right)\right)\)
                    then
                        \(\left(i^{*}, j^{*}\right) \leftarrow(i, j) ;\left(v_{\text {min }}, f_{\text {max }}\right) \leftarrow\left(v_{c}(x), f_{r}(x)\right)\)
                    end if
                    \(\left(x_{i}, x_{j}\right) \leftarrow(0,1)\)
                    end if
            end for
        end for
        if \(v_{\text {min }} \neq \infty\) then
            \(\left(x_{i^{*}}, x_{j^{*}}\right) \leftarrow(1,0)\)
            if \(v_{\text {min }}=0\) then
                    erl \(\leftarrow 0 ; f_{\text {min }} \leftarrow f_{r}(x) ; x^{*} \leftarrow x\)
            else
                iter \(\leftarrow\) iter \(+1 ; R L \leftarrow R L \cup\left\{i^{*}\right\} \cup\left\{j^{*}\right\} ;\) erl \(\leftarrow e r l+2\)
            /*UPDATE TABU STATUS*/
            \(i \leftarrow(e r l-1)\)
            while \(i \geq 0\) do
                    \(j \leftarrow R L[i]\)
                    if \(j \in R C S\) then
                        \(R C S \leftarrow R C S \backslash\{j\}\)
                    else
                        \(R C S \leftarrow R C S \cup\{j\}\)
                    end if
                    if \(|R C S|=2\) then
                        tabu \([R C S[0]][R C S[1]] \leftarrow\) iter \(;\) tabu \([R C S[1]][R C S[0]] \leftarrow\) iter
                    end if
                    \(i \leftarrow i-1\)
            end while
        end if
    end if
    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 $x_{[k]}^{*}$
of the current constrained problem $C Q K P[k]$ 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 $\operatorname{CQKP}[k-1]\left(x_{[k-1]}^{*}\right)$.

Given a feasible solution $x$, the general idea of our perturbation strategy is to remove a small number (say $s, s>0$ ) of items which are chosen from $t(s \leq$ $\left.t \leq\left(I_{1}(x)-n_{f}\right)\right)$ 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 selected items in $x$ according to the ascending order of their densities $D(x, i)$ $\left(i \in I_{1}(x)\right)$. We then remove $s$ items which are selected from the first $t$ sorted items and re-construct the solution using the greedy randomized construction procedure of Section 2.4.1, leading to a perturbed solution. This perturbed solution is further improved by using the descent procedure of Section 2.4.2. The calibration of the parameters $t$ and $s$ is discussed in Section 3.2.

To improve the diversification effect of the perturbation, we employ a shortterm memory to prevent recently removed items from being added back to the solution in subsequent iterations. Each time an item is removed from the solution, it is not allowed to be inserted to the solution in next $\operatorname{rand}(1, s)$ iterations where $\operatorname{rand}(1, s)$ takes a random value between 1 and $s$.

### 2.8 Implementation improvement

A fast incremental evaluation technique was introduced in [14] to determine rapidly the effect of the $A D D$ and $S W A P$ 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 variable $x_{i}$ produces a new solution $x^{\prime}$ whose raw objective value can be conveniently calculated in $O(1)$ time as: $f_{r}\left(x^{\prime}\right)=f_{r}(x)+\left(1-2 * x_{i}\right) * C(i, x)$, where $C(i, x)$ is the contribution of variable $x_{i}$. Therefore, any solution generated by a move operator which can be realized with constant times of flip operations can be evaluated in $O(1)$ time as well. This is the case for the $A D D$ and $S W A P$ operators which can be realized with one and two flip operations respectively. Using this fast evaluation technique leads to a significant acceleration compared to a complete evaluation which requires $\mathrm{O}\left(n^{2}\right)$ time.

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:

$$
\Delta_{j}=\left\{\begin{array}{llll}
\Delta_{j}, & \text { if } \quad j=i  \tag{8}\\
\Delta_{j}+q_{i j}, & \text { if } \quad x_{i}=1 \quad \text { and } \quad j \in N \backslash\{i\} \\
\Delta_{j}-q_{i j}, & \text { if } \quad x_{i}=0 \quad \text { and } \quad j \in N \backslash\{i\}
\end{array}\right.
$$

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

$$
\begin{equation*}
f_{r}\left(x^{\prime}\right)=f_{r}(x)+\Delta_{i} \tag{9}
\end{equation*}
$$

Similarly, a new solution $x^{\prime}$ produced by swapping items $x_{i}\left(x_{i}=1\right)$ and $x_{j}$ $\left(x_{j}=0\right)$ of the current solution $x$ can be evaluated by the following equation:

$$
\begin{equation*}
f_{r}\left(x^{\prime}\right)=f_{r}(x)-\Delta_{i}+\Delta_{j}-p_{i j} \tag{10}
\end{equation*}
$$

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 $O(1)$.

## 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 experiments on a set of 220 instances ranging from small to very large sizes. These instances can be divided into three groups:

- Group I. This group is composed of 100 small and medium sized benchmark instances generated by Billionnet and Soutif [2]. These instances, generated in the same way as in $[5,6,14,20]$, are very popular and used to test many QKP algorithms. These instances are characterized by their number of objects $n \in\{100,200,300\}$, density $d \in\{25 \%, 50 \%, 75 \%, 100 \%\}$ (i.e., number of non-zero coefficients of the objective function divided by $n(n+1) / 2)$. Each ( $n, d$ ) combination involves 10 different instances distinguished by their labels except for $(300,75 \%)$ and $(300,100 \%)$ where instances are missing. Optimal solutions are known for these instances. The instance data files can be downloaded at http://cedric.cnam.fr/~soutif/QKP/QKP.html.
- Group II. The second group includes 80 large-sized benchmark instances which are recently generated by Yang et al. [37]. These instances have a number of objects from 1000 to 2000 , a value of density from $25 \%$ to $100 \%$. Due to their large size, optimal solutions are still unknown for these instances. The instance data files are available at http://www.info.univ-angers. 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 generator that was very popular and commonly used in QKP literature [1,6,14,20]. The parameter settings for the generator are the same as well: the coefficients $p_{i j}$ of the objective function are integers that are uniformly distributed in the interval $[0,100]$; each weight $w_{j}$ is uniformly distributed in $[1,50]$; the capacity $c$ is randomly selected from $\left[50, \sum_{j=1}^{n} w_{j}\right]$. However, to ensure the hardness of the new instances of Group III, we have performed the following selection process. For each instance, we attained the best objective value of ten feasible solutions, each of which was built by randomly filling the knapsack. A gap between the objective value of the random solution and the best objective value from our IHEA algorithm was then calculated. We denote this gap as randGap. For each $(n, d)$ combination, we generated 10 instances, 5 of which having the largest randGaps were selected to join Group III. The average randGap (in percentage) of all instances in Group III is $69.36 \%$ which indicates that a randomly generated solution is rather poor. From this perspective, finding a high quality solution for these instances is a non-trivial task.

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

[^1]Table 1
Parameter settings of the IHEA algorithm

| Para. | Description | Value | Section |
| :--- | :--- | :--- | :--- |
| $r c l$ | 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 | $\min \left\{10,\left(I_{1}(x)-n_{f}\right)\right\}$ | 2.7 |
| $s$ | number of items to be perturbed | $\min \{3, t\}$ | 2.7 |
| MaxIter | max number of iterations | $\sqrt{n}+65$ | 2.3 |

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/ 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.

### 3.2 Parameter calibration

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 $(\mathrm{GHz})$ | 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 |

formed on a computer with a 3.06 GHz P 4 processor.

- A recent Dynamic Programming heuristic approach [12]. Among all algorithm variants studied in [12], the best performance was achieved by the version using $\tilde{\pi}_{i}^{3} / w_{i}$ as the item ordering rule coupled with the "fill-up and exchange" procedure proposed in [14]. This algorithm version, denoted as $\mathrm{DP}+\mathrm{FE}$, was included for our comparative study. The results of DP +FE in this study were obtained by running the source code (which was kindly given to us by the authors of [12]) on our machine. Since DP+FE is a deterministic heuristic algorithm, it was executed for a single run.
- 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 with the reference approaches due to the differences in computing hardware, termination criterion, etc. This is particularly true for the computing times. For this reason, we focus our study on the quality criterion of the solutions found. Nevertheless, we include information on computing time for indicative purposes. Following [26,31], we used the CPU frequency of our computer (AMD Opteron 41842.8 GHz ) as a basis to scale the times of the reference algorithms reported in $[35,37]$ (see Table 2 for the scaling factors).

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

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] |  |  | $\mathrm{DP}+\mathrm{FE}$ [12] |  |  | GRASP+tabu [37] |  |  | IHEA |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | SR(\%) | RPD | $\mathrm{t}(\mathrm{s})$ | SR(\%) | RPD | $\mathrm{t}(\mathrm{s})$ | SR(\%) | RPD | $\mathrm{t}(\mathrm{s})$ | 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 |

${ }^{1}$ Instance 100_100_4 is not available and is not considered when we calculate the average value for the instance class $100 \_100$.
${ }^{2}$ 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 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 time $t_{b}(s)$ of IHEA is even more interesting since the maximum time is only 0.035 seconds (for 200_50). IHEA outperforms the Min-Swarm approach in the success rate and the relative percentage deviation by consuming typically less CPU seconds. Meanwhile, IHEA dominates the deterministic $\mathrm{DP}+\mathrm{FE}$ algorithm in terms of both solution quality and computational efficiency for all instance classes. Compared to GRASP + tabu which is one of the current best performing heuristic algorithms, IHEA remains very competitive since it solves all these instances to optimality with a $100 \%$ success rate while there are 2 instances for which GRASP + tabu is not able to achieve a success rate of $100 \%$. Another interesting feature of IHEA is that its average computing time is approximately linear relative to the size of the instance which was not observed for the reference algorithms.

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

In this section, we investigate the behavior of our algorithm on the second group of 80 large instances $(n=1000$ or 2000) with unknown optima. Like 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 $\mathrm{DP}+\mathrm{FE}$ were obtained by executing a single run of its source code
on our machine while the results of GRASP+tabu were extracted from [37]. Table 4 (for instances with 1000 objects) and Table 5 (for instances with 2000 objects) summarize the comparative results. The listed indicators include the best lower bound discovered (column Best), the success rate (column SR) to attain the best lower bound, the relative percentage deviation (column RPD) and the average computing time for one trial $(t(s))$. We also report the average best time over 100 trials for our IHEA algorithm (column $t_{b}(s)$ ). The best known results are indicated in italic and the new improved results are highlighted in bold. In the last two rows, \#Bests indicates the number of italic and bold values, and $A v g$. denotes the average value for each column.

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

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

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

| INST. | DP+FE [12] |  | GRASP+tabu [37] |  |  |  | IHEA |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Best | t(s) | Best | SR(\%) | RPD | t(s) | Best | SR(\%) | RPD | t(s) | $t b(s)$ |
| 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 | $1.5 \mathrm{E}-4$ | 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 | $2.3 \mathrm{E}-4$ | 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.
This observation confirms a safe ranking of the three compared algorithms in 2 decreasing order of their performance: IHEA, GRASP+tabu and DP+FE.

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+FE [12] |  | GRASP+tabu [37] |  |  |  | IHEA |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Best | t(s) | Best | SR(\%) | RPD | t(s) | Best | SR(\%) | RPD | t(s) | $t b(s)$ |
| 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 | $4.5 \mathrm{E}-4$ | 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 | $5.1 \mathrm{E}-4$ | 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 | $4.7 \mathrm{E}-4$ | 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 | $2.1 \mathrm{E}-4$ | 424.285 | $\mathbf{2 4 8 3 5 3 4 9}$ | 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 | $1.6 \mathrm{E}-5$ | 329.877 | 14177079 | 100.000 | 0.000 | 32.008 | 0.482 |
| 2000_75_10 | 7815419 | 48717.480 | 7815755 | 78.000 | $8.7 \mathrm{E}-5$ | 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 | $3.0 \mathrm{E}-4$ | 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 | $2.2 \mathrm{E}-4$ | 188.672 | 8394562 | 100.000 | 0.000 | 18.686 | 0.361 |
| 2000_100_10 | 4923413 | 38243.750 | 4923559 | 92.000 | $1.4 \mathrm{E}-4$ | 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 |

### 13.5 Computational results on very large instances of Group III

2 We now present the last experiment on the 40 very large instances of Group III 3 with 5000 to 6000 variables with unknown optima. In addition to their size, the 4 hardness of these instances is also ensured through the selection process when ${ }_{5}$ 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 bounds $\hat{U}_{C P T}^{2}$ (the current tightest bounds), which was previously used in [37] to evaluate their algorithms. The results of $\mathrm{DP}+\mathrm{PE}[12]$ on these instances are not reported since $\mathrm{DP}+\mathrm{PE}$ requires intolerable amount of computing time (indeed, we did not obtain any result with a time limit of one week).

Our IHEA algorithm was executed 100 times for each instance. Table 6 summarizes the results: the best lower bound (column Best), the gap between the upper bound $\hat{U}_{C P T}^{2}$ and the best lower bound in percentage (column GAP, calculated by ( $\hat{U}_{C P T}^{2}-$ Best) $/$ Best $\times 100$ ), success rate (column SR), relative percentage deviation (column RPD), the average computational time for one trial (column $\mathrm{t}(\mathrm{s})$ ) and the average best solution time aver 100 trials (column $t_{b}(s)$ ). The last row (Avg.) indicates the average value of each column. From Table 6, we observe that IHEA is able to attain high quality lower bounds for all these large and difficult instances. These lower bounds are typically very close to the corresponding upper bounds. Indeed, the average gap between the best lower bound and the upper bound $\hat{U}_{C P T}^{2}$ is $1.359 \%$ for the whole instance set. Moreover, IHEA achieves a success rate of $100 \%$ for 30 out of 40 instances ( $75 \%$ ). The average success rate across all instances is $87.675 \%$. When we examine the computing time, the results are quite acceptable. Specifically, the average run time for one trial is 174.075 seconds. The best solution time is much shorter with an average value of 14.456 seconds.

## 4 Discussion

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

### 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-

Table 6
Computational results of IHEA on the 40 very large instances of Group III

| INST. | Best | Gap(\%) | 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 | $3.9 \mathrm{E}-5$ | 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 | $1.0 \mathrm{E}-4$ | 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 | 9.0E-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 |
| 6000_25_4 | 191531304 | 0.276 | 87.000 | $1.2 \mathrm{E}-5$ | 238.917 | 9.093 |
| 6000_25_5 | 36121510 | 1.423 | 100.000 | 0.000 | 208.762 | 3.447 |
| 6000_50_1 | 194344567 | 1.622 | 100.000 | 0.000 | 214.187 | 4.060 |
| 6000_50_2 | 323753804 | 0.376 | 66.000 | 9.6E-5 | 272.235 | 4.864 |
| 6000_50_3 | 31913824 | 2.502 | 100.000 | 0.000 | 220.343 | 3.015 |
| 6000_50_4 | 225556641 | 0.999 | 100.000 | 0.000 | 198.893 | 5.776 |
| 6000_50_5 | 40931924 | 1.885 | 100.000 | 0.000 | 186.351 | 6.849 |
| 6000_75_1 | 204512250 | 0.999 | 12.000 | 5.2E-5 | 267.433 | 86.722 |
| 6000_75_2 | 42422207 | 1.187 | 100.000 | 0.000 | 182.990 | 2.754 |
| 6000_75_3 | 524508156 | 0.477 | 60.000 | $3.4 \mathrm{E}-3$ | 177.873 | 24.377 |
| 6000_75_4 | 197004931 | 1.083 | 100.000 | 0.000 | 220.513 | 4.100 |
| 6000_75_5 | 74350712 | 0.344 | 100.000 | 0.000 | 282.668 | 3.822 |
| 6000_100_1 | 292257056 | 0.069 | 100.000 | 0.000 | 219.599 | 4.054 |
| 6000_100_2 | 219791358 | 0.149 | 1.000 | $9.7 \mathrm{E}-4$ | 257.679 | 122.758 |
| 6000_100_3 | 376967122 | 0.087 | 96.000 | $1.0 \mathrm{E}-6$ | 266.202 | 46.105 |
| 6000_100_4 | 355609720 | 0.058 | 100.000 | 0.000 | 245.857 | 3.710 |
| 6000_100_5 | 686364195 | 0.100 | 38.000 | 4.2E-5 | 211.295 | 69.904 |
| Avg. | - | 1.359 | 87.675 | $1.2 \mathrm{E}-4$ | 174.075 | 14.456 |

ing the best hyperplane where IHEA locates the best solution (column $k^{*}$ ), the average dimension of the initial hyperplane (Avg. $k_{0}$ ), the hyperplane dimension lower bound $\left(k_{L B}\right)$, the hyperplane dimension upper bound ( $k_{U B}$ ) and the average number of hyperplanes explored (Avg.k). Table 7 shows that the average number of hyperplanes that IHEA explores is always less than 3 for these instances. There is one case where Avg.k is exactly 2 which means TabuSearch_Engine finds improved solutions in the first hyperplane but not in the second. For the other 7 cases, TabuSearch_Engine sometimes discovers improved solutions in the second hyperplane, which explains why their

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

| INST. | $k^{*}$ | Avg. $k_{0}$ | $k_{L B}$ | $k_{U B}$ | 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 |

Avg.k value is more than 2 but less than 3. Based on this observation, we conclude that each iteration of the "hyperplane exploration" phase of IHEA typically explores a very limited number of hyperplanes which contributes to its performance. To understand why such a small number of hyperplanes is explored, we examine the initial hyperplane (Avg. $k_{0}$ ). It can be seen that the initial hyperplane is always equal or very close to the best hyperplane (see column $k^{*}$ ). Indeed, there is 1 out of 8 cases where the initial hyperplane is exactly the best hyperplane where the best solution is found, and 7 cases where the initial hyperplane is only one dimension away from the best hyperplane. Moreover, Table 7 indicates that the dimension of the initial hyperplane (column Avg. $k_{0}$ ), which is always within the interval $\left[k_{L B}, k_{U B}\right]$, is very close to $k_{U B}$. The difference between the average values of $A v g . k_{0}$ and $k_{U B}$ is only $908.00-906.75 .00=1.25$. Similar observations can be made for other instances of Group II.

### 4.2 Impact of the variable fixing strategy

As shown in Section 2.5, for a given hyperplane, IHEA has a "high quality" solution as its input. Before exploring the hyperplane with tabu search, we use the density criterion to fix a number of selected items (to the value of $1)$ and thus generate a reduced problem for tabu search. This variable fixing strategy is motivated by the idea that selected items with high density in a high quality solution are strongly determined and should not be destroyed during tabu search. To verify the usefulness of this variable fixing strategy, we conducted an experiment to compare IHEA with a variant IHEA NoVF where the variable fixing strategy is disabled (i.e., removing lines 15-17 from Algorithm 1). As such TabuSearch_Engine explores directly the search space of $C Q K P[k]$ instead of $R C P\left(V_{\text {fixed }}, C Q K P[k], x^{\prime}\right)$ (see Section 2.3).

We ran IHEA and IHEA NoVF 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)

Table 8
Comparative results of IHEA and IHEA NoVF on the benchmarks of Group II

| INST. | IHEA |  |  |  |  | $\mathrm{IHEA}_{N o V F}$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Avg.Best | Avg.SR | t(s) | Avg.\% | Avg.\% | 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 | 24676371.600 | 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 |

and average total computing time (Avg.t(s)), we also list for IHEA the average percentage of fixed variable (Avg. $\%_{F V}$ ) and average percentage of wrongly fixed variable (Avg. $\%_{W F V}$ ), where the percentage of the fixed variables is calculated by: \#fixed_variable $/ \mathrm{k} \times 100$ and the percentage of wrongly fixed variable is calculated by: \#wrongly_fixed_variable/\#fixed_variable $\times 100$. The wrongly fixed variables are identified by comparing the fixed variables to the best known solution reported in Tables 4 and 5. The last row ( Avg .) indicates the average value of some columns.

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

### 4.3 Impact of the perturbation strategy

IHEA uses a density based perturbation strategy to introduce a form of global diversification for a better exploration of the solution space (Section 2.7). To assess the impact of the adopted perturbation strategy, we conducted an experiment to compare the performance of IHEA with two variants IHEA ${ }_{R D P T}$

Table 9
Comparative results of IHEA with IHEA $_{R D P T}$ and IHEA $_{N O P T}$ on the 80 large instances of Group II [37]. The values in bold denote the best results of row Sum.

| INST. | IHEA |  |  | IHEA $_{R D P T}$ |  |  | $\mathrm{IHEA}_{N O P T}$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Avg.Best | Avg.SR | Avg.t(s) | Avg.Best | Avg.SR | Avg.t(s) | Avg.Best | Avg.SR | Avg.t( |
| 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 | 6.39 | 5900793.200 | 98.400 | 9.21 | 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 ${ }_{N O P T}$. IHEA RDPT randomly removes $s$ selected items without considering their densities while IHEA $_{N O P T}$ eliminates the perturbation phase from IHEA. This experiment was also performed on the 80 instances of Group II. As usual, each algorithm was executed 100 times on each instance.

Table 9 summarizes the results based on three indicators: 1) average best solution value (Avg.Best); 2) average success rate (Avg.SR); 3) average computing time for one trial (Avg.t(s)). The last row of the table ( $A v g$.) indicates the average of the listed values of each column. From Table 9, we observe that eliminating the perturbation phase from the IHEA algorithm causes a great deterioration of its performance in terms of both best solution value and success rate. Indeed, compared to IHEA and IHEA $A_{R D P T}$, IHEA ${ }_{N O P T}$ achieved a smaller average best solution (Avg.Best) value for 6 out of 8 instance classes and even a smaller average success rate (Avg.SR) for all 8 classes. When comparing IHEA $_{R D P T}$ with IHEA, one observes that, although IHEA ${ }_{R D P T}$ does not deteriorate the best solution value, it is less stable than IHEA by achieving a smaller average success rate for 7 out of 8 instance classes. A Wilcoxon signed rank test with a significance factor of 0.05 was applied to compare the success rates of $I H E A_{R D P T}$ and IHEA, and the resulting p-value of 0.001602 discloses that IHEA $R_{R D P T}$ is significantly worse than IHEA. Moreover, IHEA ${ }_{R D P T}$ required on average more computing time than IHEA ( 20.171 seconds v.s. 14.367 seconds). This experiment confirms that the perturbation phase of IHEA is useful and the adopted density based strategy is effective.

## 5 Conclusions

This paper deals with the NP-hard Quadratic Knapsack Problem which is a highly useful model in practice. To approximate this hard combinatorial problem, we developed an iterated "hyperplane exploration" approach mixing problem reduction techniques and local optimization with tabu search. The proposed approach introduces a hyperplane constraint to the original QKP
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 comparisons with three best performing methods on two sets of 180 well-known benchmark instances (up to 2000 items) and a set of 40 new instances (with 5000 and 6000 items). The computational experiments showed that the proposed approach competes very favorably with the state-of-the-art algorithms. Specifically, IHEA consistently attained the known optimal solution with a $100 \%$ success rate for all 100 small-sized benchmarks (with 100 to 300 objects). For the set of 80 large benchmarks with 1000 and 2000 objects, IHEA discovered 6 improved results (new best lower bounds) and attained the remaining 74 best known results. Encouraging results on 40 new very large instances (with 5000 and 6000 objects) additionally confirmed the effectiveness of our approach where the average gap between the best lower bound and the well known upper bound $\hat{U}_{C P T}^{2}$ is bounded by $1.359 \%$. The experiments also showed that the proposed approach is more computationally effective than the existing heuristics. Furthermore, we performed additional experiments to gain insight into the "hyperplane exploration" component of the proposed approach, and investigate the beneficial role of two key strategies of the proposed approach: the variable fixing strategy and the perturbation strategy.

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

For future work, there are several interesting directions that could be investigated. First, given the current IHEA algorithm, we can improve the hyperplane exploration (tabu search) by introducing adaptive memory techniques based on recency and/or frequency information projection [19]. Some advanced search frameworks like path relinking and scatter search [16] could also be integrated to reinforce the tabu search engine. Generally, under the IHEA approach, the task of hyperplane exploration can be performed by any effective search algorithm which can be either a heuristic or an exact solver. Second,
it would be useful to investigate additional methods able to identify the most "promising" hyperplanes and thus reduce the number of hyperplanes to be explored. Finally, given that the idea of hyperplane decomposition is quite general, it would be interesting to investigate its merit for solving other knapsack and related problems.

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[^1]:    $\overline{2}$ Our best solution certificates are available at: http://www.info.univ-angers. fr/pub/hao/QKPResults.zip.

