

Iterated maxima search for the maximally diverse grouping problem

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Abstract

The maximally diverse grouping problem (MDGP) is to partition the vertices of an edge-weighted and undirected complete graph into m groups such that the total weight of the groups is maximized subject to some group size constraints. MDGP is a NP-hard combinatorial problem with a number of relevant applications. In this paper, we present an innovative heuristic algorithm called iterated maxima search (IMS) algorithm for solving MDGP. The proposed approach employs a maxima search procedure that integrates organically an efficient local optimization method and a weak perturbation operator to reinforce the intensification of the search and a strong perturbation operator to diversify the search. Extensive experiments on five sets of 500 MDGP benchmark instances of the literature show that IMS competes favorably with the state-of-the-art algorithms. We provide additional experiments to shed light on the rationality of the proposed algorithm and investigate the role of the key ingredients.

Keywords: Graph grouping and clustering problems; iterated search; heuristics.

1 Introduction

Given an edge-weighted and undirected complete graph $G = (V, E, D)$, where $V = \{1, 2, \dots, n\}$ is the set of n vertices, $E = \{\{i, j\} : i, j \in V, i \neq j\}$ is the set of $n \times (n - 1) / 2$ edges, and $D = \{d_{ij} \geq 0 : \{i, j\} \in E\}$ represents the set of non-negative edge weights, the maximally diverse grouping problem (MDGP for short) is to partition the vertex set V into m disjoint subsets or groups such

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7 that the size of each group g lies in a given interval $[a_g, b_g]$ ($g = 1, 2, \dots, m$)
8 while maximizing the sum of the edge weights of the m groups. Here, a vertex
9 $v \in V$ is usually called an element, an edge weight $d_{ij} \in D$ is called the
10 diversity between elements i and j , while a_g and b_g are respectively called the
11 lower and upper limits (or bounds) of the size of group g .

12 MDGP can be expressed as a quadratic integer program with binary variables
13 x_{ig} that take the value of 1 if element i is in group g and 0 otherwise [14,24].

$$\text{Maximize } \sum_{g=1}^m \sum_{i=1}^{n-1} \sum_{j=i+1}^n d_{ij} x_{ig} x_{jg} \quad (1)$$

$$\text{Subject to } \sum_{g=1}^m x_{ig} = 1, i = 1, 2, \dots, n \quad (2)$$

$$a_g \leq \sum_{i=1}^n x_{ig} \leq b_g, g = 1, 2, \dots, m \quad (3)$$

$$x_{ig} \in \{0, 1\}, i = 1, 2, \dots, n; g = 1, 2, \dots, m \quad (4)$$

14 where the set of constraints (2) guarantees that each element is located in
15 exactly one group and the set of constraints (3) forces the size of group g is
16 at least a_g and at most b_g .

17 MDGP belongs to the category of vertex-capacitated clustering problems
18 which are a type of extensively studied combinatorial search problems and
19 can further be divided into the max-clustering problem and min-clustering
20 problem [11,12,16,20,26]. In short, the max-clustering (min-clustering) prob-
21 lem is to partition the vertices of an undirect graph $G = (V, E)$ with edge and
22 vertex weights into m mutually disjoint subsets (groups or clusters) such that
23 the sum of the vertex weights of the subsets is bounded from below by a and
24 from above by b while maximizing (minimizing) the sum of the weights of the
25 edges inside the subsets [16].

26 In addition to its theoretical signification as a typical NP-hard problem, MDGP
27 has a variety of real-world applications, like assignment of students to groups
28 [15,17,30], creation of peer review groups [7], VLSI design [28], storage allo-
29 cation of large programs onto paged memory, and creation of diverse groups
30 in companies so that people from different backgrounds work together [4]. For
31 a review of possible applications of MDGP, the readers are referred to recent
32 papers like [14,22,24,25].

33 Given the practical importance and high computational complexity of MDGP,
34 a number of exact and heuristic algorithms have been proposed in the lit-
35 erature. One of the most representative exact algorithm for MDGP is the
36 column generation approach presented in [16]. Nevertheless, local search or

37 evolutionary heuristics remain the dominant approach in the literature to find
38 high-quality sub-optimal solutions for large graphs. Examples of local search
39 heuristics includes multistart algorithm [1], Weitz-Jelassi (WJ) algorithm [27],
40 Lotfi-Cerveny-Weitz (LCW) algorithm [29], T-LCW method based on LCW
41 and tabu search [14], tabu search with strategic oscillation (TS-SO) [14], mul-
42 tistart simulated annealing (MSA) [21], variable neighborhood search (VNS)
43 [21], general variable neighborhood search (GVNS) [25], skewed general vari-
44 able neighborhood search (SGVNS) [6], iterated tabu search (ITS) [22] and
45 several graph theoretical heuristics [10]. The population-based evolutionary
46 approach includes hybrid genetic algorithm (LSGA) [9], hybrid grouping ge-
47 netic algorithm [7], hybrid steady-state genetic algorithm (HGA) [21], artificial
48 bee colony (ABC) algorithm [24], and constructive genetic algorithm [18]. Ac-
49 cording to the computational results reported on the MDGP benchmarks, the
50 heuristics T-LCW, TS-SO, HGA, MSA, VNS, ABC, GVNS, ITS, and SGVNS
51 achieved high performances at the time they were published.

52 In this paper, we propose an effective heuristic called the iterated maxima
53 search (IMS) algorithm for solving MDGP. IMS follows and extends the iter-
54 ated local search framework [19]. Though IMS shares ideas from breakout local
55 search [2,3] and three-phase local search [13], it distinguishes itself from these
56 approaches by three specific features: its local search procedure (to improve
57 the incumbent solution), the maxima search scheme (to locate other local
58 optima within a limited region of the search space) and its perturbation oper-
59 ator (to modify greatly the incumbent solution). In addition, IMS employs a
60 randomized procedure for initial solution generation. When the proposed algo-
61 rithm was assessed on five sets of 500 benchmark instances ($120 \leq n \leq 3000$)
62 commonly used in the literature, the computational results showed that the
63 algorithm achieves highly competitive results compared to the state-of-the-art
64 algorithms especially on the large-sized instances.

65 In Section 2, we describe the components of the proposed algorithm. Section 3
66 is dedicated to extensive computational assessments based on the commonly
67 used benchmarks with respect to the top performing algorithms from the
68 literature. In Section 4, the important components of the proposed algorithm
69 are analyzed and discussed. Conclusions are provided in the last Section.

70 **2 Iterated Maxima Search Algorithm for MDGP**

71 The proposed iterated maxima search (IMS) algorithm can be considered as an
72 extended iterated local search algorithm [19] and shares ideas from breakout
73 local search [2,3] and three-phase local search [13] (see Section 2.7 for more
74 discussions). IMS is composed of four basic procedures: solution initialization,
75 local search, weak perturbation, and strong perturbation. The basic idea of

76 the IMS algorithm is to provide the search algorithm with a desirable tradeoff
77 between intensification and diversification. This is achieved by iterating the
78 maxima search procedure (local search combined with weak perturbation to
79 explore a limited region around a locally optimal solution) followed by the
80 strong perturbation procedure (to displace the search to a distant region by
81 changing strongly the attained local optimum).

82 2.1 General Procedure

Algorithm 1: Main framework of iterated maxima search method for MDGP

Input: Instance I , the depth of maxima search (α), the strength of strong perturbation (η_s), the cutoff time (t_{max})

Output: The best solution s^* found

```

1 begin
2    $s \leftarrow InitialSolution(I)$            /* Sections 2.3 and 2.4 */
3    $s^* \leftarrow s$ 
4   while  $Time() \leq t_{max}$  do
5      $s \leftarrow MaximaSearch(s, \alpha)$      /* Section 2.5 */
6     if  $f(s) > f(s^*)$  then
7        $s^* \leftarrow s$ 
8     end
9      $s \leftarrow StrongPerturbation(s, \eta_s)$  /* Section 2.6 */
10  end
11  return  $s^*$ 
12 end

```

83 The IMS algorithm (Algorithm 1) starts from a feasible initial solution (Sec-
84 tion 2.2) that is obtained with a randomized construction procedure (Section
85 2.3). Then it repeats a number of iterations until a cutoff time is reached. At
86 each iteration, the incumbent solution s is improved by the maxima search pro-
87 cedure (Sections 2.4 and 2.5) and then perturbed by the strong perturbation
88 procedure (Sections 2.6). The best solution found (s^*) is updated whenever
89 it is needed and finally returned as the output at the end of the IMS algo-
90 rithm. In the rest of this section, we describe the different components of the
91 proposed algorithm.

92 2.2 Search Space, Fitness Function and Solution Representation

93 For a given MDGP instance $G = (V, E)$ with its edge diversity matrix $D =$
94 $[d_{ij}]_{n \times n}$ and the number m of groups, the search space Ω explored by the IMS
95 algorithm contains all partitions of the elements of V into m groups such that

96 the size of each group lies between its lower and upper limits. In other words,
 97 our IMS algorithm visits only feasible solutions.

98 Formally, let $P : V \rightarrow \{1, \dots, m\}$ be a partition function of the n elements of
 99 V to m groups. For each group $g \in \{1, \dots, m\}$ with lower and upper limits a_g
 100 and b_g , let $P_g = \{i \in V : P(i) = g\}$ (i.e., P_g is the set of elements of group g).
 101 Then the search space is given by:

$$102 \quad \Omega = \{P : \forall g \in \{1, \dots, m\}, a_g \leq |P_g| \leq b_g\}.$$

103 For any candidate solution $s = \{P_1, P_2, \dots, P_m\}$ of Ω , its quality or fitness is
 104 given by the objective value $f(s)$:

$$f(s) = \sum_{g=1}^m \sum_{i,j \in P_g, i < j} d_{ij} \quad (5)$$

105 Given a candidate solution $s = \{P_1, P_2, \dots, P_m\}$, we use a n -dimensional vector
 106 y (element coordinate vector) to indicate the group of each element. In other
 107 words, if element i belongs to group P_g , then $y[i] = g$ ($i \in \{1, \dots, n\}$). Addi-
 108 tionally, we use a m -dimensional vector z (group size vector) to indicate the
 109 size of each group in solution s , i.e., $z[g] = |P_g|$ ($g \in \{1, \dots, m\}$). It should
 110 be clear that any solution $s \in \Omega$ can be fully characterized by its associated y
 111 and z vectors. For this reason, we use the notation $s = \langle y, z \rangle$ to represent a
 112 solution in the rest of this section whenever this is appropriate.

113 2.3 Initial Solution

114 In the IMS algorithm, the initial solution is generated as follows. First, we
 115 construct β feasible solutions, each solution being generated in two stages.
 116 First, we pick an empty group g ($g \in \{1, \dots, m\}$), randomly select a_g ele-
 117 ments among the unassigned elements, assign them to group g , and repeat
 118 this process until all groups reach their lower bound a_g in size. Second, the
 119 remaining elements are assigned to a random group whose size is less than b_g
 120 in an one-by-one way. Finally, for each constructed solution, the local search
 121 procedure (see Section 2.4) is applied to improve its quality. The best one
 122 among those β solutions is chosen as the initial solution of our IMS algorithm.
 123 This initialization procedure is an adaptation of previous approaches used in
 124 [6,14,25].

Algorithm 2: Local Search Procedure

```
1 Function LocalSearch( $s = \langle y, z \rangle$ )
   Input: Element coordinate vector  $y[1 : n]$ , group size vector  $z[1 : m]$ 
   Output: The local optimum solution (denoted by  $\langle y, z \rangle$ )
2 Initialize  $f$ , move value matrix  $\gamma[n, m]$           /* Section 2.4.2 */
3 Improve  $\leftarrow$  true
4 while Improve = true do
5   Improve  $\leftarrow$  false
6   /* Examine the neighborhood  $N_1$  in a lexicographical order */
7   for  $v \leftarrow 1$  to  $n$  do
8     for  $g \leftarrow 1$  to  $m$  do
9       if  $(y[v] \neq g) \wedge (z[y[v]] > a_{y[v]}) \wedge (z[g] < b_g)$  then
10         $\Delta_f \leftarrow \gamma[v][g] - \gamma[v][y[v]]$  /* Calculate the move value */
11        if  $\Delta_f > 0$  then
12           $z[y[v]] \leftarrow z[y[v]] - 1$ 
13           $z[g] \leftarrow z[g] + 1$ 
14           $y[v] \leftarrow g$  /* Update the incumbent solution */
15           $f \leftarrow f + \Delta_f$ 
16          Update matrix  $\gamma$  /* Section 2.4.2 */
17          Improve  $\leftarrow$  true
18        end
19      end
20    end
21  end
22  /* Examine the neighborhood  $N_2$  in a lexicographical order */
23  for  $v \leftarrow 1$  to  $n - 1$  do
24    for  $u \leftarrow v + 1$  to  $n$  do
25      if  $y[v] \neq y[u]$  then
26         $\Delta_f \leftarrow (\gamma[v][y[u]] - \gamma[v][y[v]]) + (\gamma[u][y[v]] - \gamma[u][y[u]]) - 2d_{vu}$ 
27        if  $\Delta_f > 0$  then
28          Swap( $y, v, u$ ) /* Update the incumbent solution */
29           $f \leftarrow f + \Delta_f$ 
30          Update matrix  $\gamma$  /* Section 2.4.2 */
31          Improve  $\leftarrow$  true
32        end
33      end
34    end
35  end
36 end
37 return  $\langle y, z \rangle$ 
```

125 2.4 Local Search Method

126 For local optimization, the IMS algorithm employs a double-neighborhood
127 local search method described in Algorithm 2 (also see Sections 2.4.1 and

128 2.4.2 for details), where γ and Δ_f are defined in Section 2.4.2. Starting with an
 129 input solution, the local search method examines in a deterministic order two
 130 complementary neighborhoods N_1 and N_2 (see Section 2.4.1 for the definition
 131 of these neighborhoods), and updates the incumbent solution each time an
 132 improving neighbor solution is detected. This process terminates when the
 133 incumbent solution s can not be further improved by any neighbor solution in
 134 both $N_1(s)$ and $N_2(s)$.

135 Specifically, the local search method examines the neighborhoods N_1 and N_2
 136 in a token-ring way ($N_1 \rightarrow N_2 \rightarrow N_1 \rightarrow N_2 \rightarrow N_1 \rightarrow N_2, \dots$). When ex-
 137 amining a given neighborhood (N_1 or N_2), neighbor solutions are visited in a
 138 lexicographical order (Alg. 2, lines 7-21 for N_1 and lines 23-35 for N_2). Each
 139 time an improving neighbor solution is found, it becomes the new incumbent
 140 solution (first improvement strategy) and the search continues from this point
 141 to explore neighbor solutions within the neighborhood of the new incumbent
 142 solution (Alg. 2, lines 12-16 for N_1 and lines 28-30 for N_2). According to the
 143 algorithm, the search switches from N_1 to N_2 after examining at most $n \times m$
 144 neighbor solutions and from N_2 to N_1 after considering at most $\frac{n \times (n-1)}{2}$ solu-
 145 tions. Note that the 'if' tests in lines 9 and 25 aim at excluding solutions that
 146 do not belong to the neighborhoods N_1 and N_2 .

147 The whole local search method stops when no better solution can be found in
 148 both N_1 and N_2 and returns the best solution encountered which is a locally
 149 optimal solution with respect to N_1 and N_2 .

150 Note that though our local search method uses the same neighborhoods as
 151 the variable neighborhood descent (VND) method in [6], our way of exploring
 152 the two neighborhoods is quite different. The standard VND method starts
 153 with the first neighborhood N_1 and makes a complete exploitation of this
 154 neighborhood. It switches to the next neighborhood N_2 when a local optimum
 155 is attained with respect to N_1 . Moreover, VND switches immediately to the
 156 first neighborhood N_1 as soon as an improving solution is encountered in N_2 .
 157 VND stops when the search process reaches the end of neighborhood N_2 , i.e.,
 158 when no improving solution can be found in N_2 .

159 In the following subsections, we describe in detail the neighborhood structures
 160 and the streamlining technique for a fast neighborhood evaluation which is
 161 useful to accelerate the local search procedure.

162 2.4.1 Neighborhood Structures

163 We now define the two neighborhoods explored by the local search proce-
 164 dure, called the constrained one-move neighborhood (denoted by N_1) and
 165 swap neighborhood (N_2) respectively. For MDGP, N_1 and N_2 are two popular
 166 neighborhoods that were used in several previous studies [6,14,21,22,24,25].

167 The constrained *OneMove* neighborhood N_1 is defined as follows. Given a
 168 solution (or partition) $s = \{P_1, P_2, \dots, P_m\}$, the *OneMove* operator transfers
 169 a vertex v from its current group P_i to another group P_j such that $|P_i| > a_i$
 170 and $|P_j| < b_j$, where a_i and b_j denote respectively the lower limit of $|P_i|$
 171 and the upper limit of $|P_j|$. Let $\langle v, P_i, P_j \rangle$ designate such a move and
 172 $s \oplus \langle v, P_i, P_j \rangle$ be the resulting neighboring solution when applying the
 173 move to s . Then the neighborhood N_1 of s is composed of all possible solutions
 174 that can be obtained by applying the constrained *OneMove* operator to s . i.e.,

$$175 \quad N_1(s) = \{s \oplus \langle v, P_i, P_j \rangle : v \in P_i, i \neq j, |P_i| > a_i, |P_j| < b_j\}$$

176 One notices that this neighborhood is not applicable if $a_i = b_i$ holds for all
 177 the groups. Clearly N_1 is bounded by $O(nm)$ in size.

178 The *SwapMove* neighborhood N_2 is defined as follows. Given two vertices v
 179 and u which are located in two different groups of solution s , the *SwapMove*(v, u)
 180 move exchanges their groups to produce a neighboring solution. Thus, the
 181 neighborhood N_2 of a solution s is composed of all possible neighboring solu-
 182 tions that can be obtained by applying *SwapMove* to s , i.e.,

$$183 \quad N_2(s) = \{s \oplus \text{SwapMove}(v, u) : v \in P_i, u \in P_j, 1 \leq i < j \leq m\}$$

184 Clearly the size of N_2 is bounded by $O(n^2)$ and is usually much larger than
 185 that of N_1 since often $n \gg m$ holds.

186 2.4.2 Fast Neighborhood Evaluation Technique

187 Like [6,21,22,24,25], we adopt an incremental technique for fast evaluation of
 188 the considered neighborhood. We maintain a $n \times m$ matrix γ to effectively
 189 calculate the move value (i.e., the change of objective value) of each candidate
 190 move, where the entry $\gamma[v][g]$ represents the sum of weights between the vertex
 191 v and vertices in the group g for the current solution.

192 Given the current solution s , if a *OneMove* move, $\langle v, P_i, P_j \rangle$, is performed,
 193 the move value can be easily determined as $\Delta_f(\langle v, P_i, P_j \rangle) = \gamma[v][j] - \gamma[v][i]$,
 194 and then the matrix γ is updated accordingly. Specifically, the i -th and j -th
 195 columns of matrix γ are updated as follows: $\gamma[u][i] = \gamma[u][i] - d_{vu}$, $\gamma[u][j] =$
 196 $\gamma[u][j] + d_{vu}$, $\forall u \in V, u \neq v$, where d_{vu} is the diversity between vertices v and
 197 u . On the other hand, if a *SwapMove*(v, u) operation, which is composed of
 198 two *OneMove* operations, is performed, its move value can be calculated as
 199 $\Delta_f(\text{SwapMove}(v, u)) = (\gamma[v][y[u]] - \gamma[v][y[v]]) + (\gamma[u][y[v]] - \gamma[u][y[u]]) - 2d_{vu}$,
 200 where $y[v]$ and $y[u]$ are the group of vertex v and u in the current solution
 201 $s = \langle y, z \rangle$ (see Section 2.2).

202 The matrix γ is initialized at the beginning of each neighborhood search, and

203 is updated after each move, which can respectively be achieved in $O(n^2)$ and
 204 $O(n)$ for *OneMove* and *SwapMove*.

205 *2.5 Maxima Search Procedure with Weak Perturbation*

Algorithm 3: Maxima Search Procedure for MDGP

```

1 Function MaximaSearch( $s_0, \alpha$ )
  Input: Initial solution  $s_0$ , the depth of maxima search  $\alpha$ 
  Output: The best solution  $s_b$  found
2 begin
3    $s \leftarrow s_0$ 
4    $s_b \leftarrow \text{LocalSearch}(s)$                                 /* Section 2.4 */
5    $counter \leftarrow 0$ 
6   while  $counter < \alpha$  do
7      $s \leftarrow \text{WeakPerturbation}(s_b)$                        /* Section 2.5 */
8      $s \leftarrow \text{LocalSearch}(s)$                                /* Section 2.4 */
9     if  $f(s) > f(s_b)$  then
10       $s_b \leftarrow s$ 
11       $counter \leftarrow 0$ 
12    else
13       $counter \leftarrow counter + 1$ 
14    end
15  end
16  return  $s_b$ 
17 end

```

206 The maxima search (MS) procedure, as described in Algorithm 3, aims to
 207 detect other locally optimal solutions of better quality within a limited search
 208 region around a given input local optimum. For this purpose, it alternates
 209 between the local search procedure described in Section 2.4 and a weak per-
 210 turbation procedure explained below. Specifically, starting with the input so-
 211 lution, MS first applies the local search procedure to obtain a local optimum
 212 which becomes the incumbent solution (Alg. 3, line 4). Then, it performs the
 213 weak perturbation procedure (Alg. 3, line 7) to change slightly the incumbent
 214 solution. This is followed by a new round of the local search procedure (Alg.
 215 3, line 8) to reach a new local optimum from the perturbed solution. These
 216 two procedures are repeated until the incumbent solution can not be improved
 217 for α consecutive perturbations (α is called the depth of the MS procedure).
 218 Finally, the best solution found is returned as the result of the maxima search
 219 procedure.

220 Within the above maxima search procedure, the weak perturbation opera-
 221 tor aims to jump out of the current local optimum trap by accepting some

Algorithm 4: Weak Perturbation Operator

```
1 Function WeakPerturbation( $s_0$ )
   Input: Input solution  $s_0$ , neighborhoods  $N_1 - N_2$  defined in Section 2.4.1,
           strength of weak perturbation  $\eta_w$ 
   Output: The perturbed solution  $s_p$ 
2 begin
3    $s_p \leftarrow s_0$ 
4   for  $L \leftarrow 1$  to  $\eta_w$  do
5     Randomly pick a neighbor solution  $s \in N_1(s_p) \cup N_2(s_p)$ 
6     for  $l \leftarrow 1$  to  $|V|$  do
7       Randomly pick a neighbor solution  $s' \in N_1(s_p) \cup N_2(s_p)$ 
8       if  $f(s') > f(s)$  then
9          $s \leftarrow s'$ 
10      end
11     end
12      $s_p \leftarrow s$ 
13 end
14 return  $s_p$ 
15 end
```

222 deteriorating solutions. As shown in Algorithm 4, it realizes η_w controlled
223 *OneMove* or *SwapMove* steps (Section 2.4.1) where η_w (a parameter) is called
224 the strength of weak perturbation. Specifically, for each weak perturbation step
225 (i.e., each iteration of the outer 'for' loop of Alg. 4, line 4), we first identify
226 the best solution among randomly sampled $|V| + 1$ neighbor solutions of the
227 current solution s_p (Alg. 4, lines 5-11) and then use this best solution to re-
228 place the current solution s_p (Alg. 4, line 12), which serves as the starting
229 point for the next perturbation step. The generated solution following these
230 η_w weak perturbation steps is returned as the incumbent solution of the next
231 round of the local search procedure. Note that large samples deteriorate less
232 the current solution and we use the problem size $|V|$ to adjust the sample size.

233

2.6 Strong Perturbation

234 The maxima search procedure equipped with its weak perturbation procedure
235 helps to discover new and better local optima around an input optimum. How-
236 ever, the search can be trapped into deep local optima and weak perturbations
237 are no more sufficient for the algorithm to continue its search. Hence, our IMS
238 algorithm employs a strong perturbation procedure to jump out of such deep
239 local optimum traps. The strong perturbation procedure consecutively per-
240 forms η_s randomly selected *OneMove* or *SwapMove* moves regardless of the
241 objective value of each performed move, where η_s is called the strength of

Algorithm 5: Strong Perturbation

1 **Function** *StrongPerturbation*(s_0, η_s)

Input: Input solution s_0 , neighborhoods $N_1 - N_2$ defined in Section 2.4.1,
strength of perturbation η_s

Output: The perturbed solution s_p

2 **begin**

3 $s_p \leftarrow s_0$

4 **for** $L \leftarrow 1$ **to** η_s **do**

5 Randomly pick a neighbor solution $s \in N_1(s_p) \cup N_2(s_p)$

6 $s_p \leftarrow s$

7 **end**

8 **return** s_p

9 **end**

242 strong perturbation. In this study, η_s is empirically set as $\eta_s = \theta \times \frac{n}{m}$, where
243 θ is a parameter that is used to control the strong perturbation strength, n is
244 the size of problem instance, and m is the number of groups. The pseudo-code
245 of the strong perturbation operator is shown in Algorithm 5.

246 2.7 Motivations and Related Search Frameworks

247 Like most heuristic approaches in the literature, the proposed IMS algorithm
248 lacks a strict theoretical basis. On the other hand, the design of the IMS al-
249 gorithm relies on the well-known basic principle that an efficient algorithm
250 must ensure a suitable tradeoff between intensification and diversification of
251 its search process. To achieve this goal, the proposed algorithm employs the
252 maxima search procedure (Section 2.5 and Alg. 3) to perform an intensified
253 search around a limited search region (i.e., locate the best possible solution
254 within the nearby region around a discovered local optimum). When the max-
255 ima search procedure is trapped in a deep local optimum, the IMS algorithm
256 switches to the strong perturbation procedure (Section 2.6) to jump out of
257 the trap and displace the search to a more distant region. The analysis on
258 spatial distribution of high-quality local optima shown in Section 4.3 provides
259 additional evidences about the rationality of the proposed IMS algorithm.

260 From the perspective of algorithm design, the proposed IMS algorithm shares
261 the same framework as the three-phase search (TPS) method [13] which also
262 uses a weak (or strong) perturbation procedure to explore nearby (or distant)
263 local optima. On the other hand, unlike TPS which applies a directed per-
264 turbation procedure based on a tabu list, IMS relies on the best neighbor
265 strategy based on a random sample. IMS also shares ideas with the breakout
266 local search (BLS) method [2,3] where both the perturbation type and per-

267 turbation strength are determined in an adaptive manner. BLS has a strong
268 emphasis on an adaptive mechanism to control the application of three well-
269 separated perturbation operators (directed perturbation, random perturba-
270 tion, and frequency-based perturbation). Unlike BLS, IMS follows a simpler
271 scheme and invokes its weak perturbation procedure (embedded inside the
272 maxima search) and strong perturbation procedure deterministically.

273 As shown in the next section, the IMS algorithm equipped with its particular
274 features proves to perform very well on many MDGP benchmark instances.

275 3 Experimental Results and Comparisons

276 Following the practice of the literature, we assess the performance of our IMS
277 algorithm by presenting computational results on a large number of bench-
278 mark instances, and making comparisons with the state-of-the-art MDGP al-
279 gorithms in the literature.

280 3.1 Benchmark Instances

281 Our computational assessments are based on four sets of 460 benchmarks
282 which are extensively used in the literature¹ and a new set of 40 large scale
283 benchmarks which are adapted from the related maximum diversity problem
284 (MDP)². The details of the benchmark instances are described as follows.

- 285 • **RanReal set:** This set consists of 40 instances with equal group sizes (EGS)
286 and 40 instances with different group sizes (DGS), where the distances (or
287 diversities) between elements are a real number uniformly and randomly
288 generated in $(0, 100)$. The number of elements n varies from 120 to 960, the
289 number of groups m is between 10 and 24, and the minimum and maximum
290 group sizes a_g and b_g are in the range of $\{2, 3, \dots, 48\}$. Moreover, for the
291 EGS instances, both a_g and b_g are given by $\lfloor n/m \rfloor$.
- 292 • **RanInt set:** This set has the same structure as the RanReal set and consists
293 of 40 EGS instances and 40 DGS instances. The distances between elements
294 are an integer uniformly and randomly generated in the interval $[0, 100]$.
- 295 • **Geo set:** As the previous two sets of benchmarks, this set contains 40 EGS
296 instances and 40 DGS instances, but the distances are Euclidean distances
297 between pairs of points with random coordinates from $[0, 10]$, and the num-
298 ber of coordinates for each point is generated randomly in $[2, 21]$.

¹ Available from <http://www.opticom.es/mdgp/mdgplib.zip>

² Available from <http://www.opticom.es/mdp/#instances>

299 • **MDG-a set:** This set is composed of 11 subsets adapted from graphs of
300 the related maximum diversity problem [8], where each subset contains 20
301 instances with $n = 2000$. For the first subset, the number of groups m is set
302 to 50, the lower and upper limits of the group sizes a_g and b_g are respectively
303 fixed to 32 and 48. This subset was first adapted in [21] for MDGP, and
304 then used in [6]. The characteristics of the remaining 10 subsets are given
305 in Table 1. These 10 subsets were first adapted in [24] for MDGP and then
306 used in [6] under the name "Type1_22". For all these 220 instances, the
307 distances between elements are randomly generated between 0 to 10 using
308 an uniform distribution.

Table 1

The number of groups, lower and upper group limits for the instances in the set MDG-a.

n	m	DGS		EGS
		a_g	b_g	$a_g = b_g$
2000	50	32	48	–
2000	10	173	227	200
2000	25	51	109	80
2000	50	26	54	40
2000	100	13	27	20
2000	200	6	14	10

309 • **MDG-c set:** This new set, introduced in this paper, consists of 20 DGS
310 instances and 20 EGS instances with $n = 3000$ and $m = 50$, which are
311 adapted from graphs of the maximum diversity problem. The lower and
312 upper limits a_g and b_g of group sizes for these instances are respectively fixed
313 to $\lfloor 0.8n/m \rfloor$ and $\lfloor 1.2n/m \rfloor$ for the DGS instances. For the EGS instances,
314 both a_g and b_g are given by $\lfloor n/m \rfloor$. The distances between elements are
315 randomly generated in $[0,1000]$.

316 3.2 Parameter Setting and Experimental Protocol

Table 2

Setting of parameters

Parameters	Section	Description	Values
β	2.3	number of initial solutions	10
η_w	2.6	strength of weak perturbation	3
α	2.5	depth of maxima search procedure	{3,5}
θ	2.6	coefficient for the strength of strong perturbation	{1.0,1.5}

317 Before presenting our computational results, we first provide some basic infor-
318 mation about our experiments, including the parameter settings used by our
319 IMS algorithm, the reference algorithms, the experimental platform, and the
320 termination conditions of algorithms.

321 First, Table 2 shows the parameter setting of the IMS algorithm which was
322 achieved by a preliminary experiment. Notice that the parameter α (depth of
323 maxima search) takes 5 for the instances with $n \leq 400$ or $n/m \leq 10$, and 3

324 for the remaining instances. For the parameter θ , which is used to control the
325 strength of strong perturbation, we also use two values, (i.e., $\theta \in \{1.0, 1.5\}$),
326 where θ is set to 1.0 for small instances with $n \leq 400$ and 1.5 for the remaining
327 instances. These parameter values are used for all the following experiments
328 even though a fine tuning of some parameters would lead to better results.

329 According to the computational results reported in two most recent papers
330 [6,22], the ITS and SGVNS algorithms can be considered as the state-of-
331 the-art algorithms for MDGP. Specifically, the ITS algorithm dramatically
332 outperformed its reference algorithms, including MSA, HGA, VNS of [21] and
333 TS-SO, T-LCW of [14], and the SGVNS algorithm significantly outperformed
334 its reference algorithms, including HGA, TS-SO, ABC of [24], and GVNS of
335 [25]. Consequently, in this study we use the ITS and SGVNS algorithms as
336 the reference algorithms to assess the performance of our IMS algorithm.

337 It is worth noting that in this study all the experiments were based on the same
338 computing platform, which makes it possible to perform a rather fair compar-
339 ison between our IMS algorithm and the two reference algorithms ITS and
340 SGVNS. The source code of the ITS algorithm was kindly provided by the au-
341 thors and is available at <http://www.proin.ktu.lt/~gintaras/mdgp.html>,
342 and the executable code of the SGVNS algorithm was kindly provided by the
343 corresponding author of [6]. The IMS and ITS codes were compiled using g++
344 compiler³, and all experiments were carried out on a computing platform with
345 an Intel Xeon E5440 processor (2.83 GHz CPU and 2Gb RAM), running the
346 Linux operating system. Following the DIMACS machine benchmark proce-
347 dure, our machine requires respectively 0.23, 1.42, and 5.42 seconds for the
348 graphs r300.5, r400.5, r500.5⁴.

349 For all algorithms considered in this study, the stopping condition is a fixed
350 cutoff time limit t_{max} which depends on the size of the instances. Specifically,
351 t_{max} is set as follows: $t_{max} = 3$ seconds for $n = 120$, 20 seconds for $n = 240$,
352 120 seconds for $n = 480$ seconds, 600 seconds for $n = 960$, 1200 seconds for
353 $n = 2000$, and 3000 seconds for $n = 3000$. Finally, due to the stochastic nature
354 of the compared algorithms, each instance was independently solved 20 times
355 by each algorithm.

³ Our code will be available at <http://www.info.univ-angers.fr/pub/hao/mdgp.html>

⁴ The benchmark program (dmclique.c) and the rxxx.5 graphs are available at <ftp://dimacs.rutgers.edu/pub/challenge/graph/solvers/>

357 The RanInt, RanReal and Geo benchmarks have been widely tested to assess
 358 the performance of MDGP algorithms in the literature. The computational
 359 results of our IMS algorithm and the reference algorithms ITS and SGVNS
 360 are summarized in Tables 3–8. Column 1 of the tables gives the names of
 361 instances (Instance). Columns 2–4 report the best objective values (f_{best}) ob-
 362 tained over 20 independent runs of the compared algorithms. Columns 5–7
 363 show the average objective values (f_{avg}). The best values among the results
 364 of the competing algorithms are indicated in bold. The row '#Best' indicates
 365 the number of instances for which an algorithm performs the best among the
 366 compared algorithms. To verify whether there exists a significant difference
 367 between IMS and the reference algorithms in terms of the best and average
 368 objective values, the p -values from the non-parametric Friedman tests are re-
 369 ported in the last row of each table. A p -value smaller than 0.05 indicates a
 370 significant difference between two sets of compared results.

371 Tables 3 and 4 show that for the RanInt instances, IMS outperforms the
 372 reference algorithms. For the 40 instances with different group sizes, IMS yields
 373 the best outcomes for 29 and 36 instances in terms of the best and average
 374 objective values. For the 40 instances with equal group sizes, IMS performs the
 375 best on 32 and 26 instances in terms of the best and average objective values.
 376 Furthermore, the small p -values confirm the significance of the differences
 377 between the results of the IMS algorithm and those of two reference algorithms.

378 Tables 5 and 6 on the RanReal instances indicate that the IMS algorithm
 379 also outperforms the ITS and SGVNS algorithms on this set of benchmarks.
 380 For the 40 instances with different group sizes, IMS yields the 25 and 37 best
 381 outcomes in term of the best and average values. For the 40 instances with
 382 equal group sizes, IMS obtains the largest 'best' and 'average' values for 29
 383 and 26 instances. The Friedman tests (with p -values smaller than 0.05) confirm
 384 the statistical significance of the observed differences.

385 Tables 7 and 8 show that for the Geo instances, IMS performs significantly
 386 better than SGVNS, but performs worse than ITS. For the instances with
 387 different group sizes, IMS obtains better results than SGVNS for all instances
 388 in terms of both the best and average objective values. However, compared
 389 to the ITS algorithm, IMS yields a better and worse result respectively for 16
 390 and 24 instances in terms of the best objective value. Concerning the average
 391 objective value, IMS obtains a better and worse result respectively for 26 and
 392 14 instances compared to ITS. The p -values (> 0.05) in terms of the best and
 393 average objective values do not reveal a significant difference between IMS and
 394 ITS. However, for the instances with equal group sizes, ITS clearly dominates
 395 IMS and SGVNS.

Table 3
Comparison of the IMS algorithm with two state-of-the-art algorithms (i.e., ITS [22] and SGVNS [6]) on the RanInt instances with different group sizes.

Instance	f_{best}			f_{avg}		
	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
RanInt_n120_ds_01	51161	51097	51125	51003.45	50855.75	50920.60
RanInt_n120_ds_02	51400	51380	51366	51252.10	51204.55	51259.90
RanInt_n120_ds_03	50245	50248	50233	50144.25	50108.80	50150.50
RanInt_n120_ds_04	50394	50387	50400	50123.15	50323.30	50340.30
RanInt_n120_ds_05	49884	49996	49928	49447.30	49804.00	49803.50
RanInt_n120_ds_06	49734	49678	49701	49532.40	49496.50	49583.90
RanInt_n120_ds_07	50184	50282	50316	49743.90	50160.05	50212.90
RanInt_n120_ds_08	50459	50351	50345	50269.20	50262.05	50272.20
RanInt_n120_ds_09	50499	50429	50445	50345.05	50259.80	50322.10
RanInt_n120_ds_10	50337	50364	50327	50217.25	50256.30	50232.40
RanInt_n240_ds_01	160390	160460	160498	159964.70	160203.20	160308.50
RanInt_n240_ds_02	160019	160154	160095	159638.25	159679.50	159812.30
RanInt_n240_ds_03	160235	160211	160338	159756.60	159877.35	160071.50
RanInt_n240_ds_04	162728	162340	162473	161894.35	162001.85	162280.30
RanInt_n240_ds_05	160423	160648	160653	160177.40	160186.95	160378.50
RanInt_n240_ds_06	160944	161049	161145	160580.00	160739.70	160810.40
RanInt_n240_ds_07	159770	159950	160156	159362.70	159506.10	159734.00
RanInt_n240_ds_08	158161	157953	158087	157748.30	157666.85	157879.20
RanInt_n240_ds_09	160463	160409	160551	160060.30	160119.85	160322.00
RanInt_n240_ds_10	159924	160009	160278	159537.75	159659.00	159934.70
RanInt_n480_ds_01	389602	390304	390687	388476.85	389181.00	389623.90
RanInt_n480_ds_02	387757	388585	388972	386995.15	387679.55	388277.70
RanInt_n480_ds_03	387751	387691	388054	386584.75	386844.00	387213.70
RanInt_n480_ds_04	391604	391231	392298	390641.05	390461.90	391689.10
RanInt_n480_ds_05	388757	388818	389107	387718.15	387679.15	388374.30
RanInt_n480_ds_06	388764	389422	390029	387961.70	388465.45	389168.80
RanInt_n480_ds_07	388513	389171	389350	387879.15	388096.00	388474.70
RanInt_n480_ds_08	390230	390473	391128	389552.45	389621.65	390463.60
RanInt_n480_ds_09	388128	388388	388704	387012.65	387309.75	388001.90
RanInt_n480_ds_10	392870	393025	393193	390827.85	391957.00	392508.30
RanInt_n960_ds_01	1238944	1239019	1243609	1236212.25	1236760.85	1241662.80
RanInt_n960_ds_02	1236221	1236536	1240503	1233795.30	1234449.25	1239303.65
RanInt_n960_ds_03	1236516	1238062	1241375	1234214.00	1235002.35	1239435.05
RanInt_n960_ds_04	1237219	1238364	1241400	1235456.15	1236642.60	1239878.15
RanInt_n960_ds_05	1239017	1236447	1239833	1235692.80	1234464.35	1238354.15
RanInt_n960_ds_06	1234678	1234548	1237280	1233006.60	1232092.50	1235741.05
RanInt_n960_ds_07	1238255	1237651	1241459	1235368.65	1235281.30	1240246.50
RanInt_n960_ds_08	1234648	1234856	1238195	1232458.30	1232390.75	1236536.85
RanInt_n960_ds_09	1235323	1234310	1240169	1233074.55	1232668.80	1237532.00
RanInt_n960_ds_10	1237697	1237662	1240515	1235317.70	1236135.80	1239079.30
#Best	7	4	29	2	2	36
p-value	5.04e-4	9.55e-6		1.26e-8	1.26e-8	

Table 4
Comparison of the IMS algorithm with two state-of-the-art algorithms (i.e., ITS [22] and SGVNS [6]) on the RanInt instances with equal group sizes.

Instance	f_{best}			f_{avg}		
	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
RanInt_n120_ss_01	47909	47909	47909	47898.35	47893.25	47884.05
RanInt_n120_ss_02	47826	47826	47826	47818.60	47793.90	47794.85
RanInt_n120_ss_03	47552	47552	47552	47490.20	47475.25	47449.05
RanInt_n120_ss_04	47611	47556	47611	47538.85	47488.50	47514.45
RanInt_n120_ss_05	47148	47191	47191	47122.70	47106.65	47089.45
RanInt_n120_ss_06	46647	46641	46622	46592.05	46579.35	46556.05
RanInt_n120_ss_07	47142	47142	47142	47111.45	47085.65	47063.75
RanInt_n120_ss_08	47390	47356	47390	47369.45	47323.85	47325.25
RanInt_n120_ss_09	47660	47660	47660	47636.10	47628.15	47613.35
RanInt_n120_ss_10	47807	47807	47807	47801.75	47780.55	47778.25
RanInt_n240_ss_01	155566	155538	155474	155232.15	155369.20	155352.50
RanInt_n240_ss_02	155219	155325	155252	155088.50	155114.20	155120.55
RanInt_n240_ss_03	156325	156387	156415	156121.35	156226.85	156308.30
RanInt_n240_ss_04	156559	156643	156588	156381.25	156408.60	156430.45
RanInt_n240_ss_05	156499	156562	156479	156171.75	156185.85	156305.35
RanInt_n240_ss_06	155465	155516	155536	155149.25	155314.85	155265.95
RanInt_n240_ss_07	155770	155729	155697	155463.15	155551.10	155529.05
RanInt_n240_ss_08	155247	155398	155398	154965.05	155095.15	155068.60
RanInt_n240_ss_09	156013	155967	156012	155944.15	155800.35	155991.90
RanInt_n240_ss_10	155877	155947	155971	155670.60	155781.20	155803.05
RanInt_n480_ss_01	379455	379879	380157	378592.85	379264.40	379678.05
RanInt_n480_ss_02	379597	379628	379992	378531.60	379026.70	379482.55
RanInt_n480_ss_03	378511	379025	379067	377643.95	378490.25	378634.70
RanInt_n480_ss_04	378395	378936	379067	377815.00	378551.90	378759.80
RanInt_n480_ss_05	379627	379833	380147	378457.50	378946.45	379316.45
RanInt_n480_ss_06	379161	379304	379681	378067.85	378601.25	379013.20
RanInt_n480_ss_07	379325	379544	380022	378358.75	379068.55	379297.20
RanInt_n480_ss_08	379218	380115	380088	378435.25	379222.70	379466.85
RanInt_n480_ss_09	378383	378610	379147	377686.75	378111.20	378526.75
RanInt_n480_ss_10	379409	380291	380615	378905.25	379606.65	379791.65
RanInt_n960_ss_01	1217365	1217792	1220724	1215311.10	1215593.80	1219004.55
RanInt_n960_ss_02	1216579	1216227	1220169	1214601.85	1215048.10	1218219.00
RanInt_n960_ss_03	1217448	1217651	1220210	1215203.50	1215957.35	1218739.85
RanInt_n960_ss_04	1216950	1217392	1220242	1215775.35	1215559.60	1218289.95
RanInt_n960_ss_05	1217487	1217823	1218916	1214914.15	1215602.55	1218060.15
RanInt_n960_ss_06	1217904	1218274	1220803	1215522.80	1216142.75	1218880.75
RanInt_n960_ss_07	1218376	1217927	1220234	1215830.85	1216009.85	1219180.90
RanInt_n960_ss_08	1216778	1217721	1220555	1215293.95	1215895.80	1219391.00
RanInt_n960_ss_09	1215583	1216735	1218576	1213553.35	1214226.35	1217497.95
RanInt_n960_ss_10	1214982	1216159	1219384	1213743.10	1214343.60	1217076.40
#Best	11	13	32	10	4	26
p-value	1.01e-4	1.46e-3		1.57e-3	4.43e-3	

Table 5
Comparison of the IMS algorithm with two state-of-the-art algorithms (i.e., ITS [22] and SGVNS [6]) on the RanReal instances with different group sizes.

Instance	f_{best}			f_{avg}		
	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
RanReal_n120_ds_01	50601.64	50511.77	50471.07	50405.97	50233.42	50347.79
RanReal_n120_ds_02	50904.03	50926.60	50860.95	50691.85	50653.16	50710.78
RanReal_n120_ds_03	49935.33	50053.22	49961.99	49818.63	49769.97	49858.20
RanReal_n120_ds_04	50349.01	50362.19	50382.69	50164.48	50244.15	50269.68
RanReal_n120_ds_05	49414.58	49576.69	49642.54	49035.99	49389.44	49426.52
RanReal_n120_ds_06	50287.42	50189.78	50211.93	50120.37	50084.36	50126.83
RanReal_n120_ds_07	50074.29	50300.67	50107.47	49647.02	50033.27	50003.56
RanReal_n120_ds_08	50421.78	50471.62	50409.32	50351.31	50335.02	50323.86
RanReal_n120_ds_09	50415.22	50303.82	50339.42	50256.73	50135.17	50268.61
RanReal_n120_ds_10	49726.63	49738.82	49718.01	49552.19	49623.88	49637.11
RanReal_n240_ds_01	160122.83	160100.60	160020.56	159605.36	159658.09	159838.57
RanReal_n240_ds_02	160502.19	160195.86	160431.14	160056.73	159931.98	160238.93
RanReal_n240_ds_03	159389.94	159489.46	159404.12	159098.54	159194.52	159267.93
RanReal_n240_ds_04	161225.03	161268.00	161398.07	160540.42	160725.95	161021.04
RanReal_n240_ds_05	159474.95	159082.26	159249.91	158702.29	158863.94	158897.28
RanReal_n240_ds_06	161293.41	161149.24	160935.00	160554.40	160694.18	160817.23
RanReal_n240_ds_07	159940.05	159993.01	159919.07	159260.64	159256.38	159689.35
RanReal_n240_ds_08	158630.55	158455.65	158472.42	158194.33	158163.63	158300.69
RanReal_n240_ds_09	159707.67	159798.05	159815.04	159265.00	159426.01	159572.93
RanReal_n240_ds_10	159889.53	160116.32	160145.72	159586.36	159674.02	159897.95
RanReal_n480_ds_01	387444.56	388123.55	388623.12	386581.10	386880.96	387893.38
RanReal_n480_ds_02	386295.34	386545.55	386668.04	385302.04	385605.13	386224.71
RanReal_n480_ds_03	387474.69	387037.52	388278.66	386405.68	386385.61	387672.35
RanReal_n480_ds_04	389719.77	390468.63	390477.24	388910.57	389223.09	390126.22
RanReal_n480_ds_05	387556.78	387579.13	387778.95	386325.62	386550.27	387336.34
RanReal_n480_ds_06	388327.14	388955.10	389390.05	387713.26	388062.43	388652.59
RanReal_n480_ds_07	387953.20	388220.53	389460.58	387364.25	387277.33	387956.27
RanReal_n480_ds_08	389271.97	388704.19	389316.71	387671.57	387682.22	388606.65
RanReal_n480_ds_09	386976.68	386937.27	387387.51	385622.96	385829.80	386709.00
RanReal_n480_ds_10	391432.16	392583.25	392665.57	390233.98	391528.94	391616.68
RanReal_n960_ds_01	1237439.17	1236147.11	1239969.65	1233118.83	1233890.11	1238909.72
RanReal_n960_ds_02	1234310.30	1235681.38	1240510.37	1232084.77	1234143.93	1238715.63
RanReal_n960_ds_03	1234380.99	1235680.62	1238336.81	1232468.76	1232674.97	1236951.56
RanReal_n960_ds_04	1234687.12	1236117.09	1240460.96	1232447.56	1234544.61	1238715.10
RanReal_n960_ds_05	1232616.47	1232701.17	1237177.90	1231403.10	1231062.44	1235398.21
RanReal_n960_ds_06	1230272.69	1229937.27	1234363.75	1228455.18	1228663.53	1232633.30
RanReal_n960_ds_07	1233947.58	1235410.78	1238781.36	1232238.16	1231707.94	1237068.09
RanReal_n960_ds_08	1229287.84	1228957.27	1233177.59	1227839.29	1227748.55	1231635.91
RanReal_n960_ds_09	1234655.22	1235415.73	1239566.10	1232440.67	1233119.91	1236338.30
RanReal_n960_ds_10	1236743.27	1237850.16	1240641.54	1234957.71	1236045.50	1239307.80
#Best	8	7	25	2	1	37
p-value	1.14e-2	1.57e-3		1.26e-8	1.26e-8	

Table 6
Comparison of the IMS algorithm with two state-of-the-art algorithms (i.e., ITS [22] and SGVNS [6]) on the RanReal instances with equal group sizes.

Instance	f_{best}			f_{avg}		
	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
RanReal_n120_ss_01	47363.21	47363.21	47351.97	47320.20	47290.96	47278.28
RanReal_n120_ss_02	47243.16	47243.16	47243.16	47201.87	47174.17	47169.16
RanReal_n120_ss_03	47313.71	47313.71	47313.71	47269.91	47252.58	47270.55
RanReal_n120_ss_04	47546.81	47520.66	47546.81	47500.66	47460.04	47487.37
RanReal_n120_ss_05	46930.19	46896.02	46922.95	46862.90	46840.55	46836.60
RanReal_n120_ss_06	47253.47	47218.03	47227.14	47201.03	47159.19	47155.10
RanReal_n120_ss_07	47085.87	47085.87	47085.87	47048.75	47013.89	47016.85
RanReal_n120_ss_08	47460.13	47460.13	47460.13	47456.74	47443.28	47447.14
RanReal_n120_ss_09	47686.34	47686.34	47686.34	47651.17	47647.16	47623.66
RanReal_n120_ss_10	47415.35	47415.35	47415.35	47364.78	47370.57	47383.58
RanReal_n240_ss_01	155219.12	155213.84	155214.55	154883.12	154945.19	155014.44
RanReal_n240_ss_02	155474.95	155530.68	155503.11	155298.19	155364.94	155335.96
RanReal_n240_ss_03	155546.38	155669.29	155633.92	155285.92	155423.50	155458.48
RanReal_n240_ss_04	155275.08	155335.86	155364.27	155007.57	155194.75	155101.99
RanReal_n240_ss_05	154794.27	154978.13	154924.97	154624.80	154758.73	154751.91
RanReal_n240_ss_06	155571.81	155498.40	155671.23	155244.62	155344.28	155305.53
RanReal_n240_ss_07	155585.37	155689.23	155689.23	155388.71	155386.65	155476.73
RanReal_n240_ss_08	155578.35	155604.41	155545.42	155427.17	155432.26	155451.77
RanReal_n240_ss_09	155089.50	155084.04	155090.44	154725.08	154851.60	154828.30
RanReal_n240_ss_10	155831.39	155927.91	155880.48	155640.99	155715.16	155720.89
RanReal_n480_ss_01	377254.93	378091.43	378207.04	376577.67	377257.45	377541.47
RanReal_n480_ss_02	377084.52	377704.68	377864.04	376360.69	376868.37	377261.07
RanReal_n480_ss_03	378407.16	378727.11	379053.79	377642.01	378210.72	378523.05
RanReal_n480_ss_04	377512.67	377859.37	377964.66	376680.91	377236.63	377436.07
RanReal_n480_ss_05	377637.09	378315.79	378634.46	376933.62	377639.49	378035.78
RanReal_n480_ss_06	378561.19	379391.76	379274.93	377684.89	378435.81	378634.83
RanReal_n480_ss_07	378527.49	378960.02	379542.61	377868.64	378356.28	378830.49
RanReal_n480_ss_08	377521.79	377855.12	378204.40	376841.61	377458.17	377480.99
RanReal_n480_ss_09	377007.39	377933.93	378220.84	376381.06	377123.57	377425.71
RanReal_n480_ss_10	379490.57	379588.71	379495.84	378242.95	378988.96	378904.41
RanReal_n960_ss_01	1213571.81	1214889.59	1217164.60	1211655.10	1212393.84	1215127.66
RanReal_n960_ss_02	1215220.12	1215624.91	1218155.24	1213054.14	1213697.16	1217047.21
RanReal_n960_ss_03	1214457.16	1215262.94	1217349.78	1213049.09	1213298.63	1215606.06
RanReal_n960_ss_04	1214677.73	1215137.53	1218053.67	1213221.74	1213708.91	1217062.32
RanReal_n960_ss_05	1213355.93	1213915.65	1216203.18	1211601.14	1211816.82	1214833.11
RanReal_n960_ss_06	1213779.37	1214390.66	1217570.66	1211693.78	1212621.07	1215622.87
RanReal_n960_ss_07	1215371.11	1214000.10	1217445.63	1212882.20	1212855.81	1215974.81
RanReal_n960_ss_08	1213216.15	1213071.85	1216067.45	1211196.00	1211740.28	1214937.67
RanReal_n960_ss_09	1214408.56	1215097.64	1217955.76	1212479.70	1213411.80	1216443.45
RanReal_n960_ss_10	1216148.98	1215828.57	1218299.76	1213816.44	1214373.54	1217314.64
#Best	11	15	29	8	6	26
p-value	6.23e-05	3.08e-3		1.48e-4	4.43e-3	

Table 7
Comparison of the IMS algorithm with two state-of-the-art algorithms (i.e., ITS [22] and SGVNS [6]) on the Geo instances with different group sizes.

Instance	f_{best}			f_{avg}		
	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
Geo_n120_ds_01	111939.28	111873.75	111902.37	111911.48	111098.29	111884.65
Geo_n120_ds_02	61916.95	61890.78	61909.56	61903.64	61338.46	61902.33
Geo_n120_ds_03	52083.72	52061.00	52078.00	52073.17	51412.27	52069.82
Geo_n120_ds_04	80789.19	80759.66	80776.60	80775.83	80459.69	80764.28
Geo_n120_ds_05	121777.06	121679.46	121739.99	121735.46	120417.06	121698.37
Geo_n120_ds_06	136860.93	136815.05	136839.56	136712.49	136371.37	136817.94
Geo_n120_ds_07	108557.01	108489.35	108547.97	108466.72	107518.94	108511.23
Geo_n120_ds_08	88225.79	88172.62	88187.00	88206.58	88148.69	88178.09
Geo_n120_ds_09	95508.40	95410.84	95466.84	95474.05	94879.69	95445.76
Geo_n120_ds_10	65560.54	65521.62	65549.22	65538.04	65356.49	65531.18
Geo_n240_ds_01	200357.13	200307.82	200336.96	200303.94	199319.63	200327.31
Geo_n240_ds_02	348512.21	348406.58	348479.43	347585.05	346206.86	348465.69
Geo_n240_ds_03	217159.11	217105.66	217178.64	217124.09	214955.90	217155.76
Geo_n240_ds_04	263859.76	263765.00	263835.63	263538.75	261655.07	263587.65
Geo_n240_ds_05	313402.77	313290.69	313360.73	313377.51	312007.31	313336.36
Geo_n240_ds_06	358632.56	358456.36	358590.94	358605.22	357441.51	358550.91
Geo_n240_ds_07	341992.17	341172.78	341980.32	340415.53	339181.31	341592.84
Geo_n240_ds_08	131024.86	131024.78	131026.39	131020.88	130676.72	131021.76
Geo_n240_ds_09	410563.19	410379.34	410521.01	409945.98	408441.93	410464.95
Geo_n240_ds_10	355254.36	353823.23	355198.61	355017.34	352252.56	355184.75
Geo_n480_ds_01	580921.73	581315.05	582479.04	580805.52	576850.95	582123.61
Geo_n480_ds_02	1089043.66	1089409.66	1090000.26	1088977.03	1084763.97	1089716.53
Geo_n480_ds_03	662588.72	662622.55	664319.28	661944.19	658367.03	663591.45
Geo_n480_ds_04	836597.00	835376.73	836397.62	836532.13	831310.73	836358.87
Geo_n480_ds_05	988491.52	986287.96	988328.45	986678.57	979722.93	987742.16
Geo_n480_ds_06	1012562.54	1010237.14	1012489.37	1011750.26	1006038.94	1012037.76
Geo_n480_ds_07	864919.59	864225.44	864771.60	864710.73	860095.40	864281.45
Geo_n480_ds_08	587651.95	587419.70	587805.09	587283.15	584076.35	587506.18
Geo_n480_ds_09	666297.20	667220.91	667420.39	666229.66	663568.54	667309.42
Geo_n480_ds_10	932726.34	936532.52	937476.35	929792.10	930420.08	936650.57
Geo_n960_ds_01	3361972.63	3357246.28	3364976.99	3349073.54	3343507.03	3362203.74
Geo_n960_ds_02	1719714.70	1720538.84	1722789.69	1716091.63	1714377.84	1721443.28
Geo_n960_ds_03	3347799.90	3345716.22	3351291.12	3347722.82	3335941.16	3348867.32
Geo_n960_ds_04	3614983.35	3620711.81	3623347.13	3604535.13	3605566.68	3621476.68
Geo_n960_ds_05	2342436.81	2341962.44	2342220.13	2342276.35	2330534.53	2341420.32
Geo_n960_ds_06	3153302.03	3148820.77	3152992.29	3151552.96	3141553.49	3151442.92
Geo_n960_ds_07	1301825.26	1298267.73	1301844.91	1298534.13	1292837.36	1300216.92
Geo_n960_ds_08	1721921.20	1720719.54	1723602.17	1720286.62	1716296.69	1723335.84
Geo_n960_ds_09	1894753.44	1896003.92	1897535.27	1891513.59	1889095.78	1896214.30
Geo_n960_ds_10	2617039.54	2615485.60	2618015.72	2615978.35	2607823.21	2617741.80
#Best	24	0	16	14	0	26
p-value	2.06e-01	2.54e-10		5.78e-2	2.54e-10	

3.4 Computational Results and Comparison on the Large Scale Instances

To assess the performance of our IMS algorithm on large-sized instances, we carried out the second experiment based on the MDG-a and MDG-c benchmarks which include 11 MDG-a subsets and 2 MDG-c subsets, where each subset contains 20 instances with $n = 2000$ or 3000 . In this experiment, each instance was independently solved 20 times using the IMS, ITS, and SGVNS algorithms respectively. A summary of the results on these 13 benchmark subsets are shown in Table 9, and the detailed computational results for each subset are provided in Tables A.1 – A.13 of the appendix.

In Table 9, the first five columns indicate the characteristics of instances for each subset of benchmarks: the set name (Set), the number of groups (m), the lower and upper limits of group sizes (a_g and b_g), and the type of instances (*Type*). Each row of Table 9 corresponds to one of the 13 tested benchmark subsets and the shown results are based on the averages over all instances of each benchmark set. The row 'Average' indicates the average results of each algorithm over all subsets in terms of the best and average objective values. Once again, the non-parametric Friedman tests were used to verify the statistical significance between our IMS algorithm and the reference algorithms.

Table 8
Comparison of the IMS algorithm with two state-of-the-art algorithms (i.e., ITS [22] and SGVNS [6]) on the Geo instances with equal group sizes.

Instance	f_{best}			f_{avg}		
	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
Geo_n120_ss_01	101625.34	101582.46	101611.27	101610.59	101563.00	101595.23
Geo_n120_ss_02	54852.92	54831.10	54840.03	54846.70	54822.33	54835.58
Geo_n120_ss_03	47631.33	47615.71	47621.57	47626.08	47610.72	47616.99
Geo_n120_ss_04	73513.57	73466.35	73491.50	73498.55	73453.53	73483.01
Geo_n120_ss_05	112657.57	112621.83	112641.17	112631.14	112573.83	112613.01
Geo_n120_ss_06	125424.91	125375.10	125399.82	125404.69	125345.95	125380.47
Geo_n120_ss_07	98499.68	98448.17	98493.37	98483.28	98429.09	98466.30
Geo_n120_ss_08	79982.16	79925.82	79962.64	79963.75	79910.80	79947.92
Geo_n120_ss_09	87281.56	87217.23	87263.07	87260.55	87206.68	87243.30
Geo_n120_ss_10	60258.25	60223.82	60249.31	60248.61	60214.08	60233.23
Geo_n240_ss_01	188872.18	188820.43	188848.74	188854.87	188811.27	188833.16
Geo_n240_ss_02	330349.92	330221.98	330285.51	330303.80	330194.62	330261.08
Geo_n240_ss_03	207066.88	207004.15	207040.96	207055.28	206994.19	207028.70
Geo_n240_ss_04	246387.08	246293.80	246350.15	246364.23	246285.18	246333.52
Geo_n240_ss_05	298773.97	298663.11	298729.45	298738.96	298631.63	298700.27
Geo_n240_ss_06	338596.95	338485.52	338562.44	338566.51	338455.23	338526.47
Geo_n240_ss_07	326061.15	325947.58	326039.00	326036.28	325925.53	325995.21
Geo_n240_ss_08	126911.48	126899.34	126903.24	126908.32	126897.58	126898.69
Geo_n240_ss_09	391469.54	391315.30	391383.98	391413.51	391299.48	391365.47
Geo_n240_ss_10	339533.45	339426.07	339488.03	339506.87	339395.17	339468.43
Geo_n480_ss_01	552175.76	552029.26	552104.49	552155.33	552012.56	552078.31
Geo_n480_ss_02	1047450.18	1047180.27	1047314.11	1047387.49	1047128.56	1047241.73
Geo_n480_ss_03	633760.55	633556.01	633647.36	633729.27	633531.02	633623.07
Geo_n480_ss_04	789817.46	789565.85	789709.97	789778.49	789536.82	789559.90
Geo_n480_ss_05	945933.15	945715.47	945800.11	945887.14	945642.66	945743.46
Geo_n480_ss_06	966654.45	966380.61	966478.82	966585.10	966325.97	966431.60
Geo_n480_ss_07	827713.64	827460.21	827558.35	827658.89	827399.66	827527.35
Geo_n480_ss_08	556651.12	556507.04	556565.16	556632.18	556478.77	556538.12
Geo_n480_ss_09	636342.86	636150.41	636253.75	636319.08	636131.25	636224.49
Geo_n480_ss_10	883411.86	883126.77	883313.08	883359.36	883097.22	883232.13
Geo_n960_ss_01	3254400.00	3253897.94	3254071.56	3254283.99	3253844.76	3254022.12
Geo_n960_ss_02	1663655.10	1663453.87	1663496.02	1663632.19	1663430.65	1663471.31
Geo_n960_ss_03	3251592.49	3251133.28	3251368.68	3251534.31	3251076.91	3251289.52
Geo_n960_ss_04	3514369.69	3513845.78	3513995.60	3514217.91	3513760.67	3513948.54
Geo_n960_ss_05	2264719.61	2264438.13	2264551.72	2264687.79	2264388.84	2264524.29
Geo_n960_ss_06	3069667.72	3069224.57	3069457.37	3069579.72	3069155.74	3069358.54
Geo_n960_ss_07	1257746.77	1257645.60	1257632.82	1257733.35	1257629.61	1257624.38
Geo_n960_ss_08	1674028.54	1673798.98	1673846.57	1673989.19	1673778.03	1673825.81
Geo_n960_ss_09	1835473.14	1835246.63	1835324.69	1835440.88	1835216.53	1835289.44
Geo_n960_ss_10	2528974.50	2528612.67	2528822.78	2528919.65	2528571.34	2528761.90
#Best	40	0	0	40	0	0
<i>p</i> -value	2.54e-10	1.87e-9		2.54e-10	1.87e-9	

Table 9
Summary comparison of the IMS algorithm with two state-of-the-art algorithms (ITS [22] and SGVNS [6]) on the large instances with $n = 2000$ (220 MDG-a instances) and $n = 3000$ (40 MDG-c instances). The best results among the compared algorithms are indicated in bold.

Set	Instance set				f_{best}			f_{avg}		
	m	a_g	b_g	Type	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a	10	173	227	DGS	1133961.05	1132509.35	1135634.25	1133249.54	1131536.17	1135113.69
MDG-a	10	200	200	EGS	1115340.65	1113709.60	1116975.90	1114591.49	1112901.98	1116489.20
MDG-a	25	51	109	DGS	539418.00	539519.80	541147.35	538864.09	538965.23	540692.18
MDG-a	25	80	80	EGS	485946.35	485936.70	487501.50	485315.72	485465.81	487151.50
MDG-a	50	32	48	DGS	272656.00	273440.75	274262.10	272184.14	273105.67	273929.08
MDG-a	50	26	54	DGS	291116.55	291739.10	292585.85	290577.75	291347.52	292231.91
MDG-a	50	40	40	EGS	263767.03	264564.90	265342.55	263266.11	264211.53	265009.32
MDG-a	100	13	27	DGS	158970.90	159544.05	159905.80	158552.62	159223.94	159638.19
MDG-a	100	20	20	EGS	144118.80	144614.35	144918.35	143684.40	144325.44	144667.81
MDG-a	200	6	14	DGS	88435.70	88535.80	88721.50	88099.37	88262.95	88549.32
MDG-a	200	10	10	EGS	77208.50	76587.30	77242.80	76907.49	76459.62	77098.39
MDG-c	50	48	72	DGS	57908059.10	58034797.30	58195733.30	57830101.16	57979531.87	58149757.61
MDG-c	50	60	60	EGS	55958533.45	56087667.95	56245400.90	55877999.10	56031642.09	56201493.19
Average					9110579.39	9130243.61	9155797.86	9097953.31	9121306.14	9148601.65
<i>p</i> -value					3.12e-4	3.12e-4		3.12e-4	3.12e-4	

414 Table 9 discloses that for all 13 subsets of large instances, IMS outperforms
415 the reference algorithms ITS and SGVNS. IMS yields better results (indicated
416 in bold) for all subsets in terms of the best and average objective values.
417 Moreover, the *p*-values (all < 0.05) confirm the significance of the differences
418 between the results of IMS and those of the reference algorithms. This exper-
419 iment indicates that IMS is very competitive when it is applied to large-sized
420 instances compared to the state-of-the-art algorithms in the literature.

421 **4 Analysis and Discussions**

422 In this section, we investigate some important ingredients of the IMS algorithm
 423 to get useful insight into the behavior of the proposed algorithm. This study
 424 is based on the first subset of the MDG-a benchmark which is composed of 20
 425 DGS instances with $n = 2000$, $m = 50$, $a_g = 32$, and $b_g = 48$. We also study
 426 the spatial distribution of high-quality solutions visited by IMS to shed light
 427 on the rationality of the proposed algorithm.

428 *4.1 Influence of the Weak Perturbation Strength*

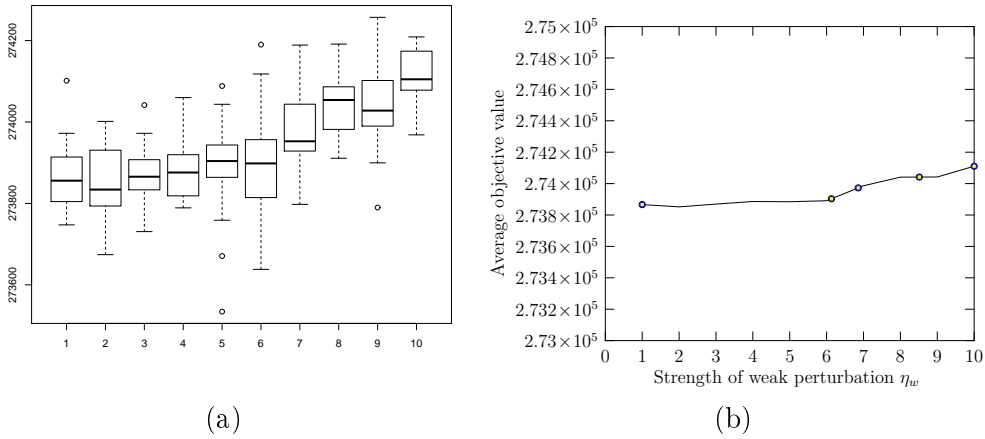


Fig. 1. Influence of the strength of the weak perturbation procedure

429 The IMS algorithm uses a weak perturbation procedure in its maxima search
 430 (Section 2.5). We carried out an experiment to analyze the influence of this
 431 component on the performance of IMS. For this study, we varied the strength
 432 (η_w) of weak perturbation within a reasonable range while keeping other pa-
 433 rameters with their default values (as shown in Table 2). The box and whisker
 434 plots of the computational results are shown in Fig. 1, where the X-axis of
 435 Fig. 1(a) indicates the test η_w values and the Y-axis indicates the objective
 436 values. As a supplement, we also plot the average objective values over the
 437 tested instances in Fig. 1(b), where the X-axis and the Y-axis respectively
 438 indicate the η_w values and the average objective values over the benchmark
 439 instances. All indicated results were based on the average over 20 independent
 440 runs with the cutoff time given in Section 3.2. Fig. 1 discloses that the perfor-
 441 mance of the IMS algorithm is not sensitive to η_w . For all the values of η_w
 442 in the interval $[1, 6]$, the algorithm obtains a similar performance. This explain
 443 why we used $\eta_w = 3$ as its default value for our experiments.

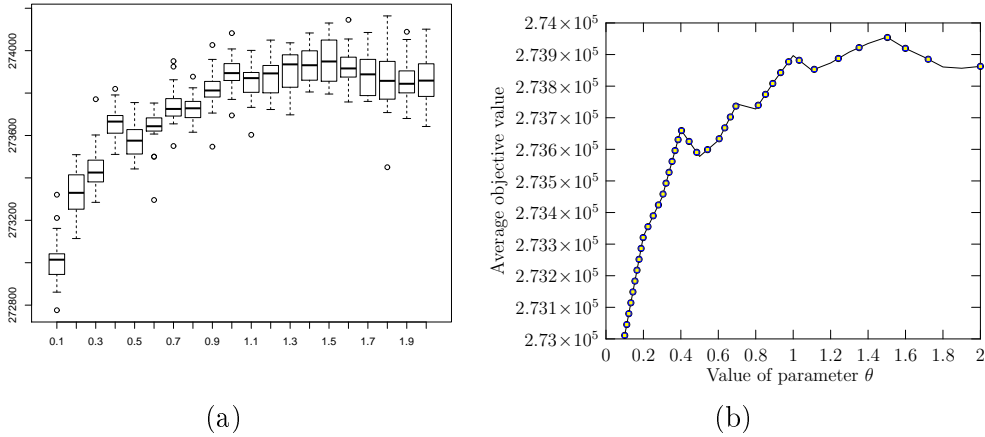


Fig. 2. Influence of the strength of the strong perturbation procedure

445 We turn now to study the influence of the strength (η_s) of strong perturbation
 446 on the IMS algorithm (Section 2.6). Since η_s is proportional to the parameter
 447 θ (recall that $\eta_s = \theta \times \frac{n}{m}$), we tested the parameter θ within a reasonable range
 448 while keeping other parameters with their default values. The computational
 449 results are shown in Fig. 2. In Fig. 2(a), the X-axis and the Y-axis respectively
 450 indicate the θ values and the objective values obtained. In Fig. 2(b), the X-
 451 axis and the Y-axis respectively indicate the θ values and the average objective
 452 values over the benchmark instances. Like in Section 4.1, these results were
 453 also based on the average over 20 independent runs.

454 One observes from Fig. 2 that the performance of the IMS algorithm is signif-
 455 icantly influenced by the setting of θ . First, small (large) θ values correspond-
 456 ing to a small (large) perturbation lead generally to a bad (high) performance.
 457 Furthermore, when θ reaches 1.5 which corresponds to a strength of $\eta_s = 60$
 458 for the tested instances, the IMS algorithm reaches its best performance. As θ
 459 further increases, the performance of the algorithm decreases gradually. This
 460 experiment shows that the IMS algorithm is sensitive to the parameter θ , and
 461 a large value is more appropriate for the large-sized instances. Therefore, in
 462 this study the default value of θ was set to 1.5 for the instances with $n > 400$,
 463 and 1.0 for other instances.

464 4.3 Spatial Distribution of High-Quality Solutions

465 To shed insight on the rationality of the proposed IMS algorithm, we carried
 466 out an experimental study on spatial distribution of high-quality local opti-
 467 mum solutions. This study, inspired by [23], helps to understand why altering

468 between maxima search and strong perturbation during the IMS process is
 469 meaningful. This study was based on 6 representative RanInt, RanReal, and
 470 Geo instances with $n = 120$. In this experiment, each instance was solved one
 471 time by running our IMS algorithm with a cutoff time of 1 minute, and the
 472 distinct high-quality local optimum solutions encountered during the run were
 473 recorded. For the 2 RanInt and 2 RanReal instances, the local optimum solu-
 474 tions with an objective value of $f \geq 0.99 \times f_B$ are considered as high-quality,
 475 where f_B represents the best objective value found in this work for the given
 476 instance. As for two 2 Geo instances, the local optimum solutions with an
 477 objective value of $f \geq 0.999 \times f_B$ are considered as high-quality.

478 Following [23], to obtain an intuitive image of the spatial distribution of
 479 high-quality local optimum solutions, we employ the multidimensional scaling
 480 (MDS) procedure to generate the distribution in Euclidean R^3 space, where
 481 the MDS procedure is composed of the following two steps.

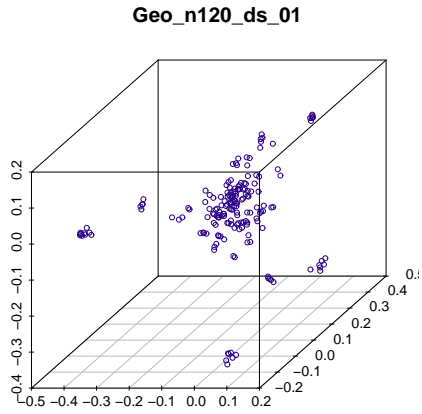
482 • Step 1: We first construct the distance matrix $D_{p \times p}$ in the real search
 483 space Ω (a n -dimensional space), where the entry $d_{ab} \in D_{p \times p}$ represents
 484 the distance between solutions s_a and s_b , and p represents the total num-
 485 ber of the local optimum solutions sampled. Given two solutions $s_a =$
 486 $(y^a[1], y^a[2], \dots, y^a[n])$ and $s_b = (y^b[1], y^b[2], \dots, y^b[n])$, we adopt the dis-
 487 tance function given in [6] to calculate their distance, which is defined as
 488 follows:

$$489 \quad d_{ab} = \frac{|(i,j):((y^a[i]=y^a[j] \wedge y^b[i] \neq y^b[j]) \vee (y^a[i] \neq y^a[j] \wedge y^b[i]=y^b[j]))|}{n^2/m}$$

490 As shown in [6], d_{ab} estimates the "fraction" of pairs belonging to the same
 491 group in one solution, but not to the same group in another solution, and
 492 it is suitable to represent the distance between two partitions.

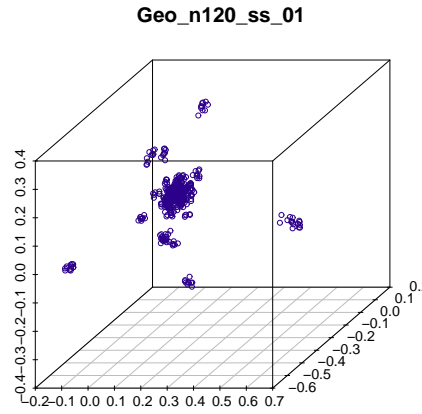
493 • Step 2: According to the distance matrix $D_{p \times p}$, we then generate p coor-
 494 dinate points in the Euclidean space R^3 by the classic *cmdscale* algorithm
 495 implemented in the R language, where each coordinate point corresponds to
 496 one of p solutions. The goal of the *cmdscale* algorithm is to map the points
 497 in n -dimensional space into Euclidean space R^3 while minimizing the dis-
 498 tance distortion. Thus, the distance between two points in R^3 approximately
 499 equals to that in the original n -dimensional space. Finally, we plot a scatter
 500 graph of the obtained points in R^3 .

501 The 3D scatter graph of the high-quality local optimum solutions produced
 502 in the experiment is plotted in Fig. 3 for each instance. Interestingly, Fig.
 503 3 discloses that high-quality local optimum solutions tend to be grouped in
 504 clusters, which has two relevant implications. On the one hand, the distances
 505 between high-quality local optimum solutions within the same cluster are in
 506 general small, which implies that it is very helpful for the search algorithm to
 507 reinforce its exploitation ability to detect other high-quality local optima in
 508 the current region of the search space. On the other hand, the local optimum
 509 solutions locating in different clusters are in general separated by a large dis-



Distribution of 183 high-quality local optima

(a)



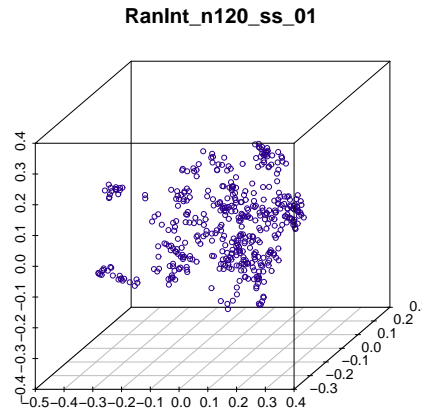
Distribution of 486 high-quality local optima

(b)



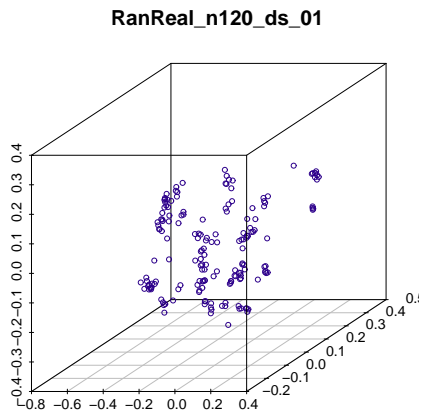
Distribution of 382 high-quality local optima

(c)



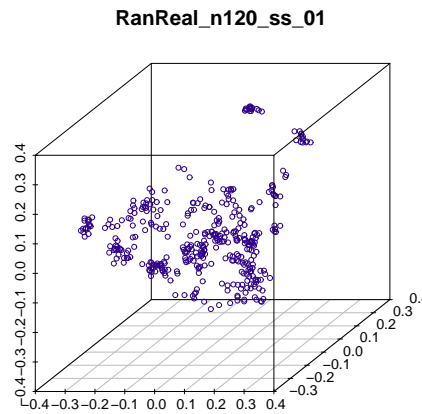
Distribution of 453 high-quality local optima

(d)



Distribution of 175 high-quality local optima

(e)



Distribution of 388 high-quality local optima

(f)

Fig. 3. Distribution of high-quality solutions produced by the IMS algorithm on the representative instances.

510 tance. To continue the search effectively, it is useful for a heuristic algorithm
511 to be able to "jump" from from one cluster to another cluster (i.e., to escape
512 from local optimum traps).

513 Based on the above analysis, the rationality of the proposed IMS algorithm
514 can be explained as follows. On the one hand, the maxima search procedure
515 uses its weak perturbation procedure to visit other (hopefully better) local
516 optima in the nearby areas of an attained local optimum (i.e., corresponding
517 to a cluster). On the other hand, the strong perturbation procedure of the IMS
518 algorithm helps the search to move from one attraction area (corresponding to
519 a cluster) to another one. As a result, the combined use of the maxima search
520 procedure and the strong perturbation procedure ensures a kind of balance
521 between intensification and diversification of its search process, which help to
522 locate high quality solutions.

523 Finally, one notices that the cluster characteristic of high-quality local opti-
524 mum solutions was previously observed for other well-known problems like
525 TSP [5] and graph coloring [23].

526 5 Conclusions

527 This paper introduced an iterated maxima search (IMS) algorithm for solving
528 the maximally diverse grouping problem (MDGP). IMS effectively integrates
529 a fast local search, a weak perturbation procedure, and a strong perturbation
530 procedure to ensure a suitable trade-off between intensification and diversifi-
531 cation of its search process. The performance of the proposed algorithm was
532 evaluated on five sets of 500 benchmark instances with various characteris-
533 tics. The experimental results showed that IMS is very competitive compared
534 to existing top performing algorithms in the literature and performs partic-
535 ularly well on large-sized instances. To provide some insight about the pro-
536 posed algorithm, we studied the influence of the weak and strong perturbation
537 procedures. We also investigated the spatial distribution of high-quality local
538 optima with the purpose of shedding light on the rationality of the proposed
539 algorithm.

540 In addition to the updated best results achieved by the proposed algorithm
541 which are useful to assess new MDGP algorithms, the key ideas of this work
542 could help to design effective heuristics for other related grouping or clus-
543 tering problems involving dense graphs. Finally, like for most heuristic and
544 metaheuristic algorithms, our current knowledge does not allow us to explain
545 theoretically why the proposed algorithm works. More effort on such funda-
546 mental aspects of heuristic search is needed in the long term with the purpose
547 of achieving a better understanding of heuristic algorithms.

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632 **A Appendix**

633 This appendix complements the presentation of Section 3.4 and contains the
634 detailed results of the IMS algorithm on the large instances with $n = 2000$
635 (220 MDG-a instances) and $n = 3000$ (40 MDG-c instances) in comparison
636 with two state-of-the-art algorithms (ITS [22] and SGVNS [6]). Tables A.1–
637 A.13 present respectively the results of the compared algorithms on each of
638 the 11 MDG-a subsets and 2 MDG-c subsets (20 instances per group) in terms
639 of the best and average objective values (based on 20 independent runs per
640 instance, see Section 3.2 for the experimental protocol). The row 'Average'
641 shows the averaged value for each subset of instances. The row '#Best' in-
642 dicates the number of instances for which an algorithm performs the best
643 among the compared algorithms. The row ' p -value' indicates the outcomes of
644 the non-parametric Friedman tests between a set of results of IMS and those
645 of a reference algorithm. The best results among the compared algorithms are
646 indicated in bold.

Table A.1
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large DGS instances with $n = 2000$, $m = 50$

Graph	Instance			f_{best}			f_{avg}		
	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	50	32	48	272874	273432	274075	272431.05	273124.65	273762.25
MDG-a_22	50	32	48	272699	273419	274335	272136.20	273107.15	274045.85
MDG-a_23	50	32	48	272689	273431	274181	272176.50	272987.45	273948.35
MDG-a_24	50	32	48	272757	273416	274075	272066.20	273069.55	273762.55
MDG-a_25	50	32	48	272579	273463	274069	272234.85	273155.00	273740.40
MDG-a_26	50	32	48	272769	273263	274466	272205.45	272991.45	273929.85
MDG-a_27	50	32	48	272205	273258	274133	272136.60	272949.10	273835.35
MDG-a_28	50	32	48	272472	273452	274228	272046.55	273076.60	273859.65
MDG-a_29	50	32	48	272811	273434	274396	272122.60	273148.55	273999.85
MDG-a_30	50	32	48	272730	273430	274316	272016.35	273107.30	273897.95
MDG-a_31	50	32	48	272900	273459	274342	272532.40	273137.00	274117.25
MDG-a_32	50	32	48	272794	273374	274303	272326.35	273080.45	273946.25
MDG-a_33	50	32	48	272692	273542	274389	272232.50	273083.35	274055.00
MDG-a_34	50	32	48	272517	273438	274379	272218.70	273177.00	273990.30
MDG-a_35	50	32	48	272486	273419	274097	272068.70	273028.50	273794.45
MDG-a_36	50	32	48	272758	273616	274172	272264.55	273068.90	273889.90
MDG-a_37	50	32	48	272280	273434	274457	271995.35	273163.80	274039.20
MDG-a_38	50	32	48	272520	273494	274382	272037.40	273228.30	274033.40
MDG-a_39	50	32	48	272815	273470	274131	272182.85	273204.25	273883.20
MDG-a_40	50	32	48	272773	273571	274316	272251.65	273225.00	274050.65
Average				272656.00	273440.75	274262.10	272184.14	273105.67	273929.08
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.2
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large DGS instances with $n=2000$ and $m = 10$.

Graph	Instance			f_{best}			f_{avg}		
	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	10	173	227	1133850	1132437	1135700	1133239.35	1131666.00	1135310.55
MDG-a_22	10	173	227	1133890	1132473	1135376	1133254.25	1131503.85	1134892.80
MDG-a_23	10	173	227	1133188	1131686	1135286	1132744.00	1130977.10	1134627.75
MDG-a_24	10	173	227	1133867	1132812	1135485	1133123.65	1131430.65	1134975.20
MDG-a_25	10	173	227	1133850	1133050	1135776	1133239.35	1131881.80	1135299.70
MDG-a_26	10	173	227	1133733	1132438	1135324	1133191.00	1131474.25	1135010.75
MDG-a_27	10	173	227	1134059	1131955	1135265	1133104.75	1130955.80	1134649.75
MDG-a_28	10	173	227	1133960	1132356	1135603	1133145.65	1131478.80	1134980.25
MDG-a_29	10	173	227	1133549	1132086	1135868	1132988.25	1131568.75	1135284.35
MDG-a_30	10	173	227	1133825	1132401	1135651	1133127.05	1131391.45	1135014.90
MDG-a_31	10	173	227	1134218	1132994	1136036	1133398.80	1132106.35	1135617.95
MDG-a_32	10	173	227	1133740	1132278	1135917	1133256.50	1131462.05	1135175.85
MDG-a_33	10	173	227	1134011	1132321	1135506	1133326.30	1131428.45	1134925.35
MDG-a_34	10	173	227	1134178	1132913	1135563	1133426.75	1131840.65	1135234.95
MDG-a_35	10	173	227	1133862	1132279	1135279	1132919.85	1131109.90	1134789.20
MDG-a_36	10	173	227	1134185	1132075	1135563	1133431.80	1131271.55	1135156.10
MDG-a_37	10	173	227	1134087	1133144	1136267	1133442.25	1132128.65	1135542.65
MDG-a_38	10	173	227	1134872	1133027	1135697	1133763.00	1131655.55	1135199.35
MDG-a_39	10	173	227	1133856	1132120	1135375	1133350.10	1131170.55	1134822.95
MDG-a_40	10	173	227	1134441	1133342	1136148	1133518.15	1132221.20	1135763.35
Average				1133961.05	1132509.35	1135634.25	1133249.54	1131536.17	1135113.69
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.3
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large EGS instances with $n=2000$ and $m = 10$.

Graph	Instance			f_{best}			f_{avg}		
	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	10	200	200	1115022	1114270	1117343	1114442.75	1113004.65	1116684.40
MDG-a_22	10	200	200	1114794	1113468	1117097	1114409.70	1112711.05	1116442.00
MDG-a_23	10	200	200	1114892	1112976	1116331	1113981.75	1112453.60	1115880.90
MDG-a_24	10	200	200	1115312	1113919	1116863	1114676.95	1112947.40	1116410.05
MDG-a_25	10	200	200	1115809	1114269	1117108	1114749.00	1113427.15	1116743.85
MDG-a_26	10	200	200	1115590	1113571	1116942	1114765.90	1112838.80	1116368.10
MDG-a_27	10	200	200	1115132	1113272	1116468	1114553.75	1112405.70	1115947.35
MDG-a_28	10	200	200	1115335	1113925	1116740	1114421.70	1112842.45	1116460.90
MDG-a_29	10	200	200	1116073	1113747	1117064	1114900.85	1112835.30	1116585.35
MDG-a_30	10	200	200	1114993	1113583	1116748	1114373.75	1112662.90	1116396.95
MDG-a_31	10	200	200	1116037	1114170	1117636	1115106.35	1113322.30	1117179.15
MDG-a_32	10	200	200	1115944	1113406	1116908	1114746.20	1112626.25	1116441.30
MDG-a_33	10	200	200	1114739	1113326	1116815	1114292.15	1112568.10	1116290.25
MDG-a_34	10	200	200	1115094	1113611	1117125	1114697.30	1113039.85	1116608.10
MDG-a_35	10	200	200	1114836	1114084	1116561	1114283.50	1112689.40	1116093.60
MDG-a_36	10	200	200	1114858	1113480	1116789	1114249.55	1112746.90	1116379.10
MDG-a_37	10	200	200	1115425	1113931	1117783	1114776.40	1113387.60	1117045.70
MDG-a_38	10	200	200	1115548	1113837	1117110	1114912.15	1113541.35	1116615.75
MDG-a_39	10	200	200	1114931	1113255	1116610	1113943.30	1112574.00	1116142.15
MDG-a_40	10	200	200	1116449	1114092	1117477	1115546.75	1113414.85	1117069.00
Average				1115340.65	1113709.60	1116975.90	1114591.49	1112901.98	1116489.20
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.4
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large DGS instances with $n=2000$ and $m = 25$.

Graph	Instance			f_{best}			f_{avg}		
	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	25	51	109	539304	539616	541130	538762.40	539050.10	540694.30
MDG-a_22	25	51	109	539732	539554	541013	539199.75	538882.55	540636.20
MDG-a_23	25	51	109	539571	539030	541352	538867.15	538663.70	540553.45
MDG-a_24	25	51	109	539549	539238	540794	538784.55	538911.85	540574.50
MDG-a_25	25	51	109	539481	539872	541283	538876.90	539156.75	540781.90
MDG-a_26	25	51	109	539321	539696	541099	538978.25	538840.85	540601.95
MDG-a_27	25	51	109	539028	539365	541084	538475.60	538794.80	540623.70
MDG-a_28	25	51	109	539560	539458	541179	539090.75	538852.30	540636.25
MDG-a_29	25	51	109	539356	539458	541492	539043.55	539005.30	540881.65
MDG-a_30	25	51	109	539467	539482	541224	538600.30	538898.80	540769.85
MDG-a_31	25	51	109	539592	539808	541215	539220.20	539184.65	540829.25
MDG-a_32	25	51	109	539738	539484	540939	539135.95	538982.75	540533.85
MDG-a_33	25	51	109	539268	539719	540958	538685.75	539054.15	540656.25
MDG-a_34	25	51	109	539567	539726	541136	538968.95	538980.60	540707.70
MDG-a_35	25	51	109	539225	539294	541054	538632.90	538743.00	540568.35
MDG-a_36	25	51	109	539375	539416	541469	538797.05	538920.90	540742.60
MDG-a_37	25	51	109	539576	539492	541183	538805.95	539108.85	540742.45
MDG-a_38	25	51	109	539367	539363	541150	538962.70	539168.40	540801.00
MDG-a_39	25	51	109	539075	539423	540920	538523.20	538810.10	540524.70
MDG-a_40	25	51	109	539208	539902	541273	538869.90	539294.25	540983.60
Average				539418.00	539519.80	541147.35	538864.09	538965.23	540692.18
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.5
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large EGS instances with $n=2000$ and $m = 25$.

Graph	Instance			f_{best}			f_{avg}		
	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	25	80	80	486046	485997	487776	485271.85	485574.30	487360.10
MDG-a_22	25	80	80	486509	486171	487472	485676.00	485437.50	487041.00
MDG-a_23	25	80	80	485690	485669	487391	485125.40	485310.00	487078.55
MDG-a_24	25	80	80	485848	485853	487382	485157.20	485532.90	487086.95
MDG-a_25	25	80	80	485819	486062	487700	485355.85	485639.90	487270.35
MDG-a_26	25	80	80	485712	486000	487443	485164.55	485368.25	487191.90
MDG-a_27	25	80	80	485532	485688	487186	484994.95	485327.50	486913.65
MDG-a_28	25	80	80	485922	485600	487340	485424.50	485336.40	487079.05
MDG-a_29	25	80	80	486329	485907	487624	485606.05	485550.20	487346.40
MDG-a_30	25	80	80	485702	486040	487319	484916.00	485510.60	486990.20
MDG-a_31	25	80	80	486403	486147	487883	485924.95	485516.45	487432.55
MDG-a_32	25	80	80	486174	485956	487254	485169.60	485478.00	486995.40
MDG-a_33	25	80	80	485676	486056	487442	485156.65	485369.50	487050.05
MDG-a_34	25	80	80	486631	486017	487620	485533.65	485594.65	487131.35
MDG-a_35	25	80	80	485440	485647	487339	485035.05	485394.20	487024.85
MDG-a_36	25	80	80	485524	485988	487417	485159.30	485475.20	487090.90
MDG-a_37	25	80	80	486137	486084	487675	485567.85	485676.05	487307.95
MDG-a_38	25	80	80	485976	485928	487711	485153.10	485225.10	487341.50
MDG-a_39	25	80	80	486005	485898	487422	485529.45	485325.75	486955.75
MDG-a_40	25	80	80	485852	486026	487634	485392.50	485673.65	487341.45
Average				485946.35	485936.70	487501.50	485315.72	485465.81	487151.50
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.6
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large DGS instances with $n = 2000$, $m = 50$, $a_g = 26$, and $b_g = 54$.

Graph	Instance			f_{best}			f_{avg}		
	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	50	26	54	291149	291749	292702	290802.40	291384.75	292343.30
MDG-a_22	50	26	54	291098	291457	292564	290700.10	291219.20	292104.55
MDG-a_23	50	26	54	290579	291553	292344	290236.45	291259.25	292023.75
MDG-a_24	50	26	54	290934	291709	292651	290386.75	291378.35	292271.05
MDG-a_25	50	26	54	291081	291826	292727	290633.45	291337.60	292415.10
MDG-a_26	50	26	54	291348	291812	292723	290380.70	291344.05	292289.20
MDG-a_27	50	26	54	291009	291530	292139	290506.30	291211.70	291842.00
MDG-a_28	50	26	54	290997	291685	292574	290511.25	291320.40	292159.20
MDG-a_29	50	26	54	291008	291731	292634	290484.05	291384.20	292220.40
MDG-a_30	50	26	54	291069	291838	292654	290428.00	291415.45	292283.10
MDG-a_31	50	26	54	291321	292093	292507	291090.65	291607.55	292273.25
MDG-a_32	50	26	54	291478	291753	292651	290647.00	291344.35	292303.15
MDG-a_33	50	26	54	291093	291682	292480	290618.00	291273.10	292194.45
MDG-a_34	50	26	54	290986	291702	292813	290638.25	291283.35	292401.75
MDG-a_35	50	26	54	290840	291689	292619	290427.75	291301.15	292252.05
MDG-a_36	50	26	54	291476	291714	292401	290579.15	291351.00	292250.85
MDG-a_37	50	26	54	291160	291781	292815	290639.15	291413.00	292425.85
MDG-a_38	50	26	54	291271	291840	292445	290676.85	291380.40	292148.60
MDG-a_39	50	26	54	291199	291642	292390	290479.05	291247.05	291960.90
MDG-a_40	50	26	54	291235	291996	292884	290689.75	291494.40	292475.75
Average				291116.55	291739.10	292585.85	290577.75	291347.52	292231.91
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.7
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large EGS instances with $n=2000$ and $m = 50$.

Instance				f_{best}			f_{avg}		
Graph	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	50	40	40	263680	264582	265422	263184.70	264259.00	265155.60
MDG-a_22	50	40	40	263929	264461	265250	263296.00	264121.60	264885.10
MDG-a_23	50	40	40	263731	264489	265146	263221.95	264092.20	264789.15
MDG-a_24	50	40	40	263675	264567	265455	263126.30	264177.40	265122.20
MDG-a_25	50	40	40	263844	264571	265363	263152.10	264225.30	265101.95
MDG-a_26	50	40	40	263837	264639	265341	263340.45	264216.75	265106.80
MDG-a_27	50	40	40	263641	264387	265383	262982.40	264095.05	265016.35
MDG-a_28	50	40	40	263628	264419	265406	263210.05	264165.35	264907.00
MDG-a_29	50	40	40	264015	264763	265375	263270.45	264246.25	264950.80
MDG-a_30	50	40	40	263457	264536	265564	263067.10	264236.85	264933.00
MDG-a_31	50	40	40	264085	264713	265452	263577.85	264323.10	265262.35
MDG-a_32	50	40	40	263893	264570	265235	263488.65	264267.60	264884.90
MDG-a_33	50	40	40	263682	264569	265285	263253.50	264215.00	264863.10
MDG-a_34	50	40	40	263564	264622	265372	263158.95	264227.50	265022.75
MDG-a_35	50	40	40	263876	264572	265304	263456.40	264149.25	265031.40
MDG-a_36	50	40	40	263674	264575	265385	263147.05	264213.35	265109.45
MDG-a_37	50	40	40	263798	264585	265378	263196.25	264324.05	265171.30
MDG-a_38	50	40	40	263879	264514	265100	263337.00	264213.25	264816.35
MDG-a_39	50	40	40	263612	264561	265133	263347.35	264136.90	264831.90
MDG-a_40	50	40	40	263841	264603	265502	263507.70	264324.90	265224.95
Average				263767.03	264564.90	265342.55	263266.11	264211.53	265009.32
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.8
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large DGS instances with $n=2000$ and $m = 100$.

Instance				f_{best}			f_{avg}		
Graph	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	100	13	27	159084	159614	160129	158583.45	159143.20	159840.15
MDG-a_22	100	13	27	159062	159462	159845	158669.95	159200.50	159630.75
MDG-a_23	100	13	27	158786	159406	159829	158413.80	159200.10	159558.05
MDG-a_24	100	13	27	158850	159477	159882	158440.15	159212.50	159671.90
MDG-a_25	100	13	27	158750	159474	159835	158437.20	159197.60	159606.05
MDG-a_26	100	13	27	158994	159538	160219	158759.90	159258.60	159795.30
MDG-a_27	100	13	27	158825	159459	160040	158487.05	159169.60	159759.30
MDG-a_28	100	13	27	159165	159442	159789	158548.45	159141.65	159448.45
MDG-a_29	100	13	27	159165	159720	159790	158570.55	159222.65	159466.30
MDG-a_30	100	13	27	158787	159446	159739	158435.35	159222.60	159468.30
MDG-a_31	100	13	27	158881	159837	159810	158514.30	159368.00	159516.70
MDG-a_32	100	13	27	159017	159525	160096	158499.25	159257.10	159815.00
MDG-a_33	100	13	27	158840	159503	159619	158470.70	159236.40	159426.20
MDG-a_34	100	13	27	158993	159680	159608	158558.45	159195.85	159405.05
MDG-a_35	100	13	27	159101	159623	159875	158625.55	159200.50	159625.15
MDG-a_36	100	13	27	159063	159445	159869	158705.10	159211.50	159627.75
MDG-a_37	100	13	27	158899	159564	160054	158554.15	159249.80	159790.70
MDG-a_38	100	13	27	158748	159456	160130	158357.90	159251.15	159828.85
MDG-a_39	100	13	27	159343	159610	159999	158802.65	159228.55	159777.65
MDG-a_40	100	13	27	159065	159600	159959	158618.50	159310.90	159706.25
Average				158970.90	159544.05	159905.80	158552.62	159223.94	159638.19
#Best				0	2	18	0	0	20
p-value				7.74e-6	3.47e-6		7.74e-6	7.74e-6	

Table A.9
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large EGS instances with $n=2000$ and $m = 100$.

Instance				f_{best}			f_{avg}		
Graph	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	100	20	20	144020	144879	144918	143619.25	144426.40	144592.80
MDG-a_22	100	20	20	143938	144536	144756	143554.95	144288.90	144549.90
MDG-a_23	100	20	20	143915	144577	144927	143505.35	144342.90	144696.95
MDG-a_24	100	20	20	144071	144794	144962	143690.95	144304.35	144707.35
MDG-a_25	100	20	20	144341	144648	145043	143635.05	144299.65	144766.50
MDG-a_26	100	20	20	144148	144601	145032	143691.65	144331.80	144626.60
MDG-a_27	100	20	20	143928	144458	144935	143617.35	144231.30	144747.70
MDG-a_28	100	20	20	144140	144557	144848	143765.70	144265.15	144644.90
MDG-a_29	100	20	20	144099	144567	144937	143831.25	144255.30	144636.80
MDG-a_30	100	20	20	144263	144628	144784	143744.45	144354.60	144500.70
MDG-a_31	100	20	20	144184	144655	144881	143852.55	144385.10	144666.35
MDG-a_32	100	20	20	143846	144693	144934	143641.50	144315.35	144701.00
MDG-a_33	100	20	20	144071	144532	144611	143667.75	144321.20	144447.00
MDG-a_34	100	20	20	144511	144573	144803	143799.00	144383.80	144576.65
MDG-a_35	100	20	20	144022	144627	144999	143682.45	144357.50	144763.65
MDG-a_36	100	20	20	143829	144543	144998	143369.80	144311.30	144788.15
MDG-a_37	100	20	20	144332	144632	144803	143779.55	144371.25	144645.50
MDG-a_38	100	20	20	144051	144585	144958	143701.05	144314.35	144656.15
MDG-a_39	100	20	20	144344	144579	145009	143794.55	144253.20	144797.55
MDG-a_40	100	20	20	144323	144623	145229	143743.75	144395.45	144843.90
Average				144118.80	144614.35	144918.35	143684.40	144325.44	144667.81
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.10
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large DGS instances with $n=2000$ and $m=200$.

Instance			f_{best}			f_{avg}			
Graph	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	200	6	14	88464	88548	88949	88139.95	88276.40	88718.70
MDG-a_22	200	6	14	88243	88536	88459	87968.15	88223.90	88318.15
MDG-a_23	200	6	14	88131	88483	88973	87800.10	88200.25	88796.70
MDG-a_24	200	6	14	88343	88464	88760	87915.65	88202.35	88597.55
MDG-a_25	200	6	14	88435	88571	89031	88030.90	88276.05	88814.00
MDG-a_26	200	6	14	88538	88642	88476	88324.75	88312.55	88322.00
MDG-a_27	200	6	14	88644	88469	88522	88126.45	88221.35	88272.05
MDG-a_28	200	6	14	88565	88454	88794	88060.65	88296.80	88656.85
MDG-a_29	200	6	14	88361	88532	89005	88001.85	88259.90	88839.35
MDG-a_30	200	6	14	88543	88560	89017	88270.80	88287.55	88811.00
MDG-a_31	200	6	14	88623	88439	88601	88363.20	88260.65	88459.75
MDG-a_32	200	6	14	88445	88502	88639	88269.85	88262.40	88456.90
MDG-a_33	200	6	14	88424	88775	88486	88147.25	88306.55	88341.10
MDG-a_34	200	6	14	88368	88490	88961	88063.85	88264.40	88790.35
MDG-a_35	200	6	14	88426	88572	88437	88070.35	88228.15	88273.80
MDG-a_36	200	6	14	88542	88590	88492	88129.15	88296.75	88340.65
MDG-a_37	200	6	14	88457	88439	88558	87943.10	88191.85	88395.35
MDG-a_38	200	6	14	88544	88442	88520	88304.75	88266.35	88325.40
MDG-a_39	200	6	14	88038	88643	88947	87750.55	88326.45	88831.10
MDG-a_40	200	6	14	88580	88565	88803	88306.05	88298.30	88625.65
Average				88435.70	88535.80	88721.50	88099.37	88262.95	88549.32
#Best				3	5	12	1	0	19
p-value				2.54e-2	2.54e-2		5.70e-5	7.74e-6	

Table A.11
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large EGS instances with $n=2000$ and $m=200$.

Instance			f_{best}			f_{avg}			
Graph	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-a_21	200	10	10	77249	76543	77175	76842.90	76438.70	76994.40
MDG-a_22	200	10	10	77214	76546	77214	76895.75	76449.15	77107.05
MDG-a_23	200	10	10	77033	76564	77234	76824.15	76464.70	77022.85
MDG-a_24	200	10	10	77092	76535	77197	76873.65	76463.75	77058.50
MDG-a_25	200	10	10	77198	76578	77229	76962.55	76461.45	77121.40
MDG-a_26	200	10	10	77234	76567	77121	76822.05	76467.90	77008.70
MDG-a_27	200	10	10	76875	76521	77131	76608.15	76441.75	77001.80
MDG-a_28	200	10	10	77216	76633	77249	76940.85	76465.05	77122.85
MDG-a_29	200	10	10	77171	76627	77339	76870.25	76463.50	77137.85
MDG-a_30	200	10	10	77470	76592	77214	77011.35	76490.35	77121.60
MDG-a_31	200	10	10	77245	76600	77302	76924.15	76452.55	77146.90
MDG-a_32	200	10	10	77168	76638	77198	76935.05	76464.00	77123.30
MDG-a_33	200	10	10	77352	76621	77396	76975.65	76478.70	77148.10
MDG-a_34	200	10	10	77316	76615	77366	76960.65	76456.60	77154.80
MDG-a_35	200	10	10	77233	76685	77236	76908.75	76470.25	77146.05
MDG-a_36	200	10	10	77150	76553	77270	76918.05	76458.15	77148.45
MDG-a_37	200	10	10	77196	76586	77302	76980.40	76452.00	77154.85
MDG-a_38	200	10	10	77226	76523	77145	76914.30	76431.70	77010.85
MDG-a_39	200	10	10	77311	76618	77261	77000.70	76441.60	77142.25
MDG-a_40	200	10	10	77221	76601	77277	76980.45	76480.55	77095.15
Average				77208.50	76587.30	77242.80	76907.49	76459.62	77098.39
#Best				6	0	15	0	0	20
p-value				3.90e-2	7.74e-6		7.74e-6	7.74e-6	

Table A.12
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large DGS instances with $n=3000$ and $m=50$.

Instance			f_{best}			f_{avg}			
Graph	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-c_1	50	48	72	57945495	58002162	58256069	57866205.40	57969360.45	58206836.25
MDG-c_2	50	48	72	57941604	58058009	58222189	57847954.50	57978365.60	58176353.85
MDG-c_3	50	48	72	57934848	58042369	58183020	57853662.10	57981548.00	58139867.15
MDG-c_4	50	48	72	57927582	58040996	58203033	57856933.15	57986655.35	58160671.30
MDG-c_5	50	48	72	57923652	58026970	58195892	57837851.55	57973993.50	58138551.15
MDG-c_6	50	48	72	57912572	58051277	58170930	57835981.70	57995787.85	58115476.40
MDG-c_7	50	48	72	57920362	58006501	58184196	57832628.50	57965788.60	58145525.85
MDG-c_8	50	48	72	57917641	58018105	58175358	57828244.60	57958586.70	58137072.20
MDG-c_9	50	48	72	57852060	58053174	58148355	57804909.10	57996436.85	58108503.85
MDG-c_10	50	48	72	57855618	58032526	58177707	57807867.05	57988658.75	58126674.90
MDG-c_11	50	48	72	57927899	58057511	58202140	57823896.80	57996449.35	58166369.45
MDG-c_12	50	48	72	57879753	58043186	58211896	57810309.90	58009313.20	58171859.25
MDG-c_13	50	48	72	57899195	58033030	58231541	57820288.55	57981936.95	58173176.70
MDG-c_14	50	48	72	57893447	58050347	58170717	57819670.60	58000079.35	58128947.60
MDG-c_15	50	48	72	57936099	58006905	58219534	57842744.00	57971202.50	58181767.65
MDG-c_16	50	48	72	57899782	58017384	58213319	57841066.40	57977613.10	58153544.70
MDG-c_17	50	48	72	57912576	58080720	58192484	57822019.25	57983021.95	58146759.40
MDG-c_18	50	48	72	57884836	58033798	58152922	57824357.45	57968806.20	58112703.35
MDG-c_19	50	48	72	57918318	58018351	58212035	57831674.95	57956907.60	58163660.60
MDG-c_20	50	48	72	57877843	58022625	58191329	57793757.60	57950125.50	58140830.60
Average				57908059.10	58034797.30	58195733.30	57830101.16	57979531.87	58149757.61
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	

Table A.13
Comparison of the IMS algorithm with two state-of-the-art algorithms on the large EGS instances with $n=3000$ and $m=50$.

Graph	Instance			f_{best}			f_{avg}		
	m	a_g	b_g	ITS [22]	SGVNS [6]	IMS	ITS [22]	SGVNS [6]	IMS
MDG-c_1	50	60	60	55977693	56095305	56253625	55910079.05	56056762.55	56218194.70
MDG-c_2	50	60	60	55969792	56090550	56272017	55890036.80	56045634.60	56226594.65
MDG-c_3	50	60	60	55997944	56130490	56262455	55867986.95	56042121.65	56208888.85
MDG-c_4	50	60	60	55959548	56076697	56257907	55901255.80	56045542.35	56219344.25
MDG-c_5	50	60	60	55966544	56082421	56234604	55866485.35	56028107.75	56200190.95
MDG-c_6	50	60	60	55942210	56117081	56243850	55881502.00	56028119.45	56202899.40
MDG-c_7	50	60	60	55944042	56086355	56236720	55872630.10	56026724.60	56183765.50
MDG-c_8	50	60	60	55935072	56055008	56249049	55884553.95	56024573.75	56218073.10
MDG-c_9	50	60	60	55906493	56057439	56235250	55851227.75	55997916.45	56188505.85
MDG-c_10	50	60	60	55920804	56107377	56179602	55812256.00	56025439.20	56157919.35
MDG-c_11	50	60	60	56010877	56095642	56238432	55875876.35	56030011.90	56197694.85
MDG-c_12	50	60	60	55952824	56067675	56267216	55872773.75	56021610.00	56196066.80
MDG-c_13	50	60	60	55954309	56068977	56273597	55868322.80	56030276.70	56201739.90
MDG-c_14	50	60	60	55990777	56097074	56270275	55892913.50	56038050.25	56211709.95
MDG-c_15	50	60	60	55945742	56076707	56252183	55891242.55	56032771.00	56215053.55
MDG-c_16	50	60	60	55960705	56140977	56249512	55877242.10	56060959.00	56215024.25
MDG-c_17	50	60	60	55958700	56079252	56226673	55891889.30	56021554.10	56181329.00
MDG-c_18	50	60	60	55947581	56061668	56240125	55879358.00	56004267.15	56175311.65
MDG-c_19	50	60	60	55949205	56063226	56225414	55875167.65	56037554.50	56204567.35
MDG-c_20	50	60	60	55979807	56103438	56239512	55897182.15	56034844.75	56206989.95
Average				55958533.45	56087667.95	56245400.90	55877999.10	56031642.09	56201493.19
#Best				0	0	20	0	0	20
p-value				7.74e-6	7.74e-6		7.74e-6	7.74e-6	