# GRASP AND PATH RELINKING FOR THE MAX-MIN DIVERSITY PROBLEM

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ABSTRACT. The Max-Min Diversity Problem (MMDP) consists in selecting a subset of elements from a given set in such a way that the diversity among the selected elements is maximized. The problem is NP-hard and can be formulated as an integer linear program. Since the 1980s, several solution methods for this problem have been developed and applied to a variety of fields, particularly in the social and biological sciences. We propose a heuristic method – based on the GRASP and path relinking methodologies – for finding approximate solutions to this optimization problem. We explore different ways to hybridize GRASP and path relinking, including the recently proposed variant known as GRASP with evolutionary path relinking. Empirical results indicate that the proposed hybrid implementations compare favorably to previous metaheuristics, such as tabu search and simulated annealing.

## 1. INTRODUCTION

The problem of maximizing diversity deals with selecting a subset of elements from a given set in such a way that the diversity among the selected elements is maximized. As stated in Kuo et al. (1993), there are basically two approaches to formulate these problems: the Max-Sum and the Max-Min models. Both have received much attention in recent years. The former, also known as the *maximum diversity problem* (MDP) has been studied in Glover et al. (1998), Silva et al. (2004), and Duarte and Martí (2007). For the *max-min diversity problem* (MMDP), both exact (Erkut, 1990) and heuristic approaches, such as simulated annealing (Kincaid, 1992), tabu search (Kincaid, 1992), and GRASP (Ghosh, 1996) have been proposed. Because of the *flat landscape* of max-min problems, these papers agree that the MMDP presents a challenge to solution methods based on heuristic optimization.

The MMDP consists in selecting a subset M of m elements (|M| = m) from a set N of n elements in such a way that the minimum distance between the chosen elements is maximized. The definition of distance between elements is customized to specific applications. As mentioned in Kuo et al. (1993) and Glover et al. (1998), the MMDP has applications in plant breeding, social problems, and ecological preservation. In most of these applications, it is assumed that each element can be represented by a set of attributes. Let  $s_{ik}$  be the state or value of the k-th attribute of element i, where  $k = 1, \ldots, K$ . The distance between elements i

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	1	<b>2</b>	3	4	<b>5</b>	6	7
1	-	4.6	6.2	2.1	3.5	3.6	4.4
<b>2</b>	4.6	-	6.6	7.1	8.2	2.4	5.3
3	6.2	6.6	-	7.3	3.3	2.4	3.8
<b>4</b>	2.1	7.1	7.3	-	5.5	1.1	2.3
<b>5</b>	3.5	8.2	3.3	5.5	-	6.4	3.4
6	3.6	2.4	2.4	1.1	6.4	-	5.4
<b>7</b>	4.4	5.3	3.8	2.3	3.4	5.4	-

FIGURE 1. Distance matrix of an instance with n = 7.

and j can be defined as

$$d_{ij} = \sqrt{\sum_{k=1}^{K} (s_{ik} - s_{jk})^2}.$$

In this case,  $d_{ij}$  is simply the Euclidean distance between *i* and *j*. The distance values are then used to formulate the MMDP as a quadratic binary problem, where for i = 1, ..., n, variable  $x_i$  takes the value 1 if element *i* is selected and 0 otherwise:

(MMDP) max 
$$z_{MM}(x) = \min_{i < j} d_{ij} x_i x_j$$
  
subject to  $\sum_{i=1}^n x_i = m$   
 $x_i = \{0, 1\}, \quad i = 1, \dots, n$ 

Erkut (1990) and Ghosh (1996) showed independently that the MMDP is NPhard. The maximum diversity problem (MDP) can be formulated in a similar way by simply replacing the objective function,  $z_{MM}(x)$ , in the formulation above with

$$z_{MS}(x) = \sum_{i < j} d_{ij} x_i x_j.$$

Although the MDP and the MMDP are related, we should not expect a method developed for the MDP to perform well on the MMDP. The example in Figure 1 illustrates that the correlation between the values of the solutions in both problems can be relatively low.

Suppose we have seven elements of which we need to select five. Furthermore, the distances between each pair of elements are given by the matrix of Figure 1. For such a small example, we can enumerate all possible solutions (selections of m out of n elements) and compute for each one the values  $z_{MS}(x)$  and  $z_{MM}(x)$ . The correlation between both objective functions is 0.52, which can be considered relatively low. Moreover, we find that the optimal solution  $x^*$  of the MDP has a value  $z_{MS}(x^*) = 54.4$  and a value  $z_{MM}(x^*) = 2.1$ . However, the optimal solution  $y^*$  of the MMDP has a value  $z_{MM}(y^*) = 3.3$ , which is relatively larger than  $z_{MM}(x^*)$ . Moreover, 30% of the solutions present a  $z_{MM}(x)$  value larger than  $z_{MM}(x^*)$ . Therefore, we should not expect a method for the MDP to obtain good solutions for the MMDP. In this paper, we restrict our attention to solution methods specifically designed for the MMDP.

In Section 2, we describe previous work. In this paper, we explore the hybridization of the GRASP, path relinking, and evolutionary path relinking methodologies to find optimal or near-optimal solutions to the MMDP. Then, we introduce our algorithms in Sections 3 and 4. Computational experiments are described in Section 5 and concluding remarks are made in Section 6.

#### 2. Previous Methods

Chandrasekaran and Daughety (1981) introduced the MMDP under the name of *m*-dispersion problem. They proposed two simple polynomial-time heuristics for the special case of tree networks. Kuby (1987) introduced the problem on general networks, proposing integer linear programming formulations with  $O(n^2)$ constraints and *n* binary variables, and tested the formulations on instances of dimension n = 25 (m = 5 and m = 10).

Erkut (1990) proposed a branch and bound algorithm and a heuristic method. The branch and bound method was able to solve problems with n = 40 in half an hour of CPU time (on an AT-compatible microcomputer with clock speed of 10 Mhz). The heuristic method consists of construction plus local search. The construction starts with the infeasible solution where all n elements are selected. To reduce the set of selected elements to m, the procedure performs  $n \cdot m$  steps. At each step, it de-selects the element  $i^*$  with an associated shortest distance. Note that given a shortest distance  $d_{ij}$  there are at least two elements with this associated distance. The method randomly selects one of them. The construction can be repeated, obtaining a different solution each time. The local search method scans the set of selected elements in search of the best exchange to replace a selected element with an unselected one. The method performs moves as long as the objective value increases and stops when no improving exchange can be found.

Kincaid (1992) proposed two heuristics for the MMDP based on exchanges: a simulated annealing (SA) heuristic and a tabu search (TS) heuristic. In a given iteration, the SA method generates a random move (an exchange between a selected and an unselected element). If it is an improving move, it is automatically made; otherwise, it still may be made with positive probability. The so-called temperature and cooling schedule in the SA that manage the evolution of this acceptance probability are implemented according to Lundi and Mess (1986). The algorithm starts with an initial temperature equal to the largest distance value and it is reduced according to the factor tfactr = 0.89. For each temperature value,  $sample_size = 10n$  moves are generated. The SA method terminates when a maximum number of iterations  $max_it = 80$  is reached (note that within this number of iterations the temperature value is still strictly positive).

The tabu search heuristic also performs exchange moves. At each iteration,  $sample_size = 10n$  moves are considered and the method performs the best admissible move among them. Admissible here refers to the tabu status. When a move is performed and a selected item i is exchanged with an unselected item j, the unordered pair (i, j) is recorded in the tabu list and is labeled tabu for tabu\_size = 20 iterations. A selected move is admissible if it is not labeled tabu, or if its value improves upon the best known solution (aspiration criterion). After max\_it = 65 iterations, the search is re-initiated from a new initial solution for diversification purposes. The author examines the performance of both methods on 30 instances of size n = 25 (in three groups of ten with different characteristics) and m ranging from 5 to 15.

Kuo et al. (1993) proposed the following improved integer linear programming formulation:

$$\begin{array}{l} \max \ Z = w \\ \text{subject to} \ \sum_{i=1}^{n} x_i = m, \\ (C - d_{ij})y_{ij} + w \leq C, 1 \leq i < j \leq n \\ x_i + x_j - y_{ij} \leq 1, \quad 1 \leq i < j \leq n \\ - x_i + y_{ij} \leq 0, \quad 1 \leq i < j \leq n \\ - x_j + y_{ij} \leq 0, \quad 1 \leq i < j \leq n \\ y_{ij} > 0, \quad 1 < i < j < n \end{array}$$

and illustrated it on small examples. The constant C takes an arbitrarily large value. The authors state that, for both exact and heuristic methods, the MMDP is harder to solve than the MDP. As reported in Section 5, we will use this formulation to solve small-size instances with an integer linear programming solver.

Ghosh (1996) proposed a solution construction procedure and a local search method. Given a set N with n elements, the construction method performs m steps as follows. Let  $M_{k-1}$  be a partial solution with k-1 elements  $(1 \le k \le m)$ . For any  $i \in N \setminus M_{k-1}$ , let  $\Delta z_{MM}(i)$  be the contribution of i to the value of the solution. Let  $\Delta z_L(i)$  and  $\Delta z_U(i)$  be, respectively, a lower and an upper bound of  $\Delta z_{MM}(i)$ .  $\Delta z_L(i)$  is computed as the minimum between the value of the current solution and the minimum distance between i and the other elements in N.  $\Delta z_U(i)$ is computed by first sorting the distances between i and the elements in  $N \setminus M_{k-1}$ and then computing the smallest among the largest m-k elements. Then  $\Delta z'(i) =$  $(1-u)\Delta z_L(i) + u\Delta z_U(i)$  is an estimate of  $\Delta z_{MM}(i)$  (where u is a random number from the U(0,1) uniform distribution). The element i<sup>\*</sup> with the largest value of the estimate is selected to be included in the partial solution:

$$M_k = M_{k-1} \cup \{i^*\}, \quad \Delta x'(i^*) = \max_{i \in N \setminus M_{k-1}} \{\Delta z'(i)\}.$$

Starting with a randomly selected element, this process is repeated until  $M_m$  is finally delivered as the output of the construction  $(|M_m| = m)$ . The local search is similar to the one introduced in Erkut (1990) and begins at the conclusion of the construction phase, attempting to improve upon an incumbent solution through neighborhood search. The neighborhood of a solution is the set of all solutions obtained by replacing one element by another. Given a solution M, for each  $i \in M$ and  $j \in N \setminus M$ , we compute the move value  $\Delta z_{MM}(i, j)$  associated with the exchange of i and j. The method scans the entire neighborhood and performs the move with the largest  $\Delta z_{MM}$  value, if it improves the current solution. The current solution is updated as well as its corresponding value. The search stops when no move improves the current solution (i.e. when  $\Delta z_{MM}(i, j) \leq 0$  for all i and j). The method performs ten global phases (construction followed by improvement) and the best solution overall is returned as the output.

```
begin GRC
1
     Sel \leftarrow \emptyset;
2
     Select i randomly from N;
3
      Sel \leftarrow \{i\};
4
      while |Sel| < m do
           d_j \leftarrow \min_{k \in Sel} d_{jk}, \forall j \in CL = N \setminus Sel;
d^* \leftarrow \max_{j \in CL} d_j;
5
6
7
            RCL \leftarrow \{j \mid d_j \ge \alpha \cdot d^*\};
            Select i^* randomly in RCL;
8
            Sel \leftarrow Sel \cup \{i^*\};
9
10 end-while;
end
```

FIGURE 2. Constructive heuristic GRC.

## 3. GRASP

The GRASP methodology was developed in the late 1980s (Feo and Resende, 1989; 1995) and the acronym was coined in Feo et al. (1994). We refer the reader to Resende and Ribeiro (2003) for a recent survey of this metaheuristic. Each GRASP iteration consists in constructing a trial solution and then applying local search from the constructed solution. The construction phase is iterative, randomized greedy, and adaptive. In this section we describe our adaptation of the GRASP methodology for the MMDP.

3.1. Construction procedures. From the previous algorithms reviewed in Section 2, we can point to two construction procedures. ErkC, the method proposed in Erkut (1990) is based on de-selecting elements, and GhoC, the one due to Ghosh (1996), is based on an estimate of the contribution of the elements. In this section, we propose two new construction methods based on the GRASP methodology.

Given a set N with n elements, the construction procedure GRC performs m steps to produce a solution with m elements as shown in Figure 2. The set Sel represents the partial solution under construction. At each step, GRC selects a candidate element  $i^* \in CL = N \setminus Sel$  with a large distance to the elements in the partial solution Sel. Specifically, it first computes  $d_j$  as the minimum distance between element j and the selected elements. Then, it constructs the restricted candidate list RCL with all the candidate (unselected) elements j with a distance value  $d_j$ within a fraction  $\alpha$  ( $0 \le \alpha \le 1$ ) of the maximum distance  $d^* = \max\{d_j \mid j \in CL\}$ . Finally, GRC randomly selects an element in RCL.

GRC implements a typical GRASP construction in which first each candidate element is evaluated by a greedy function to construct the *RCL* and then an element is selected at random from the *RCL*. We now consider GRC2, an alternative construction procedure introduced in Resende and Werneck (2004) as random plus greedy construction. In GRC2 we first randomly choose candidates and then evaluate each candidate according to a greedy function to make the greedy choice. GRC2 first constructs the restricted candidate list *RCL2* with a fraction  $\beta$  ( $0 \le \beta \le 1$ ) of the elements in *CL* selected at random. Then, it evaluates all the elements in *RCL2*, computing  $d_j$  for all  $j \in RCL2$ , and selects the best one, i.e. the element  $j^*$  such that

$$d_{j^*} = \max_{j \in BCL^2} d_j.$$

In the computational study, we discuss how search parameters  $\alpha$  and  $\beta$  affect GRC and GRC2, respectively. We also test the *reactive* variants (Reactive-GRC and Reactive-GRC2) in which the value of the parameter is randomly determined according to an empirical distribution of probabilities (Prais and Ribeiro, 2000).

During the initial constructions of Reactive-GRC (Reactive-GRC2), the value of  $\alpha$  ( $\beta$ ) is randomly selected from the set  $S = \{0, 0.1, 0.2, \dots 0.9, 1\}$  with a uniform distribution. 20% of the constructions sample from the uniform distribution while 80% sample according to the *hits* value. In each iteration, we test whether the constructed solution x(a) obtained with  $\alpha = a$  ( $\beta = a$ ), has a value  $z_{MM}(x(a))$  within a pre-established threshold of the best constructed solution so far.<sup>1</sup> In this case, we increment *hits*(a) by one unit (where *hits*(i) is initially set to zero for all  $i \in S$ ). Otherwise, *hits*(a) remains unchanged. Therefore, initially all the values considered in S have the same opportunity to be selected for construction. However, as the algorithm progresses, those values better suited for a particular instance (those that produce better constructions) are more frequently selected. In this way, the reactive construction customizes the best value (or values) of the parameter for each instance. Note that in the non-reactive variants described earlier, the selection of the parameter is made offline and adjusted to a fixed value for all the instances considered.

3.2. Local search methods. Erkut (1990) and Ghosh (1996) propose the local search method BLS, based on the best-improvement strategy, in which at each iteration the method scans the entire neighborhood in search of the best exchange (between a selected and an unselected element). In what follows, we propose two new local search methods based on the first-improvement strategy (also known as *mildest ascent*). The first method, FLS, consists in a straightforward implementation of this strategy, while the second, called improved local search (IMLS), explores the neighborhood according to an evaluation function.

Given a set N with n elements, and a solution Sel with m selected elements, we compute the following values:

$$d_i = \min_{j \in Sel} d_{ij}, \quad d^* = \min_{j \in Sel} d_j,$$

where  $d_i$  is the minimum distance of element *i* to the selected elements (those in *Sel*), and  $d^*$  is the objective function of the current solution, i.e.  $d^* = z_{MM}(Sel)$ . It is clear that to improve a solution we need to remove (and thus replace) the elements *i* in the solution for which  $d_i = d^*$ .

The FLS method scans, at each iteration, the list of elements in the solution  $(i \in Sel)$  with minimum  $d_i$  value, i.e. for which  $d_i = d^*$ . It scans the list of elements in lexicographical order, starting with a randomly selected element. Then, for each element i with a minimum  $d_i$ -value, FLS examines the list of unselected elements  $(j \in N \setminus Sel)$  in search for the first improving exchange. The unselected elements are also examined in lexicographical order, starting with a randomly selected element. The method performs the first improving move  $(Sel \leftarrow Sel \setminus \{i\} \cup \{j\})$  and updates  $d_i$  for all elements  $i \in Sel$  as well as the objective function value  $d^*$ , concluding

 $<sup>^1\</sup>mathrm{We}$  have empirically found that a conservative value of 90% for this threshold provides good results.



FIGURE 3. Local search performance

the current iteration. The algorithm repeats iterations as long as improving moves can be performed and stops when no further improvement is possible. As described below, the definition of "improving" is not limited to the objective function.

The example in Figure 3 with n = 6 and m = 4 illustrates the performance of the local search procedure. Consider the solution  $Sel = \{1, 2, 3, 4\}$ , depicted with dark circles, with a value of  $d^* = 3$  in which we perform an iteration of the FLS method. For the sake of clarity, Figure 3 only depicts some of the distances between the elements. The  $d_i$  values of the elements in the solution are  $d_1 = 3, d_2 = 3, d_2 = 3, d_3 = 3$  $d_3 = 3$ , and  $d_4 = 4$ . The FLS method selects an element with minimum  $d_i$  value, say for example i = 1. It then scans the list of unselected vertices in search for an improving move. Note, however, that when we remove element 1, elements 2 and 3 remain in the solution and therefore  $d^*$  will be equal to  $d_{23} = 3$ , regardless of the element that we introduce in the solution to replace element 1. Then, strictly speaking, we cannot find any improving exchange when we remove element 1. On the other hand, it is clear that in a certain sense the solution improves when we remove element 1, because the number of elements for which  $d^*$  is reached decreases and therefore we can say that we are closer to obtaining a better solution. This is why we consider an extended definition of improving for a given move, including not only when the move increases the value of  $d^*$ , but also when  $d^*$  remains fixed and the number of elements i with  $d_i = d^*$  is reduced. In this example, when we replace element 1 with element 5 obtaining  $Sel' = \{2, 3, 4, 5\}$ , we say that this is an improving move, because  $d^* = 3$  and  $d_i$  only matches  $d^*$  in two elements (2 and 3), which compares favorably with the initial solution Sel (in which three elements matched  $d^* = 3$ ).

The example in Figure 3 also illustrates that when we select an element for exchange, it would be better to consider not only the distance with the closest element, but also the second closest, third closest, and so on. Given an element i, let  $d_i^1, d_i^2, \ldots, d_i^k$  be its k lowest distance values between i and the m elements in the solution (k < m) sorted in increasing order ( $d_i = d_i^1$ ). In the example,  $d_1^1 = 3, d_1^2 = 4, d_2^1 = 3$ , and  $d_2^2 = 3$ . Then it is better to remove element 2 instead of element 1 because by removing element 2 the objective  $d^*$  could increase to  $d_2^3 = 4$ . Therefore, we propose a new local search method, that we call IMLS, which is based on the evaluation of the value

$$e(i) = \sum_{j=1}^{k} \frac{d_i^j}{j}$$

for elements  $i \in Sel$  with  $d_i = d^*$ , according to each element's lowest k distance values (where k is a search parameter).

The local search method IMLS selects, at each iteration, the element  $i^*$  with the lowest e(i) value among the selected elements  $i \in Sel$  with  $d_i = d^*$ . It then moves this element from the solution:  $Sel \leftarrow Sel \setminus \{i^*\}$  to the unselected set, and computes the e(s) value for all elements  $s \in N \setminus Sel$ . The method then scans the elements in  $N \setminus Sel$  in decreasing order of e(s) and performs the first improving move. If no improving move is found, the method selects the next element with lowest e(i) value among the selected elements  $i \in Sel$  with  $d_i = d^*$  and tries to find an improving move. We also apply here the definition of improving move introduced in FLS (increasing the value of  $d^*$ , or keeping  $d^*$  fixed and reducing the number of elements i with  $d_i = d^*$ ). The method stops when no further improvement is possible.

### 4. Path relinking

Path relinking (PR) was suggested as an approach to integrate intensification and diversification strategies in the context of tabu search (Glover, 1996; Glover and Laguna, 1997). This approach generates new solutions by exploring trajectories that connect high-quality solutions – by starting from one of these solutions, called an *initiating solution*, and generating a path in the neighborhood space that leads toward the other solutions, called *guiding solutions*. This is accomplished by selecting moves that introduce attributes contained in the guiding solutions, and incorporating them in an *intermediate solution* initially originated in the initiating solution.

Laguna and Martí (1999) adapted PR in the context of GRASP as a form of intensification. The relinking in this context consists in finding a path between a solution found with GRASP and a chosen elite solution. Therefore, the relinking concept has a different interpretation within GRASP since the solutions found from one GRASP iteration to the next are not linked by a sequence of moves (as in the case of tabu search). Resende and Ribeiro (2003) present numerous examples of GRASP with PR. In this section we explore the adaptation of GRASP with PR to the MMDP across different designs in which greedy, randomized, and evolutionary elements are considered in the implementation.

4.1. Greedy path relinking. Let x and y be two solutions of the MMDP, interpreted as the sets of m selected elements  $Sel_x$  and  $Sel_y$ , respectively ( $|Sel_x| = |Sel_y| = m$ ). The path relinking procedure PR(x, y) starts with the first solution x, and gradually transforms it into the second one y, by swapping out elements selected in x with elements selected in y. The elements selected in both solutions x and y,  $Sel_{xy}$ , remain selected in the intermediate solutions generated in the path between them. Let  $Sel_{x-y}$  be the set of elements selected in x and not selected in y and symmetrically, let  $Sel_{y-x}$  be the set of elements selected in y and not selected in x, i.e.

$$Sel_{xy} = Sel_x \cap Sel_y, Sel_{x-y} = Sel_x \setminus Sel_{xy}, Sel_{y-x} = Sel_y \setminus Sel_{xy}$$

Let  $p_0(x, y) = x$  be the initiating solution in the path P(x, y) from x to y. To obtain the solution  $p_1(x, y)$  in this path, we unselect in  $p_0(x, y)$  a single element  $i \in Sel_{x-y}$ , and select a single element  $j \in Sel_{y-x}$ , thus obtaining

$$Sel_{p_1(x,y)} = Sel_{p_0(x,y)} \setminus \{i\} \cup \{j\}.$$

In the greedy path relinking (GPR) algorithm, the selection of the elements i and j is made in a greedy fashion. To obtain  $p_{k+1}(x, y)$  from  $p_k(x, y)$ , we evaluate all the possibilities for  $i \in Sel_{p_k(x,y)-y}$  to be de-selected and  $j \in Sel_{x-p_k(x,y)}$  to be selected, and perform the best swap. In this way, we reach y from x in  $r = |Sel_{x-y}| = |Sel_{y-x}|$  steps, i.e.  $p_r(x, y) = y$ . The output of the PR algorithm is the best solution, different from x and y, found in the P(x, y) path (among  $p_1(x, y), p_2(x, y), \ldots, p_{r-1}(x, y)$ ).

The PR algorithm operates on a set of solutions, called *elite set* (ES), constructed with the application of a previous method. In this paper, we apply GRASP to build the elite set. If we only consider a quality criterion to populate the elite set, we could simply populate the elite set with the the best |ES| solutions generated with GRASP. However, previous studies (Resende and Werneck, 2004) have empirically found that an application of PR to a pair of solutions is likely to be unsuccessful if the solutions are very similar. Therefore, to construct ES we will consider both quality and diversity.

Initially ES is empty, and we apply GRASP for b = |ES| iterations and populate it with the solutions obtained. We order the solutions in ES from the best  $(x^1)$ to the worst  $(x^b)$ . Then, in the following GRASP iterations, we test whether the generated (constructed and improved) solution x' qualifies to enter ES. Specifically, if x' is better than the best  $x^1$ , it is put in the set. Moreover, if it is better than the worst  $x^b$  and it is sufficiently different from the other solutions in the elite set  $(d(x', ES) \ge dth)$ , it is also put in ES. The parameter dth is a distance threshold value that reflects the term "sufficiently different" and it is empirically adjusted (see Section 5). To keep the size of ES constant and equal to b, whenever we add a solution to this set, we remove another one. To maintain the quality and the diversity, we remove the closest solution to x' in ES among those worse than it in value. Figure 4 shows pseudo-code of the GRASP with PR algorithm.

The design in Figure 4 is called *static* since we first apply GRASP to construct the elite set ES and then we apply PR to generate solutions between all the pairs of solutions in ES. Given two solutions in ES, x and y, we apply path relinking in both directions, i.e. PR(x, y) from x to y and PR(y, x) from y to x. The best solution generated in both paths is subjected to the local search method for improved outcomes. As shown in Figure 4, we always keep the best solution in the elite set  $(x^1)$  during the realization of the GRASP phase and we only replace it when the new solution generated improves it in quality. The algorithm terminates when PR is applied to all the pairs in ES and the best overall solution  $x^{best}$  is returned as the output.

As aforementioned, distance is used to measure how diverse one solution is with respect to a set of solutions. Specifically, for the MMDP, let  $x_i^r$  be the value of the *i*-th variable for the elite solution  $r \in ES$ . Also let  $x_i^t$  be the value of the *i*-th variable for the trial solution t. Then, the distance between the trial solution t and the solutions in the ES is defined as

$$d(t, ES) = b \cdot m - \sum_{r=1}^{b} \sum_{i:x_i^t=1} x_i^r.$$

The formula simply counts the number of times that each selected element in the trial solution t appears in the elite solutions and subtracts this value from the maximum possible distance (i.e.,  $b \cdot m$ ). The maximum distance occurs when no

begin StaticGRASP+PR  $GlobalIter \leftarrow$  number of global iterations; 1 Apply GRASP (construction and local search) for b = |ES| iterations to populate  $ES \leftarrow \{x^1, x^2, \dots, x^b\};$ iter  $\leftarrow b + 1$ ; 3 while *iters*  $\leq$  *GlobalIter* do 4  $x \leftarrow \text{GRASP}$  construction phase; 5 $x' \leftarrow \text{GRASP}$  local search starting at x; 6 if  $z_{MM}(x') > z_{MM}(x^1)$  or  $(z_{MM}(x') > z_{MM}(x^b)$  and  $d(x', ES) \ge dth)$  then 7 $x^k \leftarrow \text{closest solution to } x' \text{ in } ES \text{ with } z_{MM}(x') > z_{MM}(x^k);$ 8 g  $ES \leftarrow ES \setminus \{x^k\};$ 10 Insert x' into ES so that ES remains sorted from best  $x^1$  to worst  $x^b$ ; 11 end-if: 12*iters*  $\leftarrow$  *iters* + 1; 13 end-while; 14  $x^{best} \leftarrow x^1$ 15 for (i = 1 to b - 1 and j = i + 1 to b do16 Apply  $PR(x^i, x^j)$  and  $PR(x^j, x^i)$  and let  $x \leftarrow$  best solution found;  $x' \leftarrow \text{local search phase of GRASP starting from } x;$ 17if  $z_{M\!,\!M}(x')>z_{MM}(x^{best})$  then 18 19 $x^{best} \leftarrow x';$ 20end-if; 21 end-for; 22 return  $x^{best}$ : end

FIGURE 4. GRASP with PR in a static variant.

element that is selected in the trial solution t appears in any of the elite solutions in ES.

An alternative implementation of GRASP with PR consists in a *dynamic* update of the elite set as introduced in Laguna and Martí (1999). In this design, each solution x' generated with GRASP is directly subjected to the PR algorithm, which is applied between x' and a solution  $x^j$  selected from *ES*. The selection is probabilistically made according to the value of the solutions. As in the *static* design, the local search method is applied to the output of PR, but now, the resulting solution is directly tested for inclusion in *ES*. If successful, it can be used as guiding solution in later applications of PR. Figure 5 shows pseudo-code for this dynamic variant.

In our computational experience, described on Section 5, we compare the static variant versus the dynamic variant with respect to both quality and speed.

4.2. Greedy randomized path relinking. Faria Jr. et al. (2005) introduced greedy randomized path relinking (GRPR) where instead of moving between the initiating and the guiding solutions in a greedy way, the moves are done in a greedy randomized fashion.

As described above for the greedy path relinking algorithm, at each step in the path from the initiating solution x to the guiding solution y, the selection of the elements i (to be de-selected) and j (to be selected) is made in a greedy fashion. In the GRPR algorithm, we construct a set of good candidates i and j for swapping and randomly select one among them. This procedure mimics the selection method employed in a GRASP construction.

begin DynamicGRASP+PR
1 $GlobalIter \leftarrow$ number of global iterations;
2 Apply GRASP (construction and local search) for $b =  ES $ iterations
to populate $ES \leftarrow \{x^1, x^2, \dots, x^b\};$
3 $iter \leftarrow b+1;$
4 while $iters \leq GlobalIter$ do
5 $x \leftarrow \text{GRASP}$ construction phase;
6 $x' \leftarrow \text{GRASP}$ local search starting at $x$ ;
7 Randomly select $x^j$ from $ES$ ;
8 Apply $PR(x', x^j)$ and $PR(x^j, x')$ and let y be the best solution found;
9 $y' \leftarrow \text{GRASP}$ local search starting at $y$ ;
10 if $z_{MM}(y') > z_{MM}(x^1)$ or $(z_{MM}(y') > z_{MM}(x^b)$ and $d(y', ES) \ge dth)$ then
11 $x^k \leftarrow \text{closest solution to } y' \text{ in } ES \text{ with } z_{MM}(y') > z_{MM}(x^k);$
12 Add $y'$ to $ES$ and remove $x^k$ ;
13 Sort <i>ES</i> from best $x^1$ to worst $x^b$ ;
14 end-if;
15 end-while;
16 $x^{best} \leftarrow x^1;$
17 return $x^{best}$ ;
end

FIGURE 5. GRASP with PR in a dynamic variant.

To obtain  $p_{k+1}(x, y)$  from  $p_k(x, y)$ , we evaluate all the possibilities for  $i \in Sel_{p_k(x,y)-y}$  to be de-selected and  $j \in Sel_{y-p_k(x,y)}$  to be selected. The candidate set C contains all these swaps, i.e.

$$C_k(x,y) = \{(i,j) \mid i \in Sel_{p_k(x,y)-y}, j \in Sel_{y-p_k(x,y)}\}.$$

Let z(i, j) be the value of the move associated with de-select i and select j in the current solution  $p_k(x, y)$  to obtain  $p_{k+1}(x, y)$ . Then,

$$z(i,j) = z_{MM}(p_{k+1}(x,y)) - z_{MM}(p_k(x,y)).$$

In step k of the path from x to y, the restricted candidate list  $RCL_k(x, y)$  of good candidates for swapping is

$$RCL_k(x,y) = \{(i,j) \in C_k(x,y) \mid z(i,j) \ge \delta z^*\},\$$

where  $z^*$  is the maximum of z(i, j) in  $C_k(x, y)$  and  $\delta$   $(0 \leq \delta \leq 1)$  is a search parameter. A pair  $(i, j) \in RCL_k(x, y)$  is randomly selected and the associated swap is performed.

In the application of PR in the GRASP with PR algorithm, we can apply the greedy variant (GPR) described in Subsection 4.1 or the randomized variant (GRPR) described in this subsection. Specifically, in the static variant we only need to apply GPR or GRPR in step 16 of the pseudo-code shown in Figure 4, and similarly in the dynamic variant we apply one or the other in step 8 of the pseudo-code in Figure 5.

4.3. Truncated path relinking. As aforementioned, path relinking explores a path in the solution space from an initiating solution  $x = p_0(x, y)$  to a guiding solution  $y = p_r(x, y)$ , where  $r = |Sel_{x-y}| = |Sel_{y-x}|$  is the number of steps from x to y.

At each intermediate solution  $p_k(x, y)$ , a restricted neighborhood of the solution is searched for the next solution in the path from  $p_k(x, y)$  to y. The neighborhood is restricted because only moves that remove element  $i \in Sel_{p_k(x,y)-y}$  and put in its place an element  $j \in Sel_{y-p_k(x,y)}$  are allowed. As the procedure moves from one intermediate solution to the next, the cardinalities of sets  $Sel_{p_k(x,y)-y}$  and  $Sel_{y-p_k(x,y)}$  decrease by one element each. Consequently, as the procedure nears the guiding solution, there are fewer allowed moves to explore and the search tends to be less effective. This suggests that path relinking tends to find good solutions near the initiating solution since it can explore the solution space more effectively around that solution. If this happens, then the effort made by path relinking near the guiding solution is fruitless.

In truncated path relinking, a new stopping criterion is used. Instead of continuing the search until the guiding solution is reached, only  $\kappa$  steps are allowed, i.e. the resulting path in the solution space is  $p_1(x, y), p_2(x, y), \ldots, p_{\kappa}(x, y)$  and the best of these solutions is returned as the path relinking solution.

4.4. Evolutionary path relinking. Resende and Werneck (2004) introduced *evolutionary path relinking* (EvPR) as a post-processing phase for GRASP with PR (see also Andrade and Resende (2007)). In EvPR, the solutions in the elite set (ES) are evolved in a similar way that the reference set evolves in scatter search (SS) (Laguna and Martí, 2003).

As in the dynamic variant of GRASP with greedy path relinking, in GRASP with EvPR we apply in each iteration the construction and the improvement phase of GRASP as well as the PR method to obtain the elite set (see steps 5 to 9 in the pseudo-code shown in Figure 5). After a pre-established number of iterations the GRASP with greedy path relinking stops. However, in GRASP with EvPR, a post-processing phase based on path relinking is applied to each pair of solutions in ES. The solutions obtained with this latter application of PR are considered to be candidates to enter ES, and PR is again applied to them as long as new solutions enter ES. This way we say that ES evolves. Figure 6 shows the pseudo-code of GRASP with EvPR in which this process is repeated for GlobalIter iterations.

GRASP with EvPR and scatter search (SS) are evolutionary methods based on evolving a small set of selected solutions (elite set in the former and reference set in the latter). We can, therefore, observe similarities between them. In some implementations of SS, GRASP is used to populate the reference set, but note that other constructive methods can be used as well. Similarly, PR can be used to combine solutions in SS, but we can use any other combination method (Martí et al., 2006). From an algorithmic point of view, we may find two main differences between these methods. The first one is that in SS we do not apply PR to the solutions obtained with GRASP (as we do in steps 7 and 8 in pseudo-code of GRASP with EvPR shown in Figure 6), but rather, we only apply PR as a combination method between solutions already in the reference set. The second difference is that in SS when none of the new solutions obtained with combinations are admitted to the reference set (elite set), it is rebuilt, removing some of its solutions, as specified in the reference set update method (Martí et al., 2006). In GRASP with EvPR we do not remove solutions from ES, but rather, we again apply GRASP (starting from step 5) and use the same rules for inclusion in the ES.

## 5. Computational experiments

This section describes the computational experiments that we performed to test the efficiency of our GRASP with path relinking procedures as well as to compare

begin GRASP+EvPR 1  $GlobalIter \leftarrow$  number of global iterations; Apply GRASP (construction and local search) for b = |ES| iterations  $\mathbf{2}$ to populate  $ES \leftarrow \{x^1, x^2, \dots, x^b\};$ for *iter* = 1, ..., *GlobalIter* do 3 4 for  $i = 1, \ldots, LocalIter$  do  $x \leftarrow \text{GRASP}$  construction phase; 56  $x' \leftarrow \text{GRASP}$  local search starting at x; Randomly select  $x^j$  from ES; 7 Apply  $PR(x', x^j)$  and  $PR(x^j, x')$  and let y be the best solution found; 8  $y' \leftarrow \text{GRASP}$  local search starting at y; 9 if  $z_{MM}(y') > z_{MM}(x^1)$  or  $(z_{MM}(y') > z_{MM}(x^b)$  and  $d(y', ES) \ge dth)$  then 10  $x^k \leftarrow \text{closest solution to } y' \text{ in } ES \text{ with } z_{MM}(y') > z_{MM}(x^k);$ 11 12Add y' to ES and remove  $x^k$ ; Sort ES from best  $x^1$  to worst  $x^b$ ; 13end-if: 14 15end-for; 16 NewSol  $\leftarrow 1$ ; while NewSol do 1718 NewSol  $\leftarrow 0$ ; Apply PR(x, x') and PR(x', x) for every pair (x, x') in ES 19 not combined before. Let y be the best solution found; 20 $y' \leftarrow \text{GRASP}$  local search starting at y; if  $z_{MM}(y') > z_{MM}(x^1)$  or  $(z_{MM}(y') > z_{MM}(x^b)$  and  $d(y', ES) \ge dth)$  then 21 $x^k \leftarrow \text{closest solution to } y' \text{ in } ES \text{ with } z_{MM}(y') > z_{MM}(x^k);$ 22Add y' to ES and remove  $x^k$ ; 23Sort *ES* from best  $x^1$  to worst  $x^b$ ; 2425NewSol  $\leftarrow 1$ ;  $x^{best} \leftarrow x^1$ : 2627end-if; 28end-while; 29end-for; 30 return  $x^1$ ; end

FIGURE 6. GRASP with EvPR.

them with the previous methods identified to be the state-of-the-art for the MMDP. We implemented the methods in Java SE 6 and solved the integer linear programming formulation described in Section 2 with Cplex 8.0. All the experiments were conducted on a Pentium 4 computer running at 3 GHz with 3 GB of RAM. We have employed three sets of instances in our experiments:

- Glover: This data set consists of 75 matrices for which the values were calculated as the Euclidean distances from randomly generated points with coordinates in the 0 to 100 range. The number of coordinates for each point is also randomly generated between 2 and 21. Glover et al. (1998) developed this test problem generator and constructed instances with n = 10, 15, and 30. The value of m ranges from 0.2n to 0.8n.
  - Geo: This data set consists of 60 matrices constructed with the same test problem generator employed in the *Glover* set. We generated twenty instances with n = 100, 250, and 500. For each value of n we consider m = 0.1n, 0.3n (generating ten instances for each combination of n and m). These instances are similar to the *geometric* instances introduced in Erkut (1990).

Ran: This data set consists of 60 matrices with random numbers. These instances are based on the generator introduced by Silva et al. (2004). As for the Geo set, we generated twenty instances with n = 100, 250, and 500 (and for each value of n we consider m = 0.1n, 0.3n). The integer random numbers are generated between 50 and 100 in all the instances except when n = 500 and m = 150 in which they are generated between 1 and 200 (to make them harder in terms of comparison among heuristics).

In each experiment, we compute for each instance the overall best solution value, *BestValue*, obtained by all executions of the methods considered. Then, for each method, we compute the relative percentage deviation between the best solution value obtained with that method and *BestValue* for that instance. We report the average of this relative percentage deviation (Dev.) across all the instances considered in each particular experiment. We finally report, for each method, the number of instances (#Best) in which the value of the best solution obtained with this method matches *BestValue*. We also report the statistic *Score* achieved by each method, as described in Ribeiro et al. (2002). For each instance, the *n\_score* of a method *M* is defined as the number of methods that found a better solution than *M*. In case of ties, all the methods receive the same *n\_score*, equal to the number of methods strictly better than all of them. We then report Score as the sum of the *n\_score* values across all the instances in the experiment. Thus, the lower the Score the better the method.

In our preliminary experimentation we consider the set of 40 instances formed with ten instances from the *Geo* set with n = 100 and ten with n = 25 and similarly from the *Ran* set (half with m = 0.1n and half with m = 0.3n). In the first preliminary experiment, we study the parameter  $\alpha$  in constructive method GRC as well as the parameter  $\beta$  in the constructive method GRC2. We run GRC and GRC2 100 times, thus obtaining 100 solutions for each method and instance pair. Table 1 reports, for this set of 40 instances and each value of  $\alpha$ , the values of Dev., #Best, and Score described above.

The results in Table 1 show that the best outcomes are obtained when the constructive method GRC2 is run with a value of  $\beta = 0.90$ . Therefore, we use this method in the rest of our experimentation.

		GI	$\operatorname{RC}(\alpha)$			GR	$C2(\beta)$		
	0.75	0.90	0.95	Reactive	0.75	0.90	0.95	Reactive	
Dev. #Best Score	$9.23\% \\ 0 \\ 277$	$2.51\% \\ 5 \\ 184$	$1.09\% \\ 10 \\ 101$	$0.81\%\ 16\ 60$	0.70% 21 41	$0.58\% \\ 21 \\ 43$	$0.66\% \\ 18 \\ 51$	$1.07\%\ 15\ 90$	-

TABLE 1. New constructive methods on *Geo* and *Ran* instances with n = 100, 250.

Method	RanC	TD2	GD2	ErkC	GhoC	GRC2
Dev. #Best Score	$22.85\% \ 0 \ 168$	23.21% 1 151	$17.10\% \\ 0 \\ 117$	$6.08\% \ 4 \ 80$	$1.68\% \\ 15 \\ 26$	$0.12\% \\ 37 \\ 4$

TABLE 2. Constructive methods on *Geo* and *Ran* instances with n = 100, 250.

In our second preliminary experiment we compare the constructive method GRC2(0.9) with the two previous constructive methods for the MMDP: ErkC, (Erkut, 1990) and GhoC (Ghosh, 1996). We also consider a random construction (RanC) in which the *m* elements in the solution are randomly selected as a baseline for comparison. In addition, we include in this experiment two previous algorithms developed for the maximum diversity problem (MDP) considered to be the best constructive methods for this variant of the problem: TD2 and GD2 (Duarte and Martí, 2007). We generate 100 solutions with each method on each instance and report the three statistics described above.

Results in Table 2 clearly show the superiority of the proposed method (GRC2) on these instances. The method is able to obtain 37 best solutions out of 40 instances. Moreover, this experiment confirms that the methods developed for the MDP provide low-quality solutions when employed to solve the MMDP. Specifically, TD2 and GD2 obtain, respectively, 23.21 and 17.10 relative percentage deviation on average, while ErkC, GhoC, and GRC2 obtain 6.08, 1.68, and 0.12 respectively. As expected, RanC obtains low-quality solutions.

In the third preliminary experiment, we compare the constructive with the local search methods for the MMDP. Specifically we target the constructive and improvement methods ErkC+BLS (Erkut, 1990) and GhoC+BLS (Ghosh, 1996). We consider the two local search methods proposed in Subsection 3.2, FLS and IMLS in combination with the constructive method GRC2. We denote by GRASP1 the constructive method GRC2(0.9) coupled with the local search FLS, and by GRASP2 the GRC2(0.9) method with IMLS. We construct and improve 100 solutions in each instance with these four methods and report the statistics of the best solutions found in Table 3. We do not report the solution methods for the MDP since, as in the previous experiment, they provide low-quality results.

Method	ErkC+BLS	GhoC+BLS	GRASP1	GRASP2
Dev. #Best Score	2.40% 8 81	0.82% 22 85	$0.24\% \\ 29 \\ 16$	$0.38\%\ 29\ 22$

TABLE 3. Local search method on *Geo* and *Ran* instances with n = 100, 250.



FIGURE 7. Solution values with construction + local search

Table 3 shows that our two new approaches based on the GRASP methodology are able to improve upon previous methods also based on construction plus local search. Specifically, GRASP1 and GRASP2 present an average percent deviation from the best solutions obtained in this experiment of 0.24 and 0.38, respectively, while ErkC+BLS and GhoC+BLS obtain 2.4 and 0.82, respectively. To complement the information shown in Table 3, Figure 7 shows the values of the 100 solutions obtained with GRASP1, GhoC+BLS, and ErkC+BLS, ordered from lowest to highest, on a *Ran* instance of dimension n = 250 and m = 25. The results shown in Figure 7 show that GRASP1 systematically obtains better solutions than the other two methods tested. Although, for the sake of simplicity, this figure only shows the results for one instance, we have found that it is representative of the evolution of the tested methods in the entire set.

In the following experiment we compare the two variants of the greedy path relinking algorithm described in Subsection 4.1. We consider both the static version in which the PR is applied after GRASP1 (pseudo-code shown in Figure 4), and the dynamic version in which the PR is executed within each iteration of GRASP1 (pseudo-code shown in Figure 5). The path relinking method depends on the parameter dth that specifies the minimum distance for a solution to enter the elite set. Table 4 reports, for the set of 40 instances considered in our preliminary experiments and four different values of dth, the average percentage deviation from the best solution obtained (Dev.), the number of best solutions (#Best), the sum of the *n\_score* values (Score), and the average CPU time (Time) in seconds.

Table 4 clearly shows that the greedy path relinking (GPR) in its dynamic variant obtains better solutions than the GPR in the static variant, although it consumes more running time (about 18 seconds on average compared with the 11 seconds of the static version). Moreover, this table also shows that the best value of *dth* in the

	Static GPR						Dynamic GPR				
dth	4	8	10	12		4	8	10	12		
Dev. #Best Score Time	0.65% 20 86 11.0s	0.63% 21 71 11.3s	0.54% 24 62 10.7s	0.76% 20 85 11.0s		0.21% 30 35 18.1s	$\begin{array}{c} 0.32\%\ 29\ 29\ 18.6 \mathrm{s} \end{array}$	0.49% 22 69 18.3s	$0.47\% \\ 22 \\ 52 \\ 18.2 s$		

TABLE 4. Greedy path relinking methods on *Geo* and *Ran* instances with n = 100, 250.

dynamic version is 4, since the method obtains an average percentage deviation of 0.21 and 30 best solutions, which compares favorably with the other values shown. We therefore set the value of dth to 4 in the following path relinking algorithms and restrict our attention to the dynamic variant.

In the next preliminary experiment we undertake to compare the greedy path relinking (GPR) algorithm considered above with the greedy randomized path relinking (GRPR) described in Subsection 4.2. We first study the effect of the parameter  $\delta$  in the performance of the GRPR algorithm, considering  $\delta = 0.1, 0.3, 0.5, 0.7,$  and 0.9. We do not reproduce the results of this experiment in a table, but we simply report that we obtain slightly better solutions with  $\delta$  set to 0.9 than with the other values (an improvement of 0.2% for the average deviation from the best solutions in this experiment). We then compare the performance of GPR and GRPR with  $\delta = 0.9$  both running for two minutes, and consider in this experiment the truncated strategy described in Subsection 4.3 in which the path is truncated when a portion depth of the solutions is explored. When depth is set to 100%, the entire path is explored (and therefore no truncation at all is applied). Alternatively, when *depth* is set to 10%, for example, only the first 10% solutions in the path are explored. Table 5 reports the statistics Dev., #Best, Score, as well as the number of paths explored (#Paths) and the average running time in seconds (PR time) that each method dedicates to the path relinking algorithm.

Table 5 shows that the GPR method provides better solutions than the GRPR, since the average percentage deviation values obtained with the former range from 0.20% to 0.26% while with GRPR these values range from 0.34% to 0.58%. As expected, as the value of the parameter *depth* increases, the time dedicated to the path relinking (PR time) also increases. Moreover, given that the total running time is set to 2 minutes in all the cases, the number of explored paths (#Paths) is reduced as *depth* increases. However, these variations (PR time and #Paths) are small since the time saved when the path is truncated is very small in this implementation because the cardinality of the neighborhood explored in the path reduces as the path approaches the guiding solution. Therefore, variations in the parameter *depth* have a small effect on the quality of the final solution obtained with the method.



FIGURE 8. Average number of best solutions in the path

Figure 8 complements the information shown in Table 5, plotting the number of best solutions found in each part of the path. The figure shows the average number of best solutions found in the first 10% of the path, the number of best solutions in the second 10% of the path (from 10% to 20%), and so on. The figure confirms the hypothesis that the best solutions are mainly obtained at the beginning of the path. However, good solutions are also obtained in the final part of the path. This fact, together with the small time saving associated with truncated the path lead us to consider in the following experiments the GPR method with *depth* set to 100%.

		Gl	PR		GRPR			
depth	50%	70%	90%	100%	50%	70%	90%	100%
Dev.	0.26%	0.23%	0.25%	0.20%	0.37%	0.34%	0.43%	0.58%
#Best	31	33	32	34	28	30	28	23
Score	18	20	14	14	39	33	43	91
#Paths	3268.95	3115.10	3026.58	3094.68	3277.18	3142.88	3111.90	3208.15
PR time	0.28s	0.30s	0.31s	0.33s	0.26s	0.30s	0.30s	0.30s

TABLE 5. Truncated GPR and GRPR methods on *Geo* and *Ran* instances with n = 100, 250.

In our final experiment, we compare our best methods with the state-of-the-art methods for the MMDP. Specifically, we consider the following six algorithms (all run for 100 global iterations except GRASP+EvPR):

- GhoC+BLS: Multi-start method (Ghosh, 1996).
  - SA: Simulated annealing (Kincaid, 1992).
  - TS: Tabu search (Kincaid, 1992).
  - GRASP1: Constructive method GRC2(0.9) coupled with the local search FLS.
    - *GPR*: Dynamic greedy path relinking in which the PR is executed within each iteration of GRASP1 with dth = 4 and depth = 100%.
- GRASP+EvPR: Evolutionary path relinking with GlobalIter = 5 (generation with GPR and evolution with PR of the elite set) and LocalIter = 20.

Tables 6, 7, and 8 report, for each method on each set of instances, the average relative percentage deviation (Dev.) between the best solution values obtained with each method and the best known, the number of instances (#Best) in which the value of the best solution obtained with each method matches the best known, the statistic Score where the lower the Score the better the method, and the average CPU time in seconds. Experiments with CPLEX 8.0 (with the Kuo et al. (1993) formulation) confirm that the best known solutions in the 75 *Glover* instances reported in Table 6 are the optimal solutions.

The problem instances in the *Glover* set (Table 6) do not provide a way of differentiating the performances of the methods that we are comparing. They are easy to solve and all the methods are capable of quickly finding the optimal solutions.

Tables 7 and 8 show the merit of the proposed procedures. Our GPR and GRASP+EvPR implementations consistently produce the best solutions with percent deviations smaller than those of the competing methods (and with number of best solutions found larger than the others). GRASP+EvPR presents a marginal improvement when compared with GPR but requires longer running times (especially for large instances). On the other hand, the GRASP1 algorithm is able to obtain relatively good solutions in short computational time, with a performance very similar to the GhoC+BLS method. The SA and TS methods perform well on small *Geo* instances (n = 100) but are clearly inferior to the others reported in our comparison when target large sized instances (n = 500). The ranking of the methods with respect to the best solutions found in the 120 *Geo* and *Ran* 

TABLE 6. Best methods – *Glover* instances

	GhoC+BLS	SA	TS	GRASP1	GPR	GRASP+EvPR
Dev. #Opt Score Time	$\begin{array}{c} 0.00\% \\ 75 \\ 0 \\ 0.03 \end{array}$	$\begin{array}{c} 0.00\% \\ 75 \\ 0 \\ 0.98 \end{array}$	$\begin{array}{c} 0.00\% \\ 75 \\ 0 \\ 1.56 \end{array}$	$\begin{array}{c} 0.00\% \\ 75 \\ 0 \\ 0.02 \mathrm{s} \end{array}$	0.00% 75 0 0.02s	$\begin{array}{c} 0.00\% \\ 75 \\ 0 \\ 0.04 \mathrm{s} \end{array}$



FIGURE 9. Search profiles on large Geo instance.

instances is: GRASP+EvPR(96), GPR(73), GRASP1(37), SA(34), TS(32), and GhoC+BLS(30).

Figure 9 shows the typical search profile for the methods that we compared. This run corresponds to the largest *Geo* instances (n = 500, m = 150) with a time limit of 60 minutes per instance and method.

		GhoC+BLS	$\mathbf{SA}$	TS	GRASP1	GPR	GRASP+EvPR
n = 100	Dev. #Best	$0.75\% \\ 10$	0.00% 19	0.00% 20	$0.76\% \\ 10$	$0.11\% \\ 16$	$\begin{array}{c} 0.09\% \\ 17 \end{array}$
	Score Time	42 2.45s	$\begin{array}{c} 1 \\ 20.96 \mathrm{s} \end{array}$	0 33.64s	44 0.68s	13 1.68s	8 3.76s
n = 250	Dev. #Best Score Time	$1.00\% \ 0 \ 65 \ 30.50 \mathrm{s}$	0.68% 6 36 220.57s	1.75% 2 73 439.68s	1.11% 1 71 5.58s	0.19% 7 18 33.44s	0.16% 14 11 65.57s
n = 500	Dev. #Best Score Time	$2.36\% \ 0 \ 56 \ 282.37 \mathrm{s}$	3.48% 0 62 1449.85s	9.27% 0 100 3633.36s	2.39% 0 61 34.99s	0.25% 7 13 788.31s	0.04% 16 4 1465.44s

TABLE 7. Best methods – Geo instances

#### GRASP AND PATH RELINKING FOR MAX-MIN DIVERSITY

		GhoC+BLS	SA	TS	GRASP1	GPR	GRASP+EvPR
n = 100	Dev.	1.71%	2.89%	3.28%	1.37%	0.61%	0.49%
	#Best	4	9	10	7	14	15
	Score	51	41	44	40	16	9
	$\mathbf{Time}$	1.37s	10.82s	33.11s	0.84s	2.96s	7.36s
n = 250	Dev.	2.01%	3.73%	7.49%	1.34%	0.81%	0.26%
	#Best	3	0	0	5	11	17
	Score	34	78	90	20	9	3
	$\mathbf{Time}$	15.98s	115.10s	$430.07 \mathrm{s}$	19.22s	$101.57 \mathrm{s}$	271.05s
n = 500	Dev.	2.95%	41.62%	41.62%	1.70%	0.18%	0.27%
	#Best	13	0	0	14	18	17
	Score	11	80	80	8	2	3
	$\mathbf{Time}$	93.05s	868.00s	$3606.49 \mathrm{s}$	99.02s	2172.38s	6349.20s

TABLE 8. Best methods - Ran instances

Figure 9 clearly shows that GRASP+EvPR outperforms the other methods over a long term horizon (3600 seconds in this experiment). Moreover, it is worthwhile noting that GRASP+EvPR obtains high quality solutions (better than the competing methods) from the first iterations (100 seconds). On the other hand, SA presents a low performance when comparing with the other three methods in this experiment.

The GRASP1 method obtains the best solutions within the first 50 seconds. However, GRASP1 by itself (without the PR post-processing) is not able to improve these initial solutions and presents a flat profile during the entire search.

## 6. Conclusions

The objective of this study has been to advance the current state of knowledge about implementations of path relinking procedures (PR) for combinatorial optimization. Unlike other evolutionary methods such as genetic algorithms or scatter search, PR has not yet been extensively studied.

In this paper, we studied the generation of solutions with GRASP and their combination with PR. We also tested four different variants of PR known as greedy PR, greedy randomized PR, truncated PR, and evolutionary PR, as well as two search strategies: static and dynamic. We performed several experiments with previously reported instances. Our experiments show that the dynamic variants of GRASP with greedy PR and GRASP with evolutionary PR are the best methods for the MMDP instances tested in this paper. Moreover, the results indicate that the proposed hybrid heuristics compare favorably to previous metaheuristics, such as tabu search and simulated annealing.

Obviously, the results that we obtained with our implementation are not all due to the strategies that we wanted to test and that we describe in Section 4. Performance was definitely enhanced by the context-specific methods that we developed for the MMDP. However, our preliminary experiments do show the merit of the mechanisms in Section 4 that we hope could become standard in future PR implementations.

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