GRASP WITH EXTERIOR PATH RELINKING FOR DIFFERENTIAL DISPERSION MINIMIZATION

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Abstract. We propose several new hybrid heuristics for the differential dispersion problem are proposed, the best of which consists of a GRASP with sampled greedy construction with variable neighborhood search for local improvement. The heuristic maintains an elite set of high-quality solutions throughout the search. After a fixed number of GRASP iterations, exterior path relinking is applied between all pairs of elite set solutions and the best solution found is returned. Exterior path relinking, or *path separation*, a variant of the more common interior path relinking, is first applied in this paper. In interior path relinking, paths in the neighborhood solution space connecting good solutions are explored between these solutions in the search for improvements. Exterior path relinking, as opposed to exploring paths between pairs of solutions, explores paths beyond those solutions. This is accomplished by considering an initiating solution and a guiding solution and introducing in the initiating solution attributes not present in the guiding solution. To complete the process, the roles of initiating and guiding solutions are exchanged. Extensive computational experiments on 190 instances from the literature demonstrate the competitiveness of this algorithm.

1. Introduction

Let $G = (V, E)$ be an undirected complete graph, where V is the set of n vertices and E the set of $\binom{n}{2}$ edges. Each edge $(u, v) \in E$ with $u, v \in V$ has an associated distance d_{uv} between u and v. Dispersion, or diversity, problems (DP) consist in finding a subset $S \subseteq V$ with m elements, such that an objective function (based on the distances between elements in S) is maximized or minimized. According to Prokopyev et al. (2009), the objective of a dispersion problem can be either to identify a subset with (i) maximum distance among its elements (diversity problems), or (ii) with maximum similarity among them (equity problems). The first class of problems has been intensively studied in the last ten years. For instance, Martí et al. (2010; 2013) and Gallego et al. (2009) present several exact, heuristic, and metaheuristic-based methods for the maximum diversity problem. Two important variants are, respectively, the sum (Maxsum DP) and minimum (Maxmin DP) of the distances in the selected set (Agca et al., 2000).

Equity problems are mainly used in the context of facility location problems, where the fairness among candidate facility locations is as relevant as the dispersion of the selected locations (Teitz, 1968). These kinds of problems also have

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applications in the context of urban public facility location (Teitz, 1968), selection of homogeneous groups (Brown, 1979a), dense/regular subgraph identification (Kortsarz and Peleg, 1993), and equity-based measures in network flow problems (Brown, 1979b). In spite of all these applications, we have identified only one previous metaheuristic-based paper on equitable problems, in which Prokopyev et al. (2009) adapt a simple generic GRASP algorithm to solve several equitable problems.

Prokopyev et al. (2009) propose four distinct equity-based functions to balance the diversity among the selected elements: the mean-dispersion function minimizes the average dispersion of the selected elements; the generalized mean-dispersion function, which is an extension of the mean-dispersion function, considers vertex-weighted graphs; and the min-sum and the min-diff dispersion functions that consider the extreme equity values of the selected elements. In this paper we focus on the last function, whose associated optimization problem is referred to as the *Minimum Differential Dispersion Problem* (Min-Diff DP).

A feasible solution of the Min-Diff problem is a set $S \subseteq V$ of m elements, where m is a given input parameter. Each feasible solution has associated with it a cost which can be can be computed as follows. Let $\Delta(v)$ be the sum of distances between a vertex $v \in S$ and the remaining elements of S. Formally,

$$\Delta(v) = \sum_{u \in S} d_{uv}.$$

The objective function of a solution S (denoted by $\mathit{diff}(S)$) is then computed as

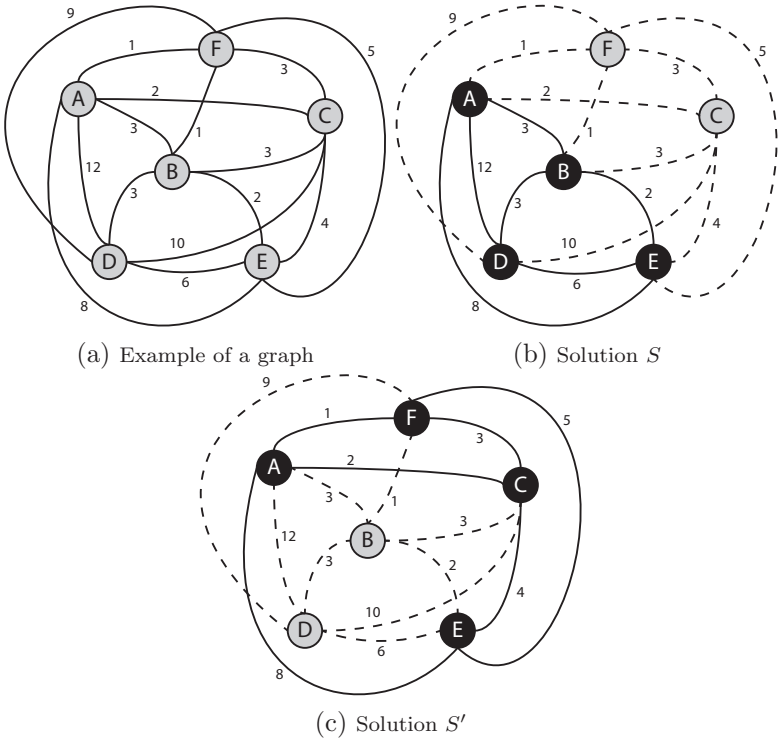
$$\mathit{diff}(S) = \max_{u \in S} \Delta(u) - \min_{v \in S} \Delta(v)$$

Therefore, the Min-Diff problem consists of finding a solution $S^\star \subseteq V$ with the minimum differential dispersion, i.e.

$$S^\star = \arg\min_{S \subseteq V_m} \mathit{diff}(S),$$

where V_m is the set of all subsets of vertices in V with cardinality m.

Figure 1a shows an example of a graph with six vertices and 15 edges with their associated distances. Figures 1b and 1c depict two possible solutions for the Min-Diff problem for $m = 4$. The selected vertices in the solution are shown in black while the edges in each solution are highlighted by solid lines. The vertices not in the solution are shown in grey while the edges not in the solution are dashed. To evaluate the quality of each solution, we first compute the $\Delta(v)$ value for all the elements in the solution. In particular, Figure 1b shows a solution where $S = \{A, B, D, E\}$, $\Delta(A) = 3{+}12{+}8 = 23$, $\Delta(B) = 3{+}3{+}2 = 8$, $\Delta(D) = 12{+}3{+}6 = 21$, and $\Delta(E) = 8{+}2{+}6 = 16$. The *diff*-value is calculated by first selecting the vertices having the highest and lowest Δ values and then taking the difference of their Δ values. In this solution, these vertices are, respectively, A and B, and therefore $\mathit{diff}(S) = \Delta(A) - \Delta(B) = 23 - 8 = 15$. If we now consider the solution $S' = \{A, C, E, F\}$ in Figure 1c, it is easy to verify that the associated objective function value is $\mathit{diff}(S') = 9$. Considering that the Min-Diff problem is a minimization problem, solution S' is better than solution S. The rationale behind this is that the distances among the elements in S' are more similar than those among the elements in S.



(a) Example of a graph (b) Solution S

(c) Solution S'

FIGURE 1. Example of two solutions on a graph with six vertices.

Prokopyev et al. (2009) present a basic mixed linear 0-1 formulation of the problem. Let L_i and U_i be lower and upper bounds on the value of $\sum_{j \in S} d_{ij}$, i.e. $L_i = \sum_{j \in S} \min\{d_{ij}, 0\}$ and $U_i = \sum_{j \in S} \max\{d_{ij}, 0\}$. Then, the mixed linear 0-1 formulation of the Min-Diff DP is as follows:

$$
\begin{array}{lll}
\min\limits_{t,r,s,x} & t & \\
s.t. & t \geq r - s, & i = 1, \ldots, n \\
& r \geq \sum\limits_{j:j \neq i} d_{ij} x_j - U_i(1 - x_i) + M^-(1 - x_i), & i = 1, \ldots, n \\
& s \leq \sum\limits_{j:j \neq i} d_{ij} x_j - L_i(1 - x_i) + M^+(1 - x_i), & i = 1, \ldots, n \\
& \sum\limits_{i=1}^{n} x_i = m & x \in \{0,1\}^n,
\end{array}
$$

where M^+ is an upper bound on the U_i values, M^- is a lower bound on the L_i values, and the binary decision variable $x_i = 1$ if and only if node $i \in S$.

The computational experiments described in Prokopyev et al. (2009) show that CPLEX 9.0 is only able to solve instances of small size (up to $|V| = 40$ and $m = 15$), requiring high CPU times (more than 2500 seconds on average). The authors also propose a generic GRASP that can be applied to different equity problems. The objective of our paper is to propose a specialized GRASP that obtains high-quality solutions for the Min-Diff problem without requiring long running times.

Additionally, we hybridize GRASP with Path Relinking for improved outcomes. Specifically, we propose in Section 2 two constructive procedures and three local search methods. We also introduce in Section 2.3 an improvement strategy based on the Variable Neighborhood Search metaheuristic. Finally, in Section 3, we consider two post-processing strategies based on Path Relinking. It is worthwhile mentioning that we apply a new variant of Path Relinking, introduced in (Glover, 2014) and called *Exterior Path Relinking*, or *Path Separation*, and which, for this problem, obtains very promising results. In Section 4, we present computational experience. We first analyze and tune the proposed algorithms and then compare our best proposal with both the GRASP of Prokopyev et al. (2009) and CPLEX 12.5.1 on the integer programming formulation proposed there and described above. Concluding remarks are outlined in Section 5.

2. GRASP

The greedy randomized adaptive search procedure (GRASP) is a metaheuristic developed in the late 1980s (Feo and Resende, 1989) and formally introduced in Feo et al. (1994). Resende and Ribeiro (2010; 2014) present recent and thorough surveys of this method. GRASP is a multi-start methodology where each iteration consists of two stages. The first is a greedy, randomized, and adaptive construction of a solution. The second stage applies an improvement method to obtain a local optimum from the constructed solution. These two phases are repeated until a termination criterion is met. The rest of this section is organized as follows. Section 2.1 presents two constructive procedures for the Min-Diff problem. Section 2.2 introduces three local search algorithms whose objective is to improve the constructed solution. Finally, Section 2.3 describes a more elaborate improvement strategy based on the Variable Neighborhood Search (VNS) metaheuristic (Mladenović and Hansen, 1997).

2.1. **Constructive methods.** GRASP constructive procedures apply a greedy function to evaluate the quality of the elements in a candidate list. Given a partial solution S, we propose the following greedy function to estimate the increment/decrement of the objective when an element $v \in V \setminus S$ is added to S. Given the complexity of the objective function evaluation in the Min-Diff problem, the definition of such a greedy function is not trivial. For the sake of simplicity, the evaluation of the greedy function consists of four steps. The first step estimates the Δ-value of vertex u (denoted by $\delta(u)$) if it is included in the partial solution:

$$\forall u \in V \setminus S \rightarrow \delta(u) = \sum_{v \in S} d_{uv}.$$

The second step estimates the variation in the Δ-values of all vertices $v \in S$ if u is included in S:

$$\forall v \in S \rightarrow \delta(v) = \Delta(v) + d_{uv}.$$

Once these δ values are computed, the third step determines whether the potential inclusion of vertex $u \in V \setminus S$ in the partial solution modifies the maximum and/or the minimum Δ-values. This values are, respectively, denoted as

$$\delta_{\max}(u) = \max \left\{ \delta(u), \max_{v \in S} \delta(v) \right\},$$

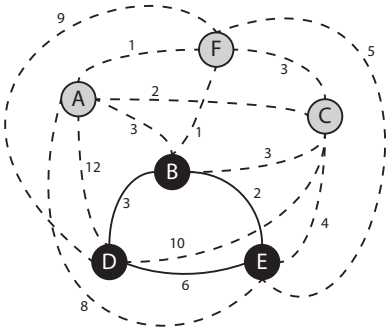
and

$$\delta_{\min}(u) = \min\left\{\delta(u), \min_{v \in S}\{\delta(v)\right\}.$$

The fourth step finally computes the greedy function g for each element $u \in V \setminus S$ as

$$g(u) = \delta_{\max}(u) - \delta_{\min}(u).$$

Let us illustrate the computation of the greedy function with an example. Figure 2a shows a partial solution $S = \{B, D, E\}$, where vertices in S are highlighted in black and the vertices in $V \setminus S$ are shown in grey. If $m = 4$, we must include one vertex from $V \setminus S$ in the current partial solution. Figure 2b shows the evaluations of the candidate vertices A, C, and F. For each candidate vertex, we compute its δ-value, as well as the δ-values for each vertex already in S. For example, if we introduce vertex A in the current partial solution, then $\delta(A) = d_{AB} + d_{AD} + d_{AE} = 3 + 12 + 8 = 23$. In addition, the inclusion of A would affect vertices B, D, and E as follows: $\delta(B) = \Delta(B) + d_{AB} = 5 + 3 = 8$; $\delta(D) = \Delta(D) + d_{AD} = 9 + 12 = 21$; $\delta(E) = \Delta(E) + d_{AE} = 8 + 8 = 16$. Then, we identify the $\delta_{\min}$ and $\delta_{\max}$-values ($\delta(B) = 8$ and $\delta(A) = 23$, respectively) and finally the greedy function value for the potential inclusion of A in the partial solution is $g(A) = \delta_{\max} - \delta_{\min} = \delta(A) - \delta(B) = 23 - 8 = 15$. Figure 2b shows that the best option is to include vertex C, with $g(C) = 11$, in the current partial solution since this insertion produces the minimum increment in the objective function ($g(A) = 15$ and $g(E) = 12$).



(a) Partial solution.

v	A	C	F
$\delta(v)$	23	17	15
$\delta(B)$	8	8	6
$\delta(D)$	21	19	18
$\delta(E)$	16	12	13
$\delta_{\min}(v)$	8	8	6
$\delta_{\max}(v)$	23	19	18
$g(v)$	15	11	12

(b) Greedy function evaluation

FIGURE 2. Example of computation of the greedy function.

Algorithm 1 shows pseudo-code for *C1*, the first constructive algorithm. It follows the standard GRASP template, by initially creating a list of candidates (CL) which contains the elements that can be added to the partial solution under construction. At this point, the CL contains all the vertices of the graph (step 2). Then, the method randomly selects the first vertex from CL (step 3) and includes it in the partial solution (step 5). The method thus iterates until it obtains a solution with m vertices (steps 6 to 13). In each iteration, *C1* calculates the maximum ($g_{\max}$) and minimum ($g_{\min}$) values of the greedy function (steps 7 to 8). After that, *C1* constructs a restricted candidate list (RCL) with all the candidates whose greedy value does not exceed a percentage α of the best greedy value (step 9). Finally,

in the last step of the iteration the method selects at random one vertex from the RCL and adds it to the solution, updating CL (steps 10 to 12).

Algorithm 1: `C1`

1: $S \leftarrow \emptyset$
2: $\text{CL} \leftarrow V$
3: $v_0 \leftarrow \texttt{SelectRandom}(\text{CL})$
4: $S \leftarrow S \cup \{v_0\}$
5: $\text{CL} \leftarrow \text{CL} \setminus \{v_0\}$
6: **while** $|S| < m$ **do**
7: $\quad g_{min} \leftarrow \min_{u \in \text{CL}} g(u)$
8: $\quad g_{max} \leftarrow \max_{u \in \text{CL}} g(u)$
9: $\quad \text{RCL} \leftarrow \{v \in \text{CL} \mid g(v) \leq g_{min} + \alpha \cdot (g_{max} - g_{min})\}$
10: $\quad v \leftarrow \texttt{SelectRandom}(\text{RCL})$
11: $\quad S \leftarrow S \cup \{u\}$
12: $\quad \text{CL} \leftarrow \text{CL} \setminus \{u\}$
13: **end while**
14: **return** S

We now consider C2, a second constructive procedure based on a different strategy introduced in Resende and Werneck (2004). Specifically, this alternative construction swaps the greedy and random stages of a standard GRASP construction. This construction template has been recently applied with success in other papers (Campos et al., 2013; Resende et al., 2010; Pantrigo et al., 2012; Duarte et al., 2011).

Algorithm 2 shows the pseudo-code of the proposed method whose first steps are similar to the ones of Algorithm 1. The differences between these constructive procedures are limited to the main loop (steps 6 to 11). In particular, C2 constructs the RCL by selecting $\alpha \times |CL|$ elements from CL at random (step 7). Then, all the elements in the RCL are evaluated with the greedy function, selecting the one which presents the minimum greedy value (step 8). Finally, the solution and the associated candidate list are updated (steps 9 and 10). The method ends when the solution becomes feasible (i.e., $|S| = m$).

The α parameter controls the greediness/randomness of the GRASP constructive procedures. Specifically, if $\alpha = 0$ the corresponding methods are purely greedy algorithms, while if $\alpha = 1$ they are totally random procedures. In Section 4 we investigate the influence of α.

2.2. **Local search procedures.** The second stage of a GRASP algorithm consists in improving the constructed solutions using a local search method, which will guide the search process to a local optimum. One of the key elements in designing a effective local search method is the definition of the move and the associated move value (change in the objective function value). In particular, for the Min-Diff problem we define $\texttt{move}(S, u, v)$ as the move that interchanges vertex $u \in S$ with vertex $v \in V \setminus S$. This move usually produces a variation in the objective function, denoted as $\texttt{move\_value}(S, u, v)$. As with the definition of the greedy function, the computation of this quantity is not trivial if we want to update the value of the

Algorithm 2: C2

$S \leftarrow \emptyset$
CL $\leftarrow V$
$v_0 \leftarrow$ `SelectRandom`(CL)
$S \leftarrow S \cup \{v_0\}$
CL $\leftarrow$ CL $\setminus \{v_0\}$
while $|S| < m$ **do**
  RCL $\leftarrow$ `SelectRandom`(CL, α)
  $u \leftarrow \arg\min_{v \in \text{RCL}} g(v)$
  $S \leftarrow S \cup \{u\}$
  CL $\leftarrow$ CL $\setminus \{u\}$
end while
return S

objective function in an incremental way. Specifically, we need to identify the subset of edges of u (associated with the removed vertex) that no longer contribute to the objective function and the subset of edges of v (associated with the inserted vertex) which will be included in the computation of the objective function. Even without performing the move, we can estimate the Δ-values of the elements in S. We denote this estimate as δ (to be consistent with the notation introduced earlier). Therefore, if we were to remove vertex u and include vertex v in the solution S, the variation of the Δ-values would be computed as

$$\forall w \in S \setminus \{u\} \rightarrow \delta(w) = \Delta(w) - d_{wu} + d_{wv}.$$

We additionally must consider the estimation of including v in S, denoted as

$$\delta(v) = \sum_{w \in S \setminus \{u\}} d_{vw}.$$

The estimation of the objective function value if we would perform the move is computed as

$$\delta_{\min} = \min \left\{ \delta(v), \min_{w \in S \setminus \{u\}} \delta(w) \right\},$$

$$\delta_{\max} = \max \left\{ \delta(v), \max_{w \in S \setminus \{u\}} \delta(w) \right\}.$$

and

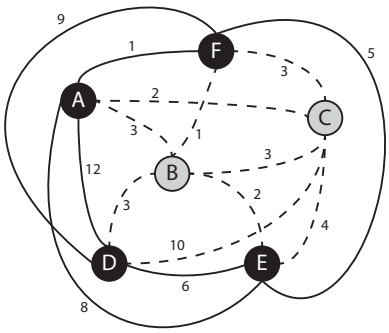
$$\mathit{MinDiff}\,(S \setminus \{u\} \cup \{v\}) = \delta_{\max} - \delta_{\min}.$$

Therefore, the move value would be finally defined as

$$\texttt{move\_value}(S, u, v) = \mathit{MinDiff}\,(S \setminus \{u\} \cup \{v\}) - \mathit{MinDiff}\,(S).$$

This way, we can quickly compute the value of the move without computing the value of the objective function from scratch. In fact, we do not really perform the move to estimate the increment/decrement of the objective function. Starting from the solution depicted in Figure 1b, we show in Figure 3a the resulting solution after performing `move`(S, B, F). Figure 3b shows a table with the computation of the δ-values defined above. Taking these values into account, the minimum and maximum values are respectively $\delta_{\min} = 15$ for F and $\delta_{\max} = 27$ for D, resulting

in a potential solution with $\mathit{MinDiff}(S \setminus \{B\} \cup \{F\}) = \delta_{\max} - \delta_{\min} = 27 - 15 = 12$. This move is accepted since it improves the current solution.



(a) Resulting solution after performing `move`(S, B, F).

v	$\delta(v)$
A	23 - 3 + 1 = 21
D	21 - 3 + 9 = 27
E	16 - 2 + 5 = 19
F	1 + 5 + 9 = 15
$\delta_{\min}$	15
$\delta_{\max}$	27
MinDiff	12

(b) Estimation of the δ-values for each vertex in the solution.

FIGURE 3. Example of the computation of `move_value`(S, B, F).

In a straightforward implementation, the complexity of computing the *MinDiff*-value is $O(m^2)$ because the method should compute, for each one of the m vertices in S, the distance to remaining $m-1$ vertices in S. However, using the proposed updating strategy defined above, the complexity reduces to $O(m)$ since it is only necessary to explore the $m-1$ vertices in S adjacent to the removed vertex and the $m-1$ vertices in S adjacent to the included vertex.

In this paper, we propose three local search procedures, denoted by LS1, LS2, and LS3, based on the move defined above. These three methods mainly differ in how the vertices are scanned. LS1 follows a best improvement template, resulting in an exhaustive search. Specifically, the method explores the vertices in the current solution S and those in $V \setminus S$. Then, it selects the best move between a vertex in S and a vertex in $V \setminus S$ (evaluating the aforementioned `move_value`). Finally, if the best move found improves the current solution, the move is made, updating the solution. The second local search method, denoted LS2, follows a first improvement template. The algorithm is similar to LS1, but instead of exploring all possible moves, it performs the first move that improves the current solution. Vertices in S and $V \setminus S$ are randomly explored to avoid focusing on the same subset of vertices. The third local search, LS3, also performs a first improvement strategy but ordering the vertices before exploring them. In order to start exploring the most promising moves, LS3 scans the vertices in S in descending order according to their Δ-values, while the vertices in $V \setminus S$ are scanned in ascending order according to their δ-values. Then, LS3 traverses both S and $V \setminus S$ performing the first move which improves the value of the current solution. The three local search methods end when no improvement is found after exploring all possible moves, returning the best solution found.

2.3. **Variable Neighborhood Search.** Variable Neighborhood Search (VNS) is a metaheuristic proposed by Mladenović and Hansen (1997) as a general framework to solve hard optimization problems. It is based on the idea of performing systematic changes of neighborhood structures within the search procedure. Heuristics based on this metaheuristic have been successfully applied to a large variety of

optimization problems (see for instance Duarte et al. (2013), Sánchez-Oro et al. (2013), Duarte et al. (2012), and Lozano et al. (2012). We refer the reader to Hansen and Mladenović (2014) for a recent survey of VNS.

An early proposal for multiple neighborhood search appeared in Glover et al. (1984) using a design based on the strategic oscillation concept. The oscillation strategy in that study was organized to apply different types of moves of varying complexity using a hierarchy of size-increasing neighborhoods in the terminology VNS has made popular. Some tabu search multiple neighborhood proposals (Glover, 1997; Glover and Laguna, 1997) are based on the interplay among classes of moves based on their distance measures, coupled with the use of memory to keep track of the attractiveness of moves from different classes. Such memory enables the search to jump between different neighborhood structures to link the most promising types of moves from each.

In this paper, we propose the use of a *Basic VNS* variant with a *Jump Neighborhood Change* strategy (Hansen et al., 2010) in place of the standard local search used in GRASP. Algorithm 3 shows the pseudo-code of the VNS. It has three input arguments: the initial solution (S), the maximum neighborhood to be explored ($k_{\max}$), and the jump magnitude (k_{step}). The initial solution is built with one of the constructive procedures described in Section 2.1. The best constructive procedure as well as the values of $k_{\max}$ and k_{step} will be experimentally determined in Section 4.

Algorithm 3: `BasicVNS`(S, k_{step}, k_{max})

1: $k \leftarrow k_{step}$
2: **repeat**
3: $\quad S' \leftarrow$ `Shake`(S, k)
4: $\quad S'' \leftarrow$ `LocalSearch`(S')
5: $\quad$ `NeighborhoodChange`(S, S'', k)
6: **until** $k = k_{max}$
7: **return** S

The algorithm mainly consists in executing three strategies: shake, local search, and neighborhood change. First, given a solution S, the shake method generates a new solution, S', in the k-th neighborhood of the current solution (step 4). In the context of the Min-Diff problem, it consists in performing k moves at random. Then, S' is improved using a local search method, producing a new improved solution S'' (step 5). We will experimentally determine the best local search among the three proposed in this paper.

The `NeighborhoodChange` function typically employed in a VNS compares the new solution S'' with the incumbent solution S obtained in the k-th neighborhood. If an improvement is obtained, k is reset to its original value (usually $k = 1$). Otherwise, the next neighborhood is considered for a further exploration (usually $k = k + 1$). In this paper, we investigate the effect on the search of the so-called *jump neighborhood search*, where the `NeighborhoodChange` function considers the parameter k_{step} to control the change of the neighborhood. Specifically, when the VNS method performs an improving move, it sets $k = k_{step}$ instead of $k = 1$. Similarly, in non-improving moves, it sets $k = k + k_{step}$ instead of $k = k + 1$. As customary in VNS, the search ends when k reaches or surpasses $k_{\max}$, returning

the best solution found. Note that the jumping strategy of this method skips some neighborhoods in the perturbation, which performs well on this type of nested neighborhoods of the same type of moves.

3. Path Relinking

Path Relinking (PR) is a metaheuristic introduced in **?** and Glover and Laguna (1997), originally proposed as a methodology to integrate intensification and diversification strategies in the context of tabu search. This metaheuristic explores trajectories that connect high-quality solutions, generating intermediate solutions that can eventually be better than the high-quality solutions being connected. Laguna and Martí (1999) adapted PR in the context of GRASP as a form of intensification. The PR algorithm operates on a set of solutions, called the *elite set* (ES), typically sorted from best (first solution in ES) to worst (last solution in ES). In this paper, we limit ourselves to consider only a quality criterion to populate the elite set. Therefore, the ES consists of the best b solutions generated with GRASP. This design is usually referred to as *static* (Resende et al., 2010), since we first apply GRASP to construct the elite set and then we apply PR to explore trajectories between all pairs of solutions in the ES.

Given two solutions in ES, S and S', the standard implementation of the path relinking (which in this paper we call *Interior Path Relinking* (IPR)) starts from the *initiating solution* S and gradually transforms it into the *guiding solution* S'. This transformation is accomplished by swapping out elements selected in S with elements in S', generating a set of *intermediate solutions*. The elements present in both solutions ($S \cap S'$) remain selected in solutions generated in the path between them. The set of elements in S and not in S' is $S \setminus S'$. Symmetrically, $S' \setminus S$ is the set of elements selected in S' and not selected in S. To obtain the first intermediate solution in this path, we remove a single element $u \in S \setminus S'$ and include a single element $v \in S' \setminus S$, thus obtaining $S_1 = S \setminus \{u\} \cup \{v\}$. Notice that S_1 can be trivially generated with the move described above. For the sake of simplicity, we denote this move as $S_1 = \texttt{move}(S, u, v)$. In general, the $k+1$-th intermediate solution is constructed from the previous solution as $S_{k+1} = \texttt{move}(S_k, u, v)$ with $u \in S_k \setminus S'$ and $v \in S' \setminus S_k$.

Given a graph with 12 vertices (labeled $\{A, B, \ldots, L\}$) and $m = 6$, let $S = \{A, B, C, D, E, F\}$ and $S' = \{A, B, C, G, H, I\}$. Figure 4 illustrates the construction of two interior paths, one from S to S' and another from S' to S. As it was aforementioned, common vertices between both solutions appear in all intermediate solutions. Solution S_1 is obtained from S by performing $\texttt{move}(S, D, G)$. Similarly, S_2 is obtained after applying $\texttt{move}(S_1, E, H)$. Notice that the reverse path is similarly constructed. In all cases, the introduced vertices are highlighted in grey.

The election of vertices u and v can be performed in a greedy or a random fashion. In particular, the greedy strategy obtains S_{k+1} from S_k by evaluating all the possibilities for $v \in S_k \setminus S'$ to be unselected and $u \in S' \setminus S_k$ to be selected, and performs the best move. On the other hand, the random strategy constructs S_{k+1} by randomly selecting a vertex $v \in S_k \setminus S'$ to be unselected and a vertex $u \in S' \setminus S_k$ to be selected. In this paper, we propose two interior path relinking methods: IPR$_G$ which constructs the paths between each pair of solutions in the ES using a greedy strategy, and IPR$_R$, which follows the random strategy. The best

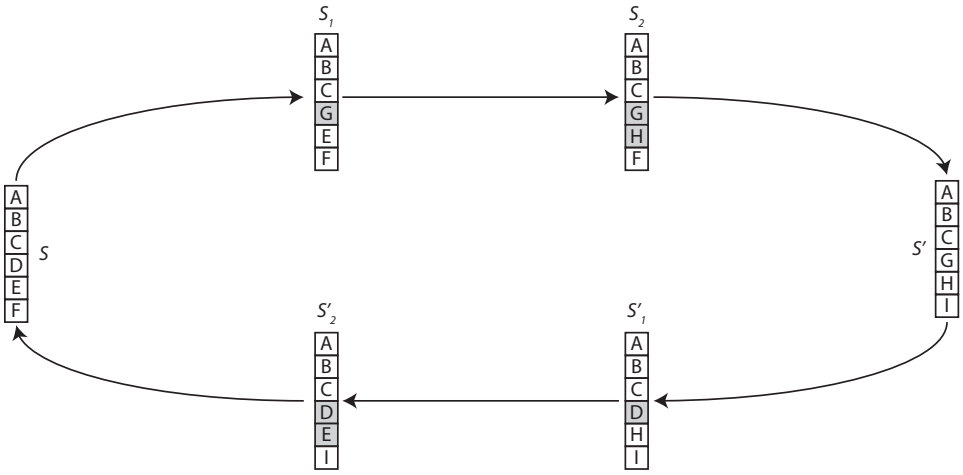


FIGURE 4. Example of two interior paths between S and S'.

solution generated in each path is subjected to the improvement method described in Section 2.3. The algorithm terminates when all pairs of solutions in the ES have been relinked, each pair by two paths. The best overall solution is returned.

Despite the widespread application of path relinking in combinatorial optimization, almost all PR implementations only consider the between-form of PR (Interior Path Relinking). This paper discusses the beyond-form of path relinking, introduced in Glover (2014) and called *Exterior Path Relinking* (EPR), and focuses on its relevance for effectively solving the MinDiff problem. Instead of introducing into the initiating solution characteristics present in the guiding solution, this new strategy introduces in the initiating solution characteristics not present in the guiding solution. Specifically, it removes from the initiating solution those elements which also belong to the guiding solution, obtaining intermediate solutions which are further away from both the initiating the guiding solutions.

The relevance of paths that go beyond the initiating and guiding solutions was broached in Glover (1997) as follows: The scope of strategies made available by path relinking is significantly affected by the fact that the term neighborhood has a broader meaning in tabu search than it typically receives in the popular literature on search methods. Often, the neighborhood terminology refers solely to methods that progressively transform one solution into another. Such neighborhoods are called transition neighborhoods in tabu search, and are considered as merely one component of a collection of neighborhoods that also include those operating in regions beyond solutions previously visited.

Given the initiating (S) and guiding (S') solutions for the MinDiff problem, the first intermediate solution in the exterior path beyond S is generated by removing a single element $u \in S \cap S'$ and adding a single element $v \in V \setminus (S' \cup S)$, thus obtaining $S_1 = S \setminus \{u\} \cup \{v\}$. Again, this solution can be directly obtained with the move operator described in Section 2.2. The $k+1$-th intermediate solution is constructed from S_k, the previous solution, as $S_{k+1} = \texttt{move}(S_k, u, v)$ with $u \in S_k \cap S'$ and $v \in V \setminus (S' \cup S_k)$. As for IPR, we propose two methods: EPR_G and EPR_R. EPR_G constructs the paths using a greedy strategy while EPR_R follows

the random strategy. Again, the best solution generated in each path is subjected to the improvement method described in Section 2.3. The algorithm terminates when all pairs of solutions in the ES have been relinked, each pair by two paths, one beyond S and the other beyond S'.

We illustrate in Figure 5 the construction of the exterior paths by considering the same graph with 12 vertices labeled $\{A, B, \ldots, L\}$ introduced earlier, with $m = 6$ and the same initiating and guiding solutions. As it can be seen, the exterior path generates solutions S_1 and S_2 by performing $\texttt{move}(S, A, J)$ and $\texttt{move}(S_1, B, K)$, respectively. It is easy to see that those intermediate solutions (i.e., S_1 and S_2 are further from S' than S). The other exterior path (starting from S' and finishing in S'_2) is constructed in a similar way. As in the previous example, the introduced vertex is highlighted in grey.

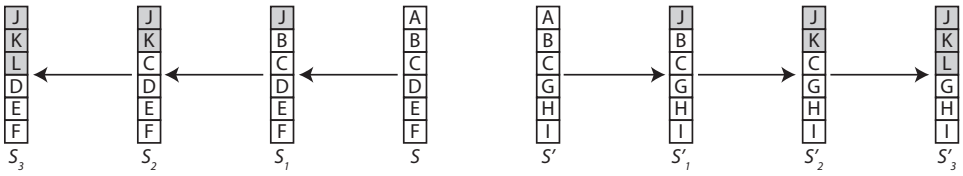


FIGURE 5. Example of two exterior paths, one beyond S and the other beyond S'.

4. Computational results

In this section, we report on the computational experiments performed to test the efficiency and effectiveness of the proposed strategies. All algorithms were implemented in Java 7 and the experiments were conducted on an Intel Core i7 2600 CPU (3.4 GHz) with 4GB of RAM. We considered the MDPLIB benchmark, which consists of three sets of instances previously used in other variants of this problem. The instances were introduced in the context of the maximum diversity problem by Duarte and Martí (2007) and can be found in `http://www.optsicom.es/mdp`. The three sets of instances are:

- **SOM**: This data set consists of 70 inter-node distance matrices of sizes ranging from $n = 25$ and $m = 2$ to $n = 500$ and $m = 200$ and were collected by Duarte and Martí (2007). They were created with a generator developed by Silva et al. (2004) and have been used in most of the previous papers dealing with the maximum diversity problem (see for example Aringhieri et al. (2008)).
- **GKD**: This data set consists of 145 inter-node distance matrices for which distance values were calculated as the Euclidean distance between pairs of randomly generated points with coordinates in the $[0, 10] \times [0, 10]$ square. The sizes of these instances range from $n = 10$ and $m = 2$ to $n = 500$ and $m = 50$. These instances were introduced in Glover et al. (1998) and generated in Duarte and Martí (2007) and Martí et al. (2010).
- **MDG**: This data set consists of 100 inter-node distance matrices with real numbers randomly selected between 0 and 10 from a uniform distribution and size varying from $n = 500$ and $m = 50$ to $n = 3000$ and $m = 600$. These

instances are extensively described in Duarte and Martí (2007), Palubeckis (2007), and Martí et al. (2013).

The experiment has two parts. In the first part, we adjust the parameters of the methods and select the best variants of the proposed algorithms on a subset of 25 representative instances from the MDPLIB. The second part is devoted to a comparison of our the best proposal with the current state-of-the-art for this problem, including the solution of the mixed linear 0-1 formulation of Prokopyev et al. (2009) with the commercial MIP solver CPLEX 12.5.1. To avoid large computing times, all the algorithms are executed for a maximum CPU time of n seconds, where $n = |V|$.

4.1. **Algorithm configuration.** The first experiment compares the two constructive methods described in Section 2.1. For GRASP, both the quality and variability of the constructed solutions are important for the success of local search. Ideally, we want to construct good solutions that are scattered about the solution space. For the Min-Diff problem we compute variability as the average number of steps in the neighborhood space among the constructed solutions. In other words, the variability between two solutions S and S' is defined as the cardinality of the set difference of the two solutions. Then, the variability of the set C of constructed solutions is defined as

$$\mathit{variability}(C) = \frac{\sum_{S \in C} \sum_{S' \in C} |S \setminus S'|}{|C|}.$$

This experiment compares the quality and variability of the solutions produced by the constructive methods C1 and C2 by considering 100 independent constructions of each. The α parameter value is set to $\mathit{random}, 0.25, 0.50, 0.75$, where *random* indicates that the method randomly selects an α value in the range $[0, 1]$ for each construction. Notice that the greater the value of α, the greater will be the expected variability of the constructed solutions. Figure 6 shows the result of this comparison where the values of quality and variability have been normalized to fall between 0 and 1. This figure shows that C2(0.50) attains the largest quality but with relatively low variability. On the other hand, one of the most randomized methods, C1(0.75), produces poor-quality solutions, but having the largest variability among all methods. Finally, C2(0.25) shows a balance between quality and variability. Specifically, it presents slightly worse quality than the best method, but considerably larger variability.

In the experiments that follow, we limit ourselves to the constructive procedures identified above as having produced the best quality, C2(0.50), the best variability, C1(0.75), and a good tradeoff between quality and variability, C2(0.25).

We next study the efficiency of the three local search methods proposed in Section 2.2 when coupled with C2(0.50), C1(0.75), and C2(0.25), the three constructive procedure chosen above. Recall that these local search procedures are: LS1 – best improvement strategy; LS2 – first improvement with random selection; and LS3 – first improvement with ordered selection. We embed them in a GRASP algorithm, constructing and improving 100 solutions. We report, for each variant, the average objective function value, Avg.; the CPU time in seconds, Time (s); the average deviation with respect to the best result found in the experiment, Dev (%); and the number of times that the method finds the best result in the experiment, #Best. For the sake of clarity, we highlight in bold font the best combination of methods.

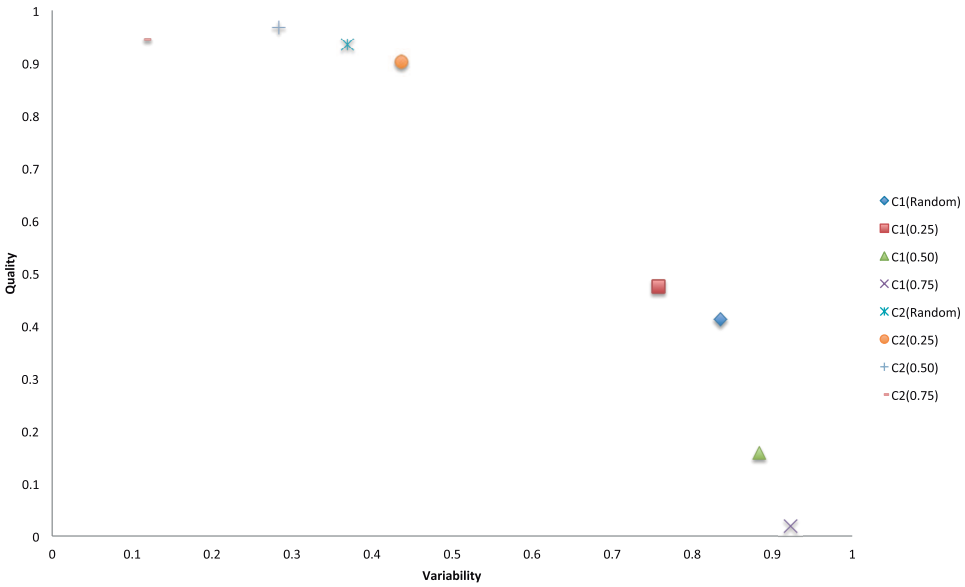


FIGURE 6. Comparison of quality and variability of the constructive methods

Table 1 shows the results obtained by the different combinations of constructive and local search procedures.

TABLE 1. Three local search methods coupled with three constructive procedures.

		Avg.	Time (s)	Dev. (%)	#Best
C1(0.75)	LS1	163.51	77.09	17.52	6
	LS2	162.65	16.95	12.18	6
	LS3	166.87	88.30	16.06	2
C2(0.25)	LS1	184.11	30.23	18.65	3
	LS2	180.16	13.08	14.72	3
	LS3	181.53	63.57	13.38	4
C2(0.50)	LS1	172.21	30.24	14.74	3
	LS2	**171.49**	**14.08**	**11.10**	**7**
	LS3	173.23	60.59	12.28	4

In this experiment C2(0.50) coupled with LS2 emerges as the best GRASP variant. It obtains the smallest deviation (11.10%) and the largest number of best solutions (7 out of 25). It is important to remark that this method ranks second (very close to the fastest algorithm) when comparing CPU times of the nine variants tested. This experiment confirms that the compromise between quality and variability is crucial in a GRASP design. We therefore select C2(0.50) with LS2 as the best variant and use it in the remaining experiments.

Next, we analyze the effect of replacing the local search component of a GRASP by a VNS (see Section 2.3). Specifically, we compare the best algorithm identified above with nine variants of GRASP with VNS local search. These VNS

procedures differ in the k_{step} and k_{max} parameters. We tested the values $k_{max} = \{0.1n, 0.2n, 0.3n\}$ and $k_{step} = \{0.01n, 0.025n, 0.05n\}$, where $n = |V|$, and denote the method by VNS(k_{step}, k_{max}). Table 2 shows that including a VNS in a GRASP procedure considerably improves the quality of the results. As a comparison of Tables 1 and 2 shows, the average objective function for constructive with local search varies from 162.65 to 184.11, while that average for constructive with VNS in place of local search varies from 136.56 to 155.11. However, as expected, the running time of the VNS grows with large values of k_{max} and/or with small values of k_{step}. To find a compromise between CPU time and quality, we select VNS(0.01, 0.1) for the next experiments, since it presents the best results in terms of average objective function (136.56) and number of best solutions found (9 out of 25). Additionally, it ranks third (out of 9 methods) when considering the average deviation (8.80%) but taking about half the CPU time (156.64 seconds) of VNS(0.01, 0.2) and VNS(0.01, 0.3) whose computing times are 226.90 and 300.81 seconds, respectively.

TABLE 2. Influence of the k_{step} and k_{max} parameters in the VNS algorithm.

		Avg.	Time (s)	Dev. (%)	#Best
	0.01	**136.56**	**156.64**	**8.80**	**9**
0.1	0.025	149.09	93.22	15.82	5
	0.05	155.11	59.16	17.68	6
	0.01	143.20	226.90	8.20	5
0.2	0.025	142.02	141.40	10.16	7
	0.05	150.79	92.54	17.38	3
	0.01	141.54	300.81	7.01	8
0.3	0.025	143.74	172.98	12.38	4
	0.05	151.47	122.31	13.72	6

To single out the contribution of the VNS we conducted an additional experiment. In particular, we compared the GRASP method in which construction is C2(0.50) and improvement is LS2 with the GRASP method in which LS2 is replaced by VNS, allowing both algorithms to run for 150 seconds, on average, which is the average running time taken by the best variant with VNS. The algorithm with VNS consistently produced better outcomes. Specifically, it obtained a lower average objective function value (136.48 versus 156.41), a lower average deviation (0.56 % versus 6.89 %) and a larger number of best solutions found (20 and 9).

We next compared the four path relinking algorithms described in Section 3 by incorporating them into the GRASP with VNS local search. Table 3 compares the methods with interior path relinking with greedy (IPR_g) and random (IPR_r) construction of the path, as well as the exterior path relinking with the same two strategies of exploring the path (EPR_g, EPR_r). Observing these results, we conclude that the greedy construction of the path consistently produces better outcomes than the random strategy. In fact, the greedy exploration of the path barely affects the computing time. This is true mainly because we use the move strategy described in Section 2.2. Another relevant observation is that the two exterior versions of PR clearly outperform the interior variants. With this, the GRASP with VNS using the EPR_g strategy emerges as the best algorithm for all statistics. We

believe that this result could be an important lesson for future implementations of path relinking.

TABLE 3. Comparison among the proposed path relinking algorithms.

	Avg.	Time (s)	Dev (%)	#Best
IPR_g	136.81	151.22	4.32	13
IPR_r	137.01	150.81	4.60	14
EPR_g	**136.23**	**156.05**	**0.80**	**20**
EPR_r	137.09	162.73	3.28	14

We conducted an additional experiment to single out the actual contribution of PR in final design of the algorithm. In particular we compare EPR_g with the best GRASP algorithm executed for the same computing time (about 150 seconds on average). EPR_g obtains a lower average deviation (0.71 % versus 5.69 %) and a larger number of best solutions found (23 versus 14).

In the remainder of the paper we refer to this GRASP with VNS and Greedy Exterior Path Relinking algorithm simply as EPR.

4.2. **Algorithm evaluation.** In Section 4.1, we identified EPR as being our best proposed procedure. We next compare it with the current state-of-the-art methods for the Min-Diff problem. These methods are a GRASP proposed by Prokopyev et al. (2009) and the commercial MIP solver CPLEX 12.5.1 on their exact formulation.

Our evaluation consists of two experiments. In the first, we compare EPR with two variants of the GRASP of Prokopyev et al. (2009), one denoted as GRASP1 which runs for 500 iterations and the other, GRASP2, which runs for 1000 iterations. In the second experiment, we compare EPR with CPLEX on all instances that fit in memory.

For the first experiment, we implemented all of the algorithms in Java with the objective of making a fair comparison with EPR. The experiments were run on the same computer. Table 4 summarizes the results of this experiment, where we consider the three sets of instances (GKD, MDG, and SOM) and the three algorithms (EPR, GRASP1, and GRASP2). The table is organized in three groups of rows (one for each type of instance). For each pair of instance type and algorithm, the table lists average solution value over all instances in the set, the average CPU time in seconds, the average percent deviation from the best known solution, and the number of times that the methods matches the best known solution.

Each algorithm was run a single time on each instance. With respect to solution quality, EPR clearly outperforms both GRASP1 and GRASP2. It should be noted that the GRASP proposed by Prokopyev et al. (2009) was designed to work on a number of equitable dispersion problems and not specifically on the MinDiff problem as EPR is designed for.

EPR found the best known solution in 188 of 190 instances, while GRASP1 and GRASP2 did so for only 12 and 18 instances, respectively. The instances for which GRASP1 and GRASP2 found the best known solution are all in the class GKD, which has the smallest instances as well as Euclidean distances, making them easier to solve as we will see later in this section in the experiments with CPLEX. In addition to not finding many best known solutions, both GRASP1 and GRASP2

TABLE 4. EPR compared with the GRASP algorithms of Prokopyev et al. (2009).

Instance set		EPR	GRASP1	GRASP2
GKD	Avg.	52.57	107.82	90.19
	Time (s)	56.99	76.03	152.07
	Dev (%)	0.00	74.19	69.69
	#Best	68	12	18
MDG	Avg.	3567.63	5981.61	5981.80
	Time (s)	1472.35	1421.10	2793.23
	Dev (%)	0.00	81.51	79.57
	#Best	100	0	0
SOM	Avg.	23.35	37.90	37.25
	Time (s)	173.41	124.40	198.82
	Dev (%)	0.00	61.54	58.18
	#Best	20	0	0
ALL	Avg.	1899.53	3200.00	3189.18
	Time (s)	814.17	789.05	1547.07
	Dev (%)	0.00	76.71	73.68
	#Best	188	12	18

found solutions that had a high percent deviation from the best known solutions, varying, on average, from 58% for GRASP2 on SOM to 81% for GRASP1 on MDG. As expected, running times for EPR were comparable to those of GRASP1, which, also as expected, were about one half of those of GRASP2.

We applied the Friedman test to the raw data obtained in the previous experiment. This test ranks each method for each instance in the data set. That is, for each instance, the method that performs the best is assigned the number 1, followed by the second best (assigned number 2), and finally the worst method receives the number 3. Then, an average ranking is calculated for each method. A small p-value associated with this test indicates that the averages are indeed significantly different. We obtained a p-value of 0.00 indicating significant difference among the methods. Additionally, the test provided the ranking in which the best method is EPR with an average ranking of 1.10, followed by GRASP2 (average ranking of 2.31), followed by GRASP1 (average ranking of 2.60).

Finally, we compare EPR with GRASP2 by considering two well-known non-parametric tests for pairwise comparisons: the Wilcoxon test and the Sign test. The former answers the question: Do the two samples (in our case, solutions obtained with EPR and GRASP2) represent two different populations? The resulting p-value of 0.00 indicates that the values compared come from different algorithms

and there are significant differences between both methods. On the other hand, the Sign test computes the number of instances on which an algorithm supersedes another. The resulting p-value of 0.00 again indicates that there are significant differences between EPR and GRASP2, confirming the superiority of the method proposed in this paper.

TABLE 5. Comparison of EPR and CPLEX (limited to 1800 seconds)

	EPR		CPLEX			
Instance	MinDiff	Time (s)	UB	LB	Time (s)	Opt
GKD-b_10_n25_m7	**23.26523**	0.312	23.26523	23.26523	1.014	1
GKD-b_11_n50_m5	**1.9261**	0.187	1.9261	1.9261	8.814	1
GKD-b_12_n50_m5	2.12104	0.171	2.0513	2.0513	9.044	1
GKD-b_13_n50_m5	**2.36231**	0.187	2.36231	2.36231	6.668	1
GKD-b_14_n50_m5	**1.6632**	0.188	1.6632	1.6632	6.428	1
GKD-b_15_n50_m5	**2.85313**	0.187	2.85313	2.85313	8.3	1
GKD-b_16_n50_m15	**42.74578**	1.389	42.74578	42.74578	54.937	1
GKD-b_17_n50_m15	**48.10761**	1.608	48.10761	48.10761	36.853	1
GKD-b_18_n50_m15	**43.19609**	1.343	43.19609	43.19609	441.016	1
GKD-b_19_n50_m15	**46.41245**	1.358	46.41245	46.41245	347.622	1
GKD-b_1_n25_m2	**0**	0	0	0	0.012	1
GKD-b_20_n50_m15	**47.71511**	1.265	47.71511	47.71511	599.622	1
GKD-b_21_n100_m10	13.83202	1.171	12.30384	0	1330.461	0
GKD-b_24_n100_m10	8.64064	1.202	9.81926	0	1500.213	0
GKD-b_26_n100_m30	168.72959	9.439	176.86238	0	1104.597	0
GKD-b_27_n100_m30	127.09726	9.72	205.76481	0	1099.519	0
GKD-b_28_n100_m30	106.37919	10.422	148.59098	0	1212.293	0
GKD-b_29_n100_m30	137.45316	10.048	176.75614	0	1091.947	0
GKD-b_2_n25_m2	**0**	0	0	0	0.018	1
GKD-b_30_n100_m30	127.47974	9.283	134.10651	0	1140.244	0
GKD-b_3_n25_m2	**0**	0.017	0	0	0.016	1
GKD-b_4_n25_m2	**0**	0.016	0	0	0.016	1
GKD-b_5_n25_m2	**0**	0.015	0	0	0.016	1
GKD-b_6_n25_m7	**12.71796**	0.173	12.71796	12.71796	0.468	1
GKD-b_7_n25_m7	**14.09875**	0.156	14.09875	14.09875	1.732	1
GKD-b_8_n25_m7	**16.76119**	0.156	16.76119	16.76119	1.186	1
GKD-b_9_n25_m7	**17.06921**	0.172	17.06921	17.06921	0.173	1
SOM-b_2_n100_m20	6	3.042	6	0	663.937	0
SOM-b_3_n100_m30	10	5.796	12	0	99.342	0
SOM-b_4_n100_m40	13	8.715	14	0	121.602	0

We compared EPR with CPLEX 12.5.1 only on the 30 instances which fit in memory for CPLEX. Most of these instances were from the GKD set. Three were from SOM and none were from MDG (the smallest instance in MDG has 500 vertices). Running times for CPLEX were limited to 1800 seconds. EPR again did 100 GRASP iterations, followed by exterior path relinking between all pairs of the ten elite set solutions. Table 5 summarizes these runs. For each instance, the table lists the solution values and CPU times in seconds for EPR, as well as the upper and lower bounds found by CPLEX and the time taken by CPLEX. The last column in the table indicates whether CPLEX was able to prove optimality. Though CPLEX was limited to 1800 seconds, it often terminated before that, even when it could not prove optimality. This occurred because its search tree could no longer fit in

memory. CPLEX was able to prove optimality in 20 of the 30 instances. In 19 of those 20 instances, EPR was able to match the value of the optimal solution in a single run. In the remaining ten instances, EPR was able to improve the upper bound found by CPLEX in eight of them, match it in one, and do worse in only one. Running times for EPR were comparable to those of CPLEX on the smaller instances and, as expected, were orders of magnitude smaller than those of CPLEX on the larger instances.

5. Conclusions

This paper proposed several new hybrid heuristics for the differential dispersion problem. The heuristics used components of GRASP, variable neighborhood search (VNS), and path relinking. To find a good configuration for our best heuristic, we considered eight constructive procedures, four local search procedures, including one based on VNS, and four path relinking strategies. The best configuration consisted of a GRASP with sampled greedy construction and VNS for local search. As opposed to the standard way of applying VNS where the starting solution is random, the sampled greedy constructed solution is used. During the search, and elite set of the best solutions found (with no repetition allowed) is built and maintained. After a fixed number of GRASP iterations, exterior path relinking is applied between all pairs of elite set solutions and the best solution found is returned.

Exterior path relinking, or *path separation*, introduced in Glover (2014) and first used here, is a variant of the more common interior path relinking. In interior path relinking, paths in the neighborhood solution space connecting good solutions are explored from between the solutions in the search for improvements. Exterior path relinking, as opposed to exploring paths between pairs of solutions, explores paths beyond those solutions. This is accomplished by considering an initiating solution and a guiding solution and introducing in the initiating solution attributes not present in the guiding solution. To complete the process, the roles of initiating and guiding solutions are exchanged.

Extensive computational experiments on 190 instances from the literature demonstrated the competitiveness of this algorithm. Not only was it able to outperform the GRASP heuristic of Prokopyev et al. (2009) and find optimal solutions to all but one of the instances that CPLEX is able to solve, it improved the CPLEX upper bound on all but one of the instances that CPLEX failed to solve.

For future research, we note the possibility of applying a form of multiple neighborhood search different from VNS by reference to the strategic oscillation (oscillating assignment) framework as implemented in Glover et al. (1984) and elaborated in Glover and Laguna (1997) ch. 9. We also observe the relevance of additional variants of exterior path relinking suggested in Glover (2014). These variants open the door to a wide variety of possibilities that invite closer examination and that may give an interesting basis for future research.

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