

Ejection chain and filter-and-fan methods in combinatorial optimization

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Abstract The design of effective neighborhood structures is fundamentally important for creating better local search and metaheuristic algorithms for combinatorial optimization. Significant efforts have been made to develop larger and more powerful neighborhoods that are able to explore the solution space more effectively while keeping computation complexity within acceptable levels. The most important advances in this domain derive from dynamic and adaptive neighborhood constructions originating in ejection chain methods and a special form of a candidate list design that constitutes the core of the filter-and-fan method. The objective of this paper is to lay out the general framework of the ejection chain and filter-and-fan methods and present applications to a number of important combinatorial optimization problems. The features of the methods that make them effective in these applications are highlighted to provide insights into solving challenging problems in other settings.

Keywords Combinatorial optimization · Metaheuristics · Tabu search · Local search · Neighborhood structures · Ejection chains · Filter-and-fan

1 Introduction

The metaheuristic area has been the focus of extensive research in the last several years, resulting in methods for solving optimization problems that have had a wide range of successful applications in business, engineering and science. Some of the most significant advances

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have occurred in the design of sophisticated compound neighborhoods coupled with candidate list strategies. The goal of these approaches is to explore the solution space effectively with a modest investment of computational effort.

The definition of an efficient neighborhood structure is important for the performance of any algorithm that iteratively explores the solution space of complex problems that typically arise in practice. Recent studies have shown that compound neighborhood structures, based on mechanisms for combining moves, have advantages over simple neighborhoods where a single move is used for the transition from one solution to another.

Important advances have been provided by ejection chain methods (Glover 1991, 1992) and a general class of multi-stream neighborhood search constructions, notably represented by the filter-and-fan method (Glover 1998; Rego and Glover 2002). An integral part of exploiting such methods stems from joining them with candidate list strategies to isolate restricted yet effective subsets of moves for consideration at each iteration. Designed properly, such strategies reinforce the intensification and diversification themes of tabu search, and provide fertile ground for the application of learning procedures.

In contrast with other more traditional types of neighborhood constructions, ejection chains and filter-and-fan methods are prototypical examples of *dynamic* and *adaptive* search approaches. Characteristically, these methods generate compound neighborhood structures, which encompass successions of interdependent (component) moves, rather than simple moves or sequences of independent moves. These methods are dynamic because the number of component moves used to compose a compound move is not determined in advance, but rather depends on the depth (or level) of the neighborhood where the best trial solution is found, which usually varies from one iteration to another. They are adaptive because the type of the neighborhood and the move itself are chosen according to the current state of the search.

This paper is an updated version of work presented in Glover and Rego (2006). We begin by presenting in Sects. 2 and 3 the fundamental principles underlying filter-and-fan and ejection chains methods, respectively. In Sects. 4 and 5, we review a number of prominent filter-and-fan and ejection chain algorithms to illustrate the application of these methods to different classes of problems and to identify the features responsible for their performance. Practical aspects of these methods are highlighted by examining the applications shown in Table 1.

These applications were selected to embrace a representative variety of models for each method and to illustrate how these methods apply to problems of different natures and complexities. Our examination constitutes a focused survey of models and applications we have encountered through direct experience, though we undertake to point out related work that provides important contributions to the areas examined.

Overall, the filter and fan methods have been notable for providing robust methods that produce solutions that match or come very close to matching those produced by the best available methods for the problem classes to which they have been applied, while requiring solution times that are significantly—in some cases dramatically—reduced by comparison

Table 1 Featured applications of filter-and-fan and ejection chain and methods

Filter and fan	Ejection chains
Facility location	Traveling salesman
Protein folding	Vehicle routing
Job shop scheduling	Crew scheduling
Capacitated minimum spanning tree	Quadratic assignment

to competing methods. (An exception occurs in the case of the job shop scheduling problem, where two tabu search implementations are more effective than all other procedures, one of them remarkably so, but the F&F method proves superior to all methods except these.) The ejection chain methods stand out in their respective applications even more prominently, often performing appreciably better than the leading challengers.

Readers who are primarily interested in outcomes can proceed immediately to Sect. 4 and (especially) Sect. 5, where applications and test results for the methods are described. Sections 2 and 3, immediately following, undertake to give a compressed description of the underlying solution methodologies, and to provide references to sources where more complete descriptions can be found.

2 Filter and fan

The filter-and-fan (F&F) method was initially proposed in Glover (1998) as a method for refining solutions obtained by scatter search, and was further extended in Rego and Glover (2002). In the latter, the method is proposed as a means for creating combined neighborhood search strategies that are particularly efficient and robust, and that can be used as complements to ejection chain approaches (whose designs are often more subtle and elaborate). Conceptually, the F&F method integrates the *filtration* and the *sequential fan* candidate list strategies used in tabu search (Glover and Laguna 1997), and can be viewed as a restricted form of tabu search that generates multiple paths in a controlled variation of a breadth-first search strategy. From a neighborhood search perspective, the method generates compound moves as a sequence of more elementary *component moves* (or submoves).

Graphically, the F&F model can be illustrated by means of a neighborhood tree where branches represent submoves and nodes identify solutions produced by these moves. An exception is made for the root node, which represents the starting solution to which compound moves are to be applied. The maximum number of levels L permitted in a single sequence of moves defines the depth of the tree. The neighborhood tree is explored breadth first, level by level. Each level is governed by the *filter candidate list* strategy that selects a subset of moves induced by the *fan candidate list* strategy. The process of selecting moves has to obey a set of *legitimacy conditions* defining associated *legitimacy restrictions* specific to the type of move utilized. The method incorporates two fundamental components: a *local search* to identify a local optimum and a *filter and fan search* to explore larger neighborhoods in order to overcome local optimality. Any time a new local optimum is found in one search strategy the method switches to the other strategy and keeps alternating this way until the filter and fan search fails to improve the current best solution.

2.1 The filter and fan search

The general F&F search procedure can be sketched as follows. Once a locally optimal solution X_o is found (in the local search phase) the best η_1 currently available moves (among the moves evaluated to establish local optimality) are used to create the level 1 of the F&F neighborhood tree. As a basis for creating the next levels, for a given level indexed by k , η_1 denotes the number of solutions that are chosen from all solutions available at level k , as a foundation for generating solutions at level $k + 1$. (For $k = 1$, there are just η_1 solutions available, so all are chosen.) For each of these η_1 solutions, denoted $X_i(k)$ ($i = 1, \dots, \eta_1$), apply η_2 moves to generate η_2 descendant solutions, thereby generating a total of $\eta = \eta_1 \cdot \eta_2$ trial solutions for level $k + 1$. At this stage, η_1 of the resulting η solutions are chosen to launch

Step 0. Generate a candidate list of component moves

- (a) Change X by performing 1-moves using a local search until a local optimum X^* is found. Let M be the set of all moves evaluated in the last iteration of the local search procedure.
- (b) Create a candidate list $M(0)$ with the η_0 highest evaluation moves of M .
- (c) Set $X^*=X$, and let X be the new starting solution, i.e. the root node of the search tree. Apply the best η_1 moves in $M(0)$ to X to create the first level of the F&F tree with solutions $X_i(1)(i=1, \dots, \eta_1)$. Set $k=1$.

Step 1. Generate the filter and fan tree

- (a) Identify the best η_2 legitimate moves derived from $M(0)$ for each solution $X_i(k)(i=1, \dots, \eta_1)$ by computing the value of the corresponding trial solution.
- (b) If the best evaluation found is better than the one of X^* , perform the associated move from $X_i(k)$ to X , the new and improved current solution. Set $X^*=X$ and go to Step 0.
- (c) Otherwise, select the best η_1 legitimate trial moves to become the members of $M(k)$.
- (d) Apply the $M(k)$ moves to the corresponding solutions $X_i(k)$ to create $X_i(k+1)$.
- (e) If $k=L$ stop. Otherwise set $k=k+1$ and repeat Step 1.

Fig. 1 The general filter-and-fan procedure

the process for the next level. The values η_1 and η_2 are input parameters, e.g. $\eta_1 = 2\eta_2$. If an improved solution (better than the local optimum X_o) is found among the trial solutions, then the method stops branching and switches back to the local search phase, taking this newly improved solution as a starting point. Otherwise, another selection takes place over the set of moves available.

The process of selecting η_2 moves has to obey a set of legitimacy restrictions that assure compatibility of the component moves used for the construction of a valid compound move. The *fan candidate list strategy* is embedded in the generation of the η trial solutions, whereas the selection of the η_1 solutions from this collection constitutes the *filter candidate list strategy*.

The basic skeleton of a general F&F procedure is as in Fig. 1. X^* denotes the best solution found so far. Let $M(k)$ be the candidate list of moves identified at level k of the F&F tree. F&F input parameters are denoted by η_0, η_1, η_2 and L represents an upper limit for the maximum number of levels of the F&F tree. The method begins by building an initial solution X .

In more general versions of the approach, *tree width* and *branch width* can vary adaptively throughout the search while the values for η_1 and η_2 are changed from level to level. In additional variants of the procedure, as when making use of constructive or destructive neighborhoods, a solution can refer to a partial solution, having some components undetermined. Local optimality is then defined relative to the determined components, or by employing a default trial completion that fills in the values of the undetermined components.

More advanced versions allow for the combination of different types of neighborhood structures and the use of adaptive memory programming as introduced in tabu search.

2.2 Refinements for higher levels of adaptive memory constructions

The F&F method can be interpreted as performing multiple threads of tabu searches from the root node of the F&F tree using a limited short-term memory component derived from the legitimacy restrictions. From this perspective a straightforward enhancement results by

creating a more general algorithm managed by two basic types of short-term memory components: e.g. a *branch-memory* that is local to each branch of the F&F tree and a *tree-memory* that is global to the F&F tree. A limited form of branch-memory is implicitly defined in the legitimacy restrictions of the tree search process. However, the inclusion of more explicit forms of memory allows different levels of flexibility by using either one of the two indicated types of memory or both memories combined. In that sense a branch-memory serves to forbid move reversals while tree-memory produces greater diversification of the search among the different branches of the tree.

Higher levels of intensification and diversification can be achieved by incorporating more advanced memory structures as prescribed in tabu search. Effective integration of memories organized at different layers provides a useful means for creating the $M(k)$ candidate lists. It also provides a vehicle for an iterative application of the F&F procedure which is executed until a given stopping criterion is met, as in general tabu search implementations. The underlying look-ahead process may also be augmented by the use of ejection chain processes (performed from nodes at the current level) as a means to determine promising component moves and dynamically update the candidate list. As in scatter search approaches, high evaluation trial solutions found throughout the ejection chain can be re-corded for further consideration. All these modifications make recourse to associated elements of tabu search and can directly turn a F&F approach into a higher level tabu search procedure.

3 Ejection chains

Ejection Chains are variable depth methods that generate a sequence of interrelated simple (component) moves to create a more complex compound move. There are several types of ejection chains, some structured to induce successive changes in problem variables and others structured to induce changes in particular types of model components (such as nodes and edges of a graph). For the original proposals of the ejection chain framework and foundations we refer the reader to Glover (1991, 1992).

Generally speaking, an ejection chain of L levels consists of a succession of operations performed on a given set of elements, where the k th operation changes the state of one or more elements which are said to be *ejected* in the $(k + 1)$ th operation. This ejection changes the state of other elements, leading in turn to further ejections, until no more operations can be made (according to pre-defined conditions). State-change steps and ejection steps typically alternate, and the options for each depend on the cumulative effect of previous steps (usually, but not necessarily, being influenced by the step immediately preceding). The conditions coordinating the ejection chain process are called *legitimacy conditions*, which are guaranteed by associated *legitimacy restrictions*. The connection between these elements will be clarified subsequently.

In the ejection chain terminology, the order in which an element appears in the chain determines its *level*. The total number of levels L is the *depth* of the ejection chain. The particular level chosen for executing a move by a local search method usually varies from one iteration to the next. The total number of levels L can likewise vary, and hence ejection chains fall within the class of *variable depth methods*. In an ejection chain framework, the solution obtained at each level k of the chain may not represent a feasible solution but may be transformed into a feasible solution by using a complementary operation called a *trial move*. The objective is to create mechanisms, namely neighborhood structures, allowing one solution to be successfully transformed into another.

More formally, let S_i be the current solution at iteration i of the local search method, and let e_k, t_k be the *ejection move* and the *trial move*, respectively, at a level k of the chain.

A neighborhood search ejection chain process consists of generating a sequence of moves $e_1, t_1, \dots, e_k, t_k, \dots, e_L, t_L$ on S_i such that the transition from solution S_i to S_{i+1} is given by performing a *compound move* $e_1, e_2, \dots, e_{k^*}, t_{k^*}$, where k^* represents the level associated with the highest quality trial solution visited during the ejection chain construction. (There is no need to save trial solutions at other levels.) In the ejection chain context we use the terms *compound move* and *transition move* interchangeably, to specify the move leading from one solution to another in an iteration of the local search procedure.

The effectiveness of such a procedure depends on the criterion for selecting component moves. More specifically, neighboring solutions obtained by an ejection chain process are created by a succession of embedded neighborhoods that lead to intermediate trial solutions at each level of the chain. However, the evaluation of ejection moves can be made independently from the evaluation of the trial moves, in which case possible trial moves are only evaluated after performing the ejection move at the same level of the chain. In this variant of the approach, the evaluation of an ejection move e_k only depends on the cumulative effect of the previous ejection moves, e_1, \dots, e_{k-1} , and is kept separate from the evaluations of trial solutions encountered along the way. The trial moves are therefore restricted to the function of finding the best trial solution that can be obtained after performing the associated ejection move.

In general, an ejection chain of L levels can be recursively evaluated by computing the ejection values for these levels and summing them to give the trial value for each level. Let $N = \{1, \dots, n\}$ represent the set of problem elements and denote a legitimate neighborhood for an element $p \in N$ by $LN(p)$, thereby identifying a subset of elements of N that do not violate the legitimacy restrictions. Also, let $\varphi(p_k, p)$ and $\delta(p_k, q)$ be respectively the values of an ejection move and trial move at a level k of the ejection chain. For the sake of simplification, we assume that the *min* function over each of the ejection and trial move evaluation functions identifies the elements p^* and q^* associated with the best ejection and best trial values found, respectively. A general ejection chain procedure for a minimization objective can be sketched as in Fig. 2.

Our preceding description of ejection chain processes simply constitutes a taxonomic device for grouping methods that share certain useful features. The value of the taxonomy, however, is evidenced by the role it has played in methods for discrete optimization problems that have proven effective across a broad range of applications. As will be seen in the applications subsequently discussed, the foregoing ejection chain framework embraces methods exhibiting a variety of compound neighborhood structures and offering advantageous properties for combining moves.

4 Filter-and-fan applications

A filter and fan algorithm requires the definition of component moves used to generate trial solutions throughout the search process. Component moves are characteristically simple moves serving as building blocks for the construction of an extended filter and fan neighborhood. As in customary local search methods, different applications require appropriate neighborhood structures to explore the solution space. The following sections illustrate how filter-and-fan has been successfully used to create effective neighborhoods for a number of applications.

4.1 Facility location

The uncapacitated facility location problem arises in bank account location planning, location of collection centers or lock-boxes, clustering analysis, location of off-shore drilling

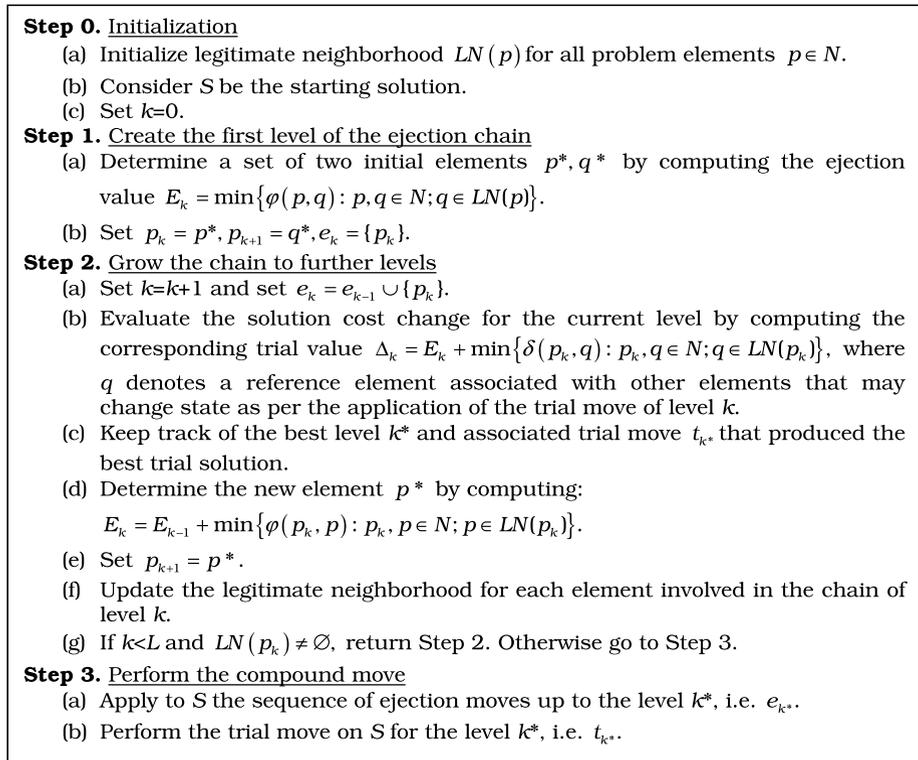


Fig. 2 An iteration of a general ejection chain procedure

platforms, machine scheduling and information retrieval, portfolio management, and design of communication networks. For a survey see Cornuéjols et al. (1990) and Gao and Robinson (1994). The basic form of the problem can be defined as follows. Given a set $S = \{1, \dots, s\}$ of warehouses or facility locations and a set $D = \{1, \dots, d\}$ of customers to be served. With each customer $j \in D$ is associated a demand b_j and c_{ij} is the transportation cost of completely serving a customer j by facility $i \in S$. Also, there is a fixed cost F_i if facility i is built (or opened). The objective is to find a set $W^* \subseteq S$ of opened facilities that minimizes the total cost. Due to the absent of capacity constraints on the facilities, customer demands may be normalized to $b_j = 1$ and for any set $W \subseteq S$ of facilities there is at least one optimal assignment where all customers are served by the nearest open facility. Consequently, a UFLP solution can be fully defined by the set of open facilities. Therefore, especially in local search, it is natural to use a vector representation $Y = (y_1, \dots, y_s)$ where $y_i = 1$ if the facility i is open and 0 otherwise.

Local search algorithms for the facility location problem typically use flip-based neighborhoods, namely, the *switch*-neighborhood that switches the status of one facility from open to closed or vice versa by flipping a single variable at a time and the *swap*-neighborhood that simultaneously closes one facility and opens another.

Greistorfer and Rego (2006) have successfully enhanced the performance of these neighborhoods by generating sequences of flip moves within a filter-and-fan approach. Computational tests, whose outcomes are described below, disclose that this method provides a significant advance for solving facility location problems effectively. The method proceeds

by performing moves that flip the value of one variable at each node of the F&F tree. A swap move implicitly results whenever in two successive nodes of a given branch of the tree, one variable flips from 0 to 1 and another variable flips from 1 to 0. The legitimacy conditions on the selection of η_2 moves are defined by tabu restrictions preventing reverse flips (that would lead to duplicated solutions) and a feasibility condition that keeps the method from closing the only open facility in the current solution. Two variants of the algorithm are developed to achieve different levels of sophistication.

The general F&F algorithm undertakes two fundamental steps. The first step is a classical local search procedure that starts with all facilities open, then improves that solution by closing the facility that locally minimizes the objective function value and the process is repeated until no improvement is possible by closing a new facility. Let M be the set of all moves evaluated in the last iteration of this descent process, then the method keeps the η_0 best moves of M to create the initial candidate list $M(0)$ for the F&F tree used in the next step.

Two variants of the algorithm are implemented to achieve different levels of sophistication and performance. In a more rudimentary design, memory structures are limited to the tabu restrictions implicitly defined in the legitimacy conditions specified above. In a more advanced design, the method is enhanced by exploring multilevel candidate lists, which extends the legitimacy conditions with a validity check, with respect to the current depth of the search, that has its counterpart in the notion of admissibility in tabu search memories. Accordingly, the evaluation of a move may not exclusively rely on the net change in the objective function value created by the move but may include a bias factor introduced by memory considerations used to guide the search at different layers. In the present algorithm, layers are associated with two consecutive levels of the F&F tree that are subsequently and alternatively checked with respect to the solution cost changes yielded by the corresponding moves. As a result of these effects, improving moves are always kept in the tree; however if in the previous level a non-improving move was performed and if none of the moves available improve the solution at the current level, a reverse flip move that transforms the current solution back to the one in the previous level is allowed, denoting a relaxation by cost of one of the legitimacy constraints.

It is shown that the simple version is competitive with state-of-the-art algorithms, but fails to find 2 optimal solutions out of 45 classical benchmark problems. Overall this algorithm produces solutions that are on average exceedingly close to optimal, while consuming a very small amount of computation time—yielding solutions that are on average 0.04% above optimality in an average computation time of 2.78 seconds.

The more advanced version of the method was implemented with the goal of producing still better outcomes and specifically of tackling the new 60 instances currently known as the hardest UFLP data sets in literature. This version succeeded in finding all best know solutions for the previous 45 instances and achieved an average deviation of only 0.03% above the optimal solutions for the hardest 60 instances. The total time required to solve these hard problems averaged less than 3.5 seconds (on a Pentium IV, 1.7 GHz CPU desktop computer).

The exceedingly high quality of these results discloses that the filter-and-fan approach provides a very effective framework to explore the solution space in facility location problems and suggests its use in other more complex variants of these problems.

4.2 Protein folding

A protein's function is closely related to its 3D structure, and therefore to determine how a protein functions one must know its 3D conformation. The Protein Folding Problem (PFP)

is the problem of predicting the three-dimensional (3D) structure of a protein given only the protein's sequence of amino acids. This is a fundamental yet open problem in the fields of biological chemistry and protein science, and has recently attracted attention in bioinformatics and computational biology. The PFP is central in a number of practical applications including the designing of new proteins having desirable functions in pharmaceutical, food, and agriculture industry (Lengauer 1993). Informative overviews of the PFP and its applications can be found in Richards (1991) and Chan and Dill (1993).

The PFP is a notoriously difficult combinatorial problem due to the combinatorial explosion of valid conformations as the number of amino acids in the chain increases. Due to the complex nature of the PFP, the so-called HP lattice model proposed by Dill (1985) constitutes a well established simplification for algorithm assessment.

Rego et al. (2009a) consider the two-dimensional (2D) version of the HP lattice model and propose a F&F algorithm for the solution of the associated PFP. A sequence of H and P amino acids is configured as a path on a two-dimensional (2D) lattice to define a valid conformation. The path designation implies that the conformation is both connected and self-avoiding, i.e., no amino acids can collide in the same cell of the lattice. (In graph theory terminology, such a path is called *node simple*.) The energy function is defined by the number of pairs of H nodes that are *adjacent* in the lattice and not *consecutive* in the chain. Each of these pairs, generally called an H-H contact, decreases the energy value by one unit. The objective is to find a conformation that minimizes the total energy of the given amino acid sequence, which therefore corresponds to maximizing the number of H-H contacts.

In this application, the F&F approach is used to seek an effective guidance strategy within a simpler neighborhood by extending the so-called *pull-move* neighborhood (Lesh et al. 2003). To elaborate the algorithm we first describe the associated *component moves* defined by the pull-move neighborhood structure.

A pull-move is initiated by moving one node of the current conformation to one of its empty diagonal adjacent positions in the square induced by the node and one of its adjacent neighbors in the sequence. Depending on the structure of the conformation the displacement of the initiating node may require other nodes to change their current positions in order to preserve connectivity. Nodes displaced by a pull move are only allowed to occupy vacant adjacent positions in the lattice. Consequently, the preservation of connectivity results in a self-avoiding path. Rego et al. make use of only three types of pull-moves designated by *filling*, *single-pull* and *multiple-pull*, according to the number of nodes that are pulled by the first displaced node. The *filling* move is the simplest pull-move, displacing a single node in the structure. A valid conformation is obtained by simply moving a node to its diagonal adjacent position. A *single-pull*, on the other hand, requires another node to change position after the initiating node takes a new position. The *multiple-pull* move extends the single-pull move to achieve connectivity in more complex structures that become disconnected upon performing the simpler move. Figure 3 shows an example of the filter and fan neighborhood for a 2D HP model with 20 amino acids, where $\eta_1 = \eta_2 = 2$ and $L = 3$. The negative numbers denote the energy value of the corresponding conformation.

A conformation of energy -6 (represented by the root node) denotes a local optimum determined by the local search phase. The first level of the filter and fan neighborhood is then generated by applying the $\eta_1 = 2$ best moves to the root conformation. The next level is created by applying the $\eta_2 = 2$ best pull-moves to each of the conformations in the current level, thus generating $\eta_1 \cdot \eta_2 = 4$ trial conformations from which a new set of $\eta_1 = 2$ best conformations is chosen to initiate the next level. If at one level more than η_1 solutions exist with the same objective value preference is given to solutions that derive from different parent conformations. In the figure, the η_2 different conformations derived

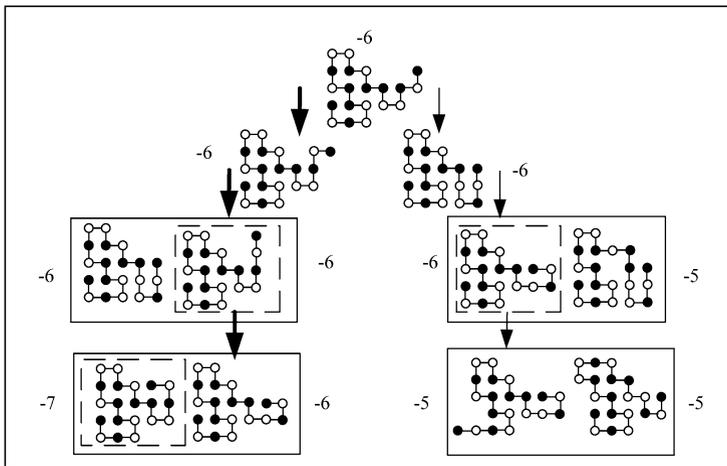


Fig. 3 Filter-and-fan neighborhood tree for the 2D HP model of the PFP

from the same parent conformation are contained within the rectangles delimited by solid lines whereas the η_1 best conformations selected at each level are contained within “interior rectangles” delimited by dotted lines. The method continues expanding the neighborhood until the improved conformation of energy -7 is found in level 3 of the filter and fan tree. The compound move leading to the improved conformation is then identified by the path indicated by the dark arrows. Note that to continue the tree search after obtaining the new local optimum, the method will restrict attention to solutions in the left-hand side branches as a basis for extending the tree.

Diversification strategies that utilize memory of elite solutions and their attributes (either in direct or statistical form) to drive the search into new regions plays a critical role in the leading metaheuristic algorithms for the PFP. Rego et al. (2009a) explore mechanisms for achieving an intelligent form of diversification within a filter-and-fan approach making use of a simple tabu search structure. The algorithm alternates between single-path and multiple-path tabu searches using component moves provided by the pull-move neighborhood, subject to short-term memory controls.

Computational results for a standard set of benchmark problems show that the F&F algorithm performs more robustly and efficiently than the current leading algorithms, requiring only a single solution trial to obtain best known solutions to 9 out of 11 problems. By contrast, the best of the alternative methods require a hundred or more trials in the typical case to obtain best solutions to these 9 problems. For one of the instances this algorithm required hundreds of runs and 78 hours of wall clock time to find the best solution, while the filter-and-fan algorithm finds this solution in approximately 12 seconds on an equivalent computer. On the remaining 2 problems, a single trial of the F&F method obtains a solution one unit away from the best known solution, again yielding a performance that is not matched by some of the best competitors that are allowed to run for a hundred or more trials.

The success of the algorithm in performing more efficiently and robustly than alternative state-of-the-art algorithms owes to two fundamental components: (i) the dynamic and adaptive feature of the search method in exploiting the neighborhood structure employed; and (ii) the interplay between the tabu search and the tree search phases, which creates a strategic oscillation between intensification and diversification. Further improvements are anticipated to result by incorporating longer-term tabu search memory components to achieve

higher levels of intensification, and by means of vocabulary building strategies that incorporate ejection chain methods and path-relinking.

4.3 Job shop scheduling

The Job Shop Scheduling Problem (JSSP) is a notoriously difficult problem in combinatorial optimization. The problem finds its application in manufacturing industries and has a pivotal role in many supply chains that integrate production planning and scheduling. In a supply chain environment, production planning and scheduling models are often incorporated into a unified framework, sharing information and interacting with one another in order to optimize the production of different products over multiple facilities. The output of the planning process serves as an input to the scheduling process, which is often analyzed as a job shop scheduling problem. Planning and scheduling models may also interact with other types of logistics models such as inventory models, facility location models and transportation models. For an extensive coverage of planning and scheduling models and applications in various supply chains settings, see Pinedo (2006).

The JSSP can be defined by a set of machines specialized to perform ordered operations unique for every job. No machine can perform more than one operation at a time, each operation has fixed time duration, and preemption is not allowed. The goal is to minimize the makespan, which is the duration of the longest job in the schedule.

Beam search is a classical tree search method typically used in the optimization of complex scheduling systems, including the JSSP (Sabuncuoglu and Bayiz 1999). However more advanced forms of tree search neighborhood approaches have been recently proposed that have proved more effective than beam search for solving scheduling problems.

In particular, Balas and Vazacopoulos (1998) consider a specialized neighborhood tree for the JSSP that leads to one of the most effective algorithms for this problem. Making use of this neighborhood, Rego and Duarte (2009) developed a filter-and-fan (F&F), which can also be viewed as a natural generalization of *beam search* and which includes the B&V neighborhood tree as a special case. The basic structure of the algorithm may be described as follows.

The most rudimentary version of the classical *shifting bottleneck procedure* (SBP) (Adams et al. 1988) is used as a constructive method to generate an initial feasible solution. At each step the machine with longest processing time (i.e. the bottleneck machine) among the ones that have not been scheduled is selected for scheduling and the method stops when all machines are scheduled. It is well-known that this procedure does not produce high quality solutions by itself, but provides a convenient means to rapidly generate initial feasible solutions for more advanced algorithms.

The F&F algorithm starts from the solution generated by the SBP and iteratively improves this solution by alternating between the local search and the tree search phases. The method considers two types of neighborhoods N_1 (Aarts et al. 1994) and N_2 (Nowichi and Smutnicki 1996) based on classical moves that swap two adjacent operations in the critical path (i.e. the longest path in the problem graph that represents the solution). Typically, N_1 swaps arcs that are internal to the blocks of operations in the same machine while N_2 exploits interactions between adjacent blocks by swapping arcs linking operations in different blocks. Depending on the search strategy both types of moves can be used for the local search as well as to define elementary moves in the F&F tree.

The search starts with the N_1 neighborhood. Any time a local optimum is found (in the local search phase) the best $M(0)$ moves (among the M moves evaluated to establish local

optimality) are used to create the first level of the F&F neighborhood tree. The next levels are created using $\eta_1 = 16$ and $\eta_2 = 8$. The method stops branching as soon as an improved solution is found, the maximum number of levels $L = 15$ is reached, or if there is no more legitimate candidate moves to evaluate.

In case a global improvement is found in the tree search the new best solution is made the starting solution for another run of the local search procedure. However, if the solution at the root node cannot be improved, the method switches back to the local search starting with the best trial solution encountered in the tree search and using neighborhood N_2 . In this case, the list M determined in the last run of the local search procedure, and so made up of type N_1 moves, is now extended with new candidates of type N_2 . The new list $M(0)$ is created using the best moves of each type in equal number. The objective is to allow the algorithm to combine both types of neighborhoods throughout the F&F tree.

The performance of the algorithm was evaluated on a set of 43 benchmark problems belonging to two classical sets known as LA and FT.

The analysis of the computational results shows that the F&F algorithm produces solutions that are on average at 0.28% above the optimum (or best known) solutions for the LA testset and that are optimal for all FT instances. The algorithm is also very fast, finding its best solutions in relatively short time (on a 1.7 GHz Pentium IV 256 MB): less than 6 seconds on average for the LA problems and no more than 21 seconds on average for the FT class. Also, only 1 second of running time was enough for the algorithm to find optimal solutions for 23 out of 29 instances that the method successfully solved to optimality.

The resulting F&F approach has also been compared to two leading methods that were established to be the best among thirteen methods tested in a recent study by Gonçalves et al. (2005): (1) a hybrid genetic algorithm/local search (GA/LS) method developed as part of the study, and (2) a tabu search (TS) approach by Nowichi and Smutnicki (1996), which emerged the clear winner of all methods examined. The performance of the present F&F approach with regard to solution quality places it next after the TS approach, with an average relative deviation from the best known solutions of 0.27%, as compared to 0.05% for the TS approach and 0.39% for the hybrid GA/LS approach. The F&F approach also falls between these two methods in solution speed, running about one order of magnitude slower than the TS approach, but about two orders of magnitude faster than the GA/LS approach (after adjusting for differences in computers). However, the F&F procedure emerges as significantly more robust than the other two methods in the time required to find best solutions. F&F times range from 1 to 52 seconds with a standard deviation of 11.9, while the TS times range from less than 1 second to 623 seconds with a standard deviation of 147.6, and the GS/LS times range from 13 to 3745 seconds with a standard deviation of 1183.0. However, it is to be noted that another TS algorithm for the JSSP has recently emerged that appears to be substantially better yet in relation to both speed and robustness. The tabu search approach due to Grabowski and Wodecki (2005), applied to the same testbed, yields solutions having an average relative deviation of 0.04% from the best known solution, while consuming about 1.03 seconds (on a 333 MHz CPU), which would translate into an insignificant amount of time if runs were performed on a faster computer like the ones used by the F&F and the GA/LS algorithms.

4.4 Capacitated minimum spanning tree

The capacitated minimum spanning tree problem (CMST) has been addressed extensively in the literature for its importance in modeling and practical applications in the design of communication networks. It also emerges in applications in distribution, transportation and

logistics (see Gavish 1982, 1991). From the modeling standpoint, the problem constitutes a relaxation of the classical capacitated vehicle routing problem, which in turn is central in many other more complex problems. Comprehensive reviews of methods and solution approaches appear in Amberg et al. (1996) and in Mathew and Rego (2006).

The CMST problem can be stated as follows. Given a complete undirected graph $G = (V_0, A)$, where $V_0 = \{v_0, v_1, \dots, v_n\}$ is a vertex (node) set and $A = \{(v_i, v_j) \mid v_i, v_j \in V; i \neq j; j \neq 0\}$ is an arc set. Let v_0 denote a special *central* node (root), and let $V = V_0 \setminus \{v_0\}$ be a set of *terminal* nodes requiring a specified demand d_i . $C = (c_{ij})$ is an $n \times n$ matrix associated with A , where c_{ij} is a non-negative weight (distance or cost) on arc (v_i, v_j) if there is an arc between v_i and v_j . Otherwise c_{ij} is infinity. The CMST problem consists of finding a minimum cost tree T spanning all nodes of G , so that the sum of the demands in each sub-tree incident to the root node does not exceed a fixed arc capacity Q . When all the nodes $v_i \in V$ have the same demand the problem is referred to as the homogeneous demand CMST problem.

Successful approaches to the CMST problem involve high complexity multi-exchange neighborhoods that take advantage of the basic tree-based and node-based neighborhoods used in tabu search algorithms to address the problem. Node-based neighborhoods generate moves that transfer a node from one sub-tree to another or exchange nodes between sub-trees, while tree-based neighborhoods transfer sub-trees between different sub-trees.

The evaluation of node-based or tree-based neighborhoods in dense graphs requires $O(n^2)$ effort, and the effort to evaluate a combination of L of these moves is $O(n^L)$, and hence grows exponentially with L . A potentially best combination of L moves can be evaluated with significantly less effort if the combination is thought of as a compound move consisting of individual moves evaluated progressively using the filter-and-fan strategy.

The effectiveness of the filter-and-fan method for implementing complex compound moves that improve the local optima with only a modest increase in computational effort is examined in Rego and Mathew (2009). This algorithm uses a design of the F&F approach wherein the descent phase is replaced with a tabu search phase and the tree search is continued after a local optimum is found, allowing local optimality to be overcome in any level of the tree except for leaf nodes. In addition the method employs a neighborhood structure that brings about two types of strategic oscillation: (1) cycling between feasibility and infeasibility and (2) cycling between node-based shift moves and tree-based shift moves. Strategic oscillation is a specialized tabu search technique that operates by orienting the search with respect to some boundary (or collection of boundaries). In a one-sided oscillation, which is appropriate for the present setting, whenever such a boundary is reached the algorithm changes direction according to a specified search mechanism. In this algorithm changing direction involves switching to the alternate neighborhood structure. The memory structures used include short term memory defined by the classical tabu restrictions and aspiration criteria together with critical event memory to bring about strategic oscillation. A brief description of the algorithm follows.

A complete evaluation of both the node-based and tree-based neighborhood, starting from the initial solution X_o , is performed by incorporating penalty costs for moves that lead to infeasible solutions. The method selects a set of η_0 best moves that lead to solutions with the lowest objective function values. From among these moves a subset of the η_1 best moves (which can be either node-based or tree-based) are executed to form η_1 different solutions. For each of these solutions, η_2 highest evaluating moves from the original η_0 are selected. From the union of the η_2 moves for all η_1 solutions, the best η_1 moves are executed to produce η_1 new solutions. This process extends for L levels of the F&F tree (in a diversification phase) or until the best solution is improved upon (in an intensification phase), in

which case the process is repeated from the beginning using the best solution encountered throughout the tree to re-initiate the tabu search phase. In this manner the filter-and-fan approach executes simple tree-based and node-based shift moves that consist of at most L moves. The compound move composed of these shift moves avoids the computational overhead required for the complete neighborhood evaluation necessary to determine the exact best L -compound move. Additionally, to prevent cycling in the solution space, the most recent moves executed are maintained as tabu active for a stipulated number of iterations.

Computational tests performed using standard benchmark problems revealed that this algorithm produced results that compare favorably to a number of prior metaheuristic algorithms and rivals the best. Tests carried on a total of 125 instances comprising 45 heterogeneous demand problems and 80 homogeneous demand problems demonstrated that the algorithm found the best known solutions in 70 of these 125 instances with an overall deviation of 0.65% on average. In addition, the average execution time for the F&F approach proved to be significantly smaller than that of the state-of-the-art competitors on comparable platforms.

For an appropriate comparative analysis, runs were performed in a similar manner and on the same groups of instances used to test the alternative algorithms. To do this, recourse was made to the study of Amberg et al. (1996), which tested a simulated annealing algorithm and six variants of a tabu search algorithm on 70 homogeneous-demand instances. The various algorithms differ by the type of neighborhood and the method used to manage the tabu restrictions in the tabu search algorithms.

Results obtained for 12 independent runs of each algorithm disclosed that a run of the F&F algorithm is better than any of the runs of these algorithms. In particular, it is shown that even if all seven variants of these algorithms are taken together and the best overall run for each individual problem is chosen, the average quality of the solutions produced by the F&F algorithm across all problems exceeds the quality of such best solutions by 0.43%, indicating a clear dominance of the F&F algorithm over these alternative strategies for the CMST. Similar analysis reveals a significant advantage of the F&F algorithm over the tabu search implementation of Sharaiha et al. (1997) and the adaptive reasoning technique (ART) of Patterson et al. (1999) across all problem categories. More competitive approaches are due to Ahuja et al. (2001) who propose two very large-scale neighborhood search (VLSN) approaches based on multi-exchanges of node-based and tree-based neighborhoods, respectively. These neighborhoods are used to create two different variants of a tabu search and a GRASP algorithm. Tests on 2 groups of problems of different sizes and characteristics indicate that the F&F algorithm performs better than one of the GRASP variants for the first group and better than the other GRASP variant for the other group. Similarly, the F&F algorithm performs better than one of the TS variants for a group of problems and is very competitive with the other variant for the other group. As an overall assessment, the F&F approach outperforms a GRASP and a TS variant. A considerable advantage of the F&F algorithm concerns the significantly reduced amount of solution time it requires relative to the solution times required by each of the 4 variants of the competing algorithms.

These results clearly indicate the impact of the neighborhood structure in the performance of metaheuristic strategies, disclosing that node-based neighborhoods prove more effective for solving homogeneous-demand problems while tree-based neighborhoods prove more effective for solving heterogeneous-demand problems. To take advantage of the complementary features of the two types of neighborhoods, a strategy that unifies node-based and tree-based into a composite multi-exchange neighborhood has been proposed in Ahuja et al. (2003). Their neighborhood search is powered by an exact dynamic programming solution method aimed at finding the best move in the composite neighborhood. This enhanced

approach finds all best known solutions for the 75 problems tested (out of the 125 considered by the F&F algorithm), and so proves relatively more effective, although to achieve this result the method requires more than four times as much effort as the F&F method (on a similar computer) to find solutions of the same or exceedingly similar quality.

5 Ejection chain applications

5.1 Traveling salesman

The Traveling Salesman Problem (TSP) consists in finding a minimum distance tour of n cities, starting and ending at the same city and visiting each other city exactly once. In spite of the simplicity of its problem statement, the TSP is remarkably challenging and is the most studied problem in combinatorial optimization, having inspired well over a thousand publications.

In graph theory, the problem can be defined on a graph $G = (V, A)$, where $V = \{v_1, \dots, v_n\}$ is a set of n vertices (nodes) and $A = \{(v_i, v_j) \mid v_i, v_j \in V, i \neq j\}$ is a set of arcs, together with a non-negative cost (or distance) matrix $C = (c_{ij})$ associated with A . The problem is considered to be symmetric (STSP) if $c_{ij} = c_{ji}$ for all $(v_i, v_j) \in A$, and asymmetric (ATSP) otherwise. Elements of A are often called edges (rather than arcs) in the symmetric case. The version of STSP in which distances satisfy the triangle inequality ($c_{ij} + c_{jk} \geq c_{ik}$) is the most studied special case of the problem. The STSP (ATSP) consists in determining the Hamiltonian cycle (circuit), often simply called a *tour*, of minimum cost.

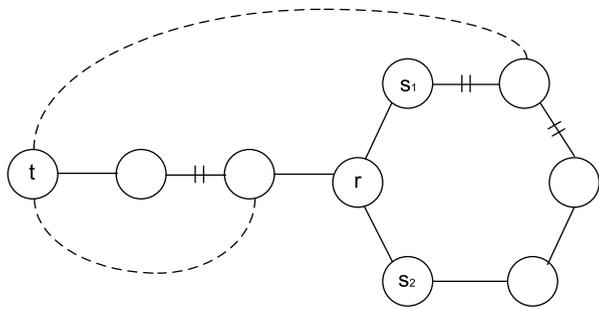
The importance of identifying effective heuristics to solve large-scale TSP problems prompted the “8th DIMACS Implementation Challenge”, organized by Johnson et al. (2000) and solely dedicated to TSP algorithms.

Ejection chain methods lead the state-of-the-art in local search heuristics for the traveling salesman problem (TSP) and likewise have successfully been applied to a cardinality-constrained variant of the problem (Cao and Glover 1997). The most effective local search approaches for the classical TSP primarily originate from the Stem-and-Cycle (S&C) ejection chain method (Glover 1992) and the widely acclaimed Lin-Kernighan (LK) procedure (Lin and Kernighan 1973), which can be viewed as an instance of an ejection chain method. These two types of TSP ejection chain approaches typically proceed by disconnecting a subpath and reconnecting it with different components at each level of the chain, and as a consequence are generally called *subpath ejection chain methods*.

5.1.1 Subpath ejection chains for the TSP

Subpath ejection chain methods for the TSP start from an initial tour and iteratively attempt to improve the current solution, generating moves coordinated by a *reference structure*. The LK approach uses a Hamiltonian path as the reference structure to generate moves throughout the neighborhood construction. By contrast, the S&C ejection chain method is based on the stem-and-cycle reference structure, which is a spanning subgraph of G consisting of a path called a *stem* connected to a *cycle* by a single node called the *root* node. The two nodes adjacent to the root in the cycle are called *subroots* and the node on the end of the stem opposite the root is called the *tip* of the stem. In a subpath ejection chain, once a reference structure is created from the initial TSP tour, ejection moves consist of transforming the reference structure into another of the same type and suitably structured trial moves are used to generate feasible tours at each level of the chain.

Fig. 4 The S&C reference structure and associated ejection moves



The LK method starts by generating a low order k -opt move (with $k \leq 4$) and then creates a Hamiltonian path by deleting an edge adjacent to the last edge added. This completes the first level of the LK process. In succeeding levels each ejection move consists of linking a new edge to the unique degree 1 node that was adjacent to the last edge added, followed by deleting the sole edge whose removal will generate another Hamiltonian path. A trial move consists of linking the two endpoints of the current Hamiltonian path, thus creating a feasible tour.

By contrast, the S&C method creates the initial S&C reference structure from a TSP tour by adding an edge to link two nodes of the tour and removing one of the edges adjacent to one of those nodes. Each ejection move then adds an edge that links the tip node to any other node on the graph, except for the one adjacent to the tip, and removes one of the edges adjacent to that node. Two different ejection moves are possible depending on whether the node to be linked to the tip lies in the stem or in the cycle. If such node lies in the stem there is only one possibility to eject a subpath, which results from deleting the only possible adjacent edge that creates a feasible structure; otherwise two possible subpaths may be ejected by deleting either adjacent edge.

The S&C structure and the nature of its ejection moves are illustrated in Fig. 4. In the figure, the S&C structure is represented by dark edges with nodes t , r , s_1 and s_2 denoting the tip, the root and the two subroots of the structure, respectively. Dotted lines denote edges to be added by each type of ejection move and the associated possible edges to be deleted by the move are marked by the small parallel lines crossing them.

Trial solutions are obtained by adding an edge from the tip to one of the subroots and deleting the edge between this subroot and the root.

Both theoretical and experimental studies have demonstrated that the S&C ejection chain method is more general and powerful than the LK approach. Notably, the reference structure in the LK approach is very close to being a valid TSP solution (it only requires adding a single edge to close the gap between the two nodes of degree 1 and thus obtain a tour). As a result, the structure implicitly limits the different types of moves it can generate and consequently makes only one trial solution available from a given Hamiltonian path. The S&C reference structure, on the other hand, yields two trial solutions (except in the case of a degenerate structure when the tip and root nodes coincide, in which case the structure corresponds to a tour). Another fundamental difference is that the S&C procedure generates *dynamic alternating paths* while the classical LK approach generates *static alternating paths*. A theoretical analysis of the differences between the types of paths generated by S&C and LK procedures is provided in Funke et al. (2005), which includes a demonstration that the LK neighborhood is strictly contained in the S&C neighborhood. The authors also show that even a generalization of the LK approach that incorporates generalized alternating paths cannot reach solutions accessible to the S&C neighborhood.

5.1.2 The symmetric TSP

An effective algorithm design and implementation of the S&C ejection chain method was first proposed by Rego (1998a) for the STSP and subsequently enhanced in Gamboa et al. (2005, 2006a). In the latter, the authors have adopted the *two-level tree* data structure described in Fredman et al. (1995) that is used to support the most efficient LK implementations reported in the DIMACS Challenge (e.g. those of Johnson and McGeoch 1997; and Helsgaun 2000; Applegate et al. 2003). The upgraded S&C algorithm also incorporates a variety of neighbor lists, thus providing the algorithm with additional options not available in the previous version.

The generation of moves throughout the ejection chain process is based on the definition of a set of rules and legitimacy restrictions on the set of edges that are allowed to be used in subsequent steps of an ejection chain. The algorithm is implemented as a local search improvement method in the sense that no meta-strategy is used to guide the search beyond local optimality. Also, the method always stops after n iterations of the *re-routing* strategy fail to improve the best solution found so far. (Re-routing consists of starting an S&C ejection chain from a different route node.) This makes the implementation of the S&C algorithm simpler than LK implementations that make use of additional supplementary techniques such as caching distances, and other implementation tricks.

Maintaining the fundamental rules of the original algorithm (described in Rego 1998a) unchanged, improvements on the data structures and the use of appropriate candidate list strategies made the modified version of the S&C algorithm more efficient and effective for solving very large-scale problems.

In Gamboa et al. (2006a, 2006b) the authors report the outcomes of an extensive series of tests on problems ranging from 1000 to 3,000,000 nodes, showing that by using data structures and candidate lists routinely included in state-of-the-art TSP solution software, the S&C algorithm clearly outperforms all implementations of the LK procedure. Specifically, it is shown that S&C approach finds better solutions than all of the leading LK variants for about 70% of the problems tested. Conspicuously, the 70% advantage of the S&C approach refers to a comparison with the most effective variant of the LK procedure. The second best variant of the LK approach is dominated by the S&C approach in approximately 97% of the problems. Some LK variants included in the DIMACS challenge failed to find even a single solution better than the S&C approach over all 59 problems tested.

5.1.3 The asymmetric TSP

The S&C is a fundamental component of several other reference structures used in the creation of ejection chain methods. A direct generalization of the S&C reference that has special advantages for the ATSP is called the Doubly-Rooted (DR) S&C (Glover 1996), which considers two root nodes instead of one. The doubly rooted structure has two forms: a *bicycle* in which the roots are connected by a single path, joining two cycles, and a *tricycle* in which the two roots are connected by three paths, thereby generating three cycles. In the DR structure the definition of subroot is extended to include any node adjacent to a root node, regardless of whether it is in the cycle or in the stem.

Ejection moves consist of adding a new edge linking one of the subroots to an arbitrary node on the graph and deleting the edge between this subroot and the associated root, causing the selected arbitrary node to become the new root.

The trial solutions available to the doubly-rooted structure are those generated by the union of the trial solutions available to the single-rooted S&C structure obtained by deleting

any edge linking a root node to a cycle subroot. Such a subroot becomes the tip of the S&C, while the (root) node that remains with three incident edges becomes the S&C root.

Rego et al. (2006) provide a comparative study of the DR neighborhood structure and the generalized LK neighborhood for the ATSP proposed in Kanellakis and Papadimitriou (1980) and recently used in the current state-of-the-art local search algorithm for the ATSP by Cirasella et al. (2001). Computational experiments on a standard testbed exhibits superior performance for the DR neighborhood over its LK counterpart, revealing that a straightforward implementation of a DR ejection chain algorithm outperforms the best local search algorithms and obtains solutions comparable to those obtained by the current most advanced iterative local search algorithms specially designed for the ATSP, while requiring dramatically smaller computation time.

Out of 28 instances for which results are available for KP, in only 4 instances did the KP algorithm manage to find tours that are slightly better than those found by the DR algorithm. For the remaining 24 instances, the DR algorithm found 3 tours of similar quality and 21 of superior quality compared to those produced by the KP algorithm. In some cases the quality of solutions found by the DR algorithm exceeded that of the KP algorithm by as much as 5.5%. Even more impressive is the performance of the DR algorithm compared to the sophisticated iterative local search variant (iKP) of the basic KP algorithm (Cirasella et al. 2001). Considering the whole set of 47 benchmark instances both iKP and DR algorithms find an equal number of best solutions (28). Among these, a 0.00% gap from optimality is achieved on 9 instances by the iKP algorithm and on 17 instances by the DR algorithm. Also, the iKP algorithm requires significantly more computational time on average than the DR algorithm. In some cases the iKP algorithm requires 2 hours compared to less than 50 seconds for the DR algorithm (which finds tours of better quality).

5.1.4 Advances on data structures for large STSPs

An effective data representation is crucial for the efficiency of search algorithms for the TSP and particularly important for large STSP instances. The nature of these algorithms necessitates the use of certain basic tour operations involving subpath reversal and traversal. The computational effort that must be devoted to these operations becomes increasingly pronounced with larger problem instances.

The 2-level tree (Chrobak et al. 1990) has for many years been considered the preeminent choice for representing the tour, retaining that reputation until the recent emergence of the k -level satellite tree proposed by Osterman and Rego (2003). The classical 2-level tree divides the tour into approximately $n^{1/2}$ segments each containing as many nodes as grouped under a parent node, where a doubly linked list is used to connect both segments and client nodes within the segments. A worst case cost of $O(n^{1/2})$ for tour operations may be achieved with the 2-level tree representation.

The theory behind the 2-level tree contributes much to the latest developments on TSP data structures. Its effectiveness has been demonstrated by independent implementations due to Fredman et al. (1995), Gamboa et al. (2005, 2006a) and numerous participants in the DIMACS TSP Challenge (Johnson et al. 2000).

The k -level satellite tree expands upon the 2-level tree to allow the tree to be divided into k levels instead of two. This is accomplished by partitioning the tour nodes into segments containing roughly $n^{1/k}$ nodes each, and the resulting segments are grouped into *parent segments* containing about $n^{1/k}$ segments each. A fundamental feature of this k -level satellite tree is the *satellite list* structure, also proposed by Osterman and Rego (2003) as symmetric counterpart of the classical doubly-linked list structure. The satellite list represents a tour

without implying a fixed orientation, making it useful for representing symmetric paths or cycles. It can operate in the same capacity as the doubly-linked list and is equally efficient in terms of both memory and computation of *previous* and *next* queries. Because the satellite list avoids a fixed orientation, the subpath reversal operation can be performed in constant time, whereas for the linked list, every pointer associated with nodes in the reversed path in the list must be changed to reflect the appropriate orientation. A satellite design for the k -level tree is important, not only because of subpath reversal, but also because *next* and *previous* queries do not need to access *parent* nodes. The resulting benefit is substantial, considering the frequency of the need for these operations and the fact that the cost of accessing a parent node varies with the problem size when the data structure is designed optimally.

As shown in Osterman and Rego (2003), when k is chosen optimally, a path between two client nodes in the tree can be traversed with a complexity of $O(\log n)$ rather than $O(n^{1/2})$. This result indicates that an optimally designed k -level tree is the most efficient structure proposed to date.

5.2 Vehicle routing

The Vehicle Routing Problem (VRP) is a generic name given to a class of problems in which a set of routes for a fleet of vehicles, based on one or several depots, must be determined for a number of geographically dispersed *cities* or *customers*, subject to side constraints. The problem is central in the fields of transportation, distribution and logistics and provides a general model for a wide range of practical applications.

Let $G = (V, A)$ be a graph where $V = \{v_0, v_1, \dots, v_n\}$ is a vertex (or node) set, and $A = \{(v_i, v_j) \mid v_i, v_j \in V, i \neq j\}$ is an arc (or edge) set. Consider a *depot* to be located at v_0 and let $V' = V \setminus \{v_0\}$ denote a set of n cities (or client locations). A non-negative *cost* or *distance* matrix $C = (c_{ij})$ is associated with every arc of A . It is assumed that m identical vehicles are used, each with capacity Q , and their number is a decision variable (or can be fixed depending on the application). Vehicles make pickups or deliveries but not both. With each vertex v_i is associated a quantity q_i ($q_0 = 0$) of some goods to be delivered by a vehicle and a service time δ_i ($\delta_0 = 0$) required by a vehicle to unload the quantity q_i at v_i . The VRP consists of determining a set of m vehicle routes of minimal total cost, starting and ending at a depot v_0 , such that every vertex $v_i \in V'$ is visited only once by precisely one vehicle, where the total quantity assigned to each route does not exceed the capacity Q and the total duration (travel plus service times) of any vehicle route does not surpass a given bound D . Hence in this context the cost c_{ij} is taken to be the travel time between the two associated cities.

Drawing on the fact that ejection chain methods have proved very efficient for solving large scale traveling salesman problems, generalizations of some of these methods have been developed to deal with multiple routes as required in general vehicle routing problems.

5.2.1 Node-based ejection chains for the VRP

Node-based ejection chain methods derive from extensions of customary single node insertion and exchange neighborhoods that have been found useful in several classes of graph problems including: machine scheduling, clustering, graph-coloring, vertex covering, maximum clique or independent problems, vehicle routing problems, generalized and quadratic assignment problem, and the traveling salesman problem, just to cite a few.

Typical node insertion (or shift) neighborhoods involve removing a node from one route and inserting it into another, while typical node exchange (or swap) neighborhoods involve

interchanging nodes between routes. In neighborhood search, these insertion and swapping operations are also performed within a given route (instead of across routes) as a way to re-optimize the associated TSP defined over the nodes of this route. Since the worst case complexity of evaluating a single node insertion and node exchange neighborhood is $O(n^2)$, creating compound neighborhoods by combinations of these moves requires an effort that grows exponentially with the number of moves considered in combination. More precisely, the best compound neighborhood of k moves can be generated and evaluated with $O(n^k)$ effort. Embedding these simple neighborhoods in an ejection chain framework can notably reduce this effort (Glover 1991).

Rego (2001) develops an ejection chain neighborhood for the VRP that implements a *multi-node insertion* move and a *multi-node exchange* move to yield an important form of *combinatorial leverage*. Specifically, the number of moves represented by a level k neighborhood is multiplicatively greater than the number of moves in a level $k - 1$ neighborhood, but the best move from the neighborhoods at each successive level can be determined by repeating only the effort required to determine a best first level move.

The ejection chain starts by identifying a node pair v_i, v_j that yields the best (highest evaluation) ejection move that disconnects node v_i from its current position and inserts it into the position currently occupied by node v_j . For subsequent levels, ejection moves consist of selecting a new candidate node to be ejected by the previously ejected node, and then repeating until no other legitimate node exists for ejection. Such an ejection process creates an intermediate structure at each level of the chain where the associated ejected node, say v_k ($k = j$ for the first level), is temporarily disconnected from the tour. However a trial solution can be obtained by: (1) inserting node v_k between two nodes v_p and v_q and adding an arc linking the original predecessor and successor of v_i to close the route—a *multi-node insertion move*; or (2) simply by relocating the last ejected node v_k to occupy the vacant position left by the node v_i that initiates the chain—a *multi-node exchange move*.

This composite ejection chain neighborhood has been embedded in a tabu search algorithm, named TabuChain, which is designed to use frequency-based adaptive memory and strategic oscillation to allow for temporary violation of the capacity or maximal route duration constraints. Both sequential and parallel versions of the algorithm have been implemented. The parallel version is based on a synchronous model of parallel searches that allows for a more extensive exploration of the solution space than the basic sequential version. Also, different levels of parallelization are used in order to accelerate the search process. One takes advantage of an ejection chain property that permits ejection and trial moves to be evaluated separately by different processors, potentially reducing the time per iteration by half. Another level of parallelization consists of launching separate processes to re-optimize each individual route. The sequential and parallel methods, each in its own category, remain among the most effective algorithms available for the VRP, producing solutions that are on average 0.77% and 0.55% above the best known solutions for the classical fourteen-instance testbed of Christofides et al. (1979).

Node-based ejection chain approaches have also been successfully applied to clustering problems by Dorndorf and Pesch (1994). Principles similar to those underlying the node-based ejection chain method discussed for the VRP are developed and explored in Yagiura et al. (2004) to provide an effective algorithm for the generalized assignment problem.

5.2.2 Subpath ejection chains for the VRP

Another type of ejection chain approach for the VRP concerns a subpath ejection chain method proposed in Rego (1998b). A fundamental feature of this method is the *flower reference structure* that generalizes the stem-and-cycle (S&C) reference structure (discussed in

Sect. 5.1) to a multiple routing context. The flower structure is defined as a spanning subgraph of G , which consists of a path called *stem* attached to multiple cycles representing routes. In the original paper several components of the flower structure are termed differently than their equivalents in the S&C structure; however to facilitate the discussion in this paper we stick with the terms already introduced for the S&C. Therefore, the node that lies on the intersection of a stem and a cycle is called a *root* and the nodes adjacent to a root are called *subroots*. Likewise, the node at the opposite end of the stem from the root is referred to as the *tip* of the stem. In the flower structure the *root* node always identifies the *depot* and hence these two terms may be used interchangeably.

The consideration of multiple cycles in the flower reference structure extends the ejection and trial moves of the stem-and-cycle to encompass a number of other possibilities. Starting from a given VRP solution, the ejection move to create a flower structure may simply delete one of the edges incident to the root (depot), thus transforming a cycle into a stem, which is also a basic move to deal with routes containing a single city. Such a move that only deletes one edge without adding another may be referred here to as a *drop move* to differentiate it from the moves that replace one edge with a new one and so may be called *add-drop moves*. Similarly, a trial move that transforms a flower structure into a VRP solution may simply link the tip directly to the depot to close the route. Such a trial move may be called a *route-creation move*. By contrast, the type of S&C trial move that links the tip node to one of the subroots and deletes the associated edge incident to the root may be called *route-extension move*, since it extends a route to include the clients currently in the stem that is made to join that route. Depending on the type of ejection and trial moves considered for an ejection chain, the number of vehicle routes can vary: the number decreases if the chain starts with an ejection move that deletes an edge incident to the root and then applies a route-extension trial move, whereas the number increases if the chain starts by applying an add-drop move to one of the routes and a route-creation move is used to obtain a new trial solution.

An important feature of the algorithm concerns the choice of the chain starting rules. Since it is possible to create a flower structure from a given VRP solution by deleting one edge without adding another, such a step always results in a cost reduction in relation to the current solution. Moreover, as the longest edges are usually selected to be deleted, this leads to the outcome that the proper add-drop S&C move will rarely be chosen to start the chain. To avoid this situation, the algorithm considers a penalty factor to provide a more appropriate evaluation of the two types of ejection moves. Experimental tests carried out on problems with different characteristics disclosed that randomly varying this penalty within specific intervals (of real values) was highly advantageous. Different tradeoffs can be obtained in evaluating the two types of moves that initiate an ejection chain depending on three ranges of values as follows. For negative values the drop move is highly penalized, hence an add-drop initiating move is performed. If these values are positive and less than 1, initiating drop moves are again penalized in relation to add-drop moves, but not so strongly. Finally, values greater than 1 yield greater penalties for the add-drop initiating moves and hence favor drop moves to be performed.

Although the Flower reference structure preserves the same properties as the S&C structure and so succeeds in generating dynamic alternating paths and cycles, the violation of the alternating path construction that is caused by an ejection chain process in the VRP setting is less restrictive than in the TSP setting. This increases the move options for the VRP, yielding a heuristic advantage. In this setting, periodically limiting the moves to generate an ordinary alternating path rather than a dynamic alternating path turned out to be useful to avoid modifying adjacent edges at the same step of the algorithm. Nevertheless, such a modification was not completely forbidden in order to allow the most promising changes to

be carried out. In sum, on one hand it is sometimes desirable not to simultaneously modify two adjacent edges as a means of inducing some degree of diversification; on the other hand it can also sometimes be desirable to allow such a modification to provide some intensification of the search and possibly reach deeper local optima where new best solutions may be found.

The implementation of this subpath ejection chain method relies on a tabu search guidance to prevent the method from generating flower structures already considered at previous levels of the chain. Guidance by tabu search is also used to govern the creation of alternating paths within the context of the legitimacy conditions used in the algorithm, which as in the case of the TSP problem assure that a given solution can be transformed into any other.

To gauge its performance, the Flower algorithm was tested on an extended set of 30 problems from the literature, which include the classical fourteen-instance set of Christofides et al. (1979), three real-world problems taken from Fisher (1994) and twelve instances considered in Taillard (1993) and Rochat and Taillard (1995). The original goal in creating the Flower algorithm was to produce high-quality solutions rapidly rather than striving to find (new) best solutions, and hence no recourse was made to sophisticated forms of TS guidance—in contrast to TabuChain (previously described) and a number of other algorithms in the literature. Comparisons with algorithms sharing a similar goal of rapid convergence reveal that the Flower algorithm is clearly superior to all of them, producing better solutions and also requiring less running time. When compared with other classes of algorithms that make advanced use of metaheuristic guidance, the Flower algorithm compares quite favorably to these as well, especially when good solutions must be found quickly. In particular, the algorithm is very fast in finding solutions that are within the range of 1% of the best known solution.

5.3 Crew scheduling

The general crew scheduling problem (CSP) can be formulated as seeking the minimum number of crews necessary to cover a set of trips with duties that have to satisfy a number of regulations and operational constraints.

Cavique et al. (1999) address a CSP arising in train transportation and develop a subgraph ejection chain method embedded in a tabu search algorithm for the solution of the problem. The algorithm relies on the definition of a number of terms generally used in crew scheduling, which can be introduced in the context of the problem at hand.

The set of trips to be performed by each train defines a *timetable*. A *trip* is a one way movement of a train between two *terminal* points, the smallest period (or elementary crew activity) into which the timetable can be divided. A trip has five attributes: train number, starting place and time, finishing place and time. A *block* is a set of all trips produced by the same train, and the set of consecutive trips in a block, covered by the same crew, is called a *piece of work* (or *piece*). A *block partition* is a set of non-overlapping pieces of work that exactly covers a block. In this application, a complete duty may be formed by one or two pieces or work, a meal break, the report and clear time and a possible reserve period. The set of contractual and operational constraints include specific relief points, bounds on the durations of pieces of work, report and clear times, duty duration, and possible intervals for meal breaks. A duty that satisfies all problem constraints is called a *feasible duty* and a set of feasible duties covering all trips makes up a feasible *schedule*. The objective of the CSP is to find a feasible schedule with a minimum number of crews (duties) needed to operate the train line.

The subgraph ejection chain method and associated tabu search procedure for this problem may be described as follows. In contrast with the node based and subpath ejection

chain methods, the present method considers a *subgraph* as the elementary component to be ejected at each level of the ejection chain process. The method explores a specialized *block partition* technique that underlies the formulation of the *maximum cardinality matching problem* (MCMP) of a non-bipartite graph $G = (P, D)$. The method is divided into three fundamental procedures: *block partition*, *graph generation*, and *duty achievement*. In the first step, the block partition procedure divides the blocks into k feasible pieces of work, creating the node set $P = (p_1, \dots, p_k)$. In the second step, the matching graph G is built by linking pairs of pieces for all possible duties, creating the edge set $D = \{(p_i, p_j) \mid p_i, p_j \in P\}$. Finally, in the third step, a MCMP algorithm is applied to find a maximal matching of pieces to create a schedule. In the solution of the MCMP, the matched nodes represent duties with two pieces and the free (or unmatched) nodes are duties with only one piece of work. Under this model the CSP reduces to the problem of finding the block partition that produces a schedule with a minimum number of duties over all possible partitions.

The enormous number of alternatives to partition the set of blocks for a given timetable entails a very large and complex solution space for which effective search algorithms must be designed. The algorithm considers a tabu search approach based on an embedded neighborhood structure that gives rise to a subgraph ejection chain method defined as follows. A neighborhood structure N is decomposed in two substructures N_1 and N_2 , which separates the neighborhood space into two subsets. N_1 is an intermediate structure responsible for generating a set of new pieces of work that will replace pieces of the current graph $G_i = (P_i, D_i)$ transforming it into another graph $G_{i+1} = (P_{i+1}, D_{i+1})$. N_2 is a structure defining the set of edges in G_{i+1} associated with feasible duties. The complete neighborhood structure N is defined by any possible sequence of moves $e_1, t_1, \dots, e_k, t_k, \dots, e_L, t_L$ such that $e_k \in N_1$ and $t_k \in N_2$, representing an ejection chain of L levels. Accordingly, the transition from a solution (schedule) S_i to a solution S_{i+1} can be obtained by a sequence of moves $e_1, e_2, \dots, e_{k^*}, t_{k^*}$ with e_{k^*} and t_{k^*} denoting the ejection move and trial move, respectively, at level k^* where the best trial solution was found.

In the algorithm, ejection moves are defined by three types of elementary operations (1) *shift operation*, which shifts the extreme of a piece to the right or to the left, transferring one or more trips between adjacent pieces, (2) *cut operation*, which splits one piece into two pieces, and (3) *merge operation*, which combines two pieces into a single piece. Each of these operations that modify the configuration of certain nodes require deleting (or ejecting) a subgraph involving the modified nodes and certain edges adjacent to them, which thereby entails the creation of another subgraph associated with the new configuration of the nodes that have been modified by the ejection move. Under this conception, an ejection move at level k deletes (ejects) a subgraph G_i^{k-} of G_i^k ($G_i^k = G_i$) and adds another subgraph G_i^{k+} to the current graph transforming G_i^k into $G_i^{k+1} = G_i^k \setminus G_i^{k-} \cup G_i^{k+}$. The associated trial move for the current level may be given by solving the MCMP on graph G_i^{k+1} , thus yielding a new feasible schedule. Due to the inherent time complexity of determining an exact solution for the MCMP at each level of the chain, the algorithm considers a *trial function* that implicitly reflects the potential quality of the trial solution that could be reached. Once the chain ends, the explicit evaluation of N_2 is carried out by solving the MCMP on the graph $G_{i+1} = G_i^{k^*}$, where k^* represents the level of the chain where the best value of the trial function was found.

A set of six real time tables involving over 700 trips and up to 26 trains (number of blocks) is used in order to test the performance of the algorithm. The quality of the solutions is evaluated on the basis of three correlated performance measures: the percent improvements to the number of duties obtained by alternative schedulers, the matching ratio (i.e. percentage of duties with two pieces of work), and the average number of driving hours per

duty. The results disclose that the ejection chain algorithm performs extremely well across the three evaluation criteria. The algorithm finds better schedules than previous methods for all problems tested, reducing the number of duties, improving the distribution of the crew's workload and finding higher matching ratios.

5.4 Quadratic assignment

The quadratic assignment problem (QAP) is a classical combinatorial optimization problem that has garnered much attention due to both its large number of applications and its solution complexity. Originally used to model a location problem in the 1950's, the QAP is computationally very difficult to solve which makes it an ideal candidate for testing new algorithmic approaches. While facility location problems remain the most popular application area for the quadratic assignment problem, many other applications for this problem exist including scheduling problems, statistical data analysis, information retrieval, as well as problems in transportation. The attractiveness of the QAP is also due to the fact that many other combinatorial optimization problems can be formulated as a QAP, including: the traveling salesman problem, the maximum clique problem and the graph partitioning problem. (See Cela (1998) for a survey of both classical and practical applications.)

In the context of facility location problems, the QAP can be stated as follows. Given a set $F = \{f_1, \dots, f_n\}$ of n facilities to be placed in exactly n locations represented by the set $L = \{l_1, \dots, l_n\}$. Let $A = (a_{ik})$ be a matrix of *distances* between pairs of locations $l_i, l_k \in L$, and an associated matrix $B = (b_{ji})$ of *flows* to be transmitted (or shipped) between pairs of facilities $f_j, f_i \in F$. The objective is to find a minimum cost assignment of facilities to locations considering both the flow of materials between facilities and the distance between locations.

In mathematical terms, each assignment can be defined as a permutation p of the underlying index set $N = \{1, \dots, n\}$. Hence, if facility j is assigned to location i and facility l is assigned to location k , the cost of the flow between facilities $j = p(i)$ and $l = p(k)$ is $a_{ik}b_{p(i)p(k)}$. The QAP is the problem to find a permutation vector $p \in P_n$ that minimizes the total assignment cost, where P_n is the set of all possible permutations of N . Such a formulation can be generically described as

$$\text{Minimize } \sum_{p \in P_n} \sum_{i=1}^n \sum_{j=1}^n a_{ij} b_{p(i)p(j)}.$$

Heuristic approaches for the QAP abound in the literature wherein local search is commonly used as a basic component to explore the solution space. Local search methods rely on the exploration of a defined neighborhood. In the case of the QAP, this neighborhood is typically a 2-exchange neighborhood that swaps the location of two facilities at each step of the local search process. The exploration of larger neighborhoods where the simultaneous movement of k nodes of the permutation can be examined is attractive though computationally very demanding.

Ahuja et al. (2007) introduce a very large scale neighborhood search (VLSN) for the QAP, which constitutes an important advance in the creation of more complex neighborhoods for the problem. This algorithm iteratively examines all paths (or exchanges of nodes) of increasing depth, where the maximum depth is a specified parameter. The VLSN algorithm considers all moves (or a defined subset of moves) of a given depth before proceeding to the next depth. Due to the computational complexity of the full path enumeration scheme presented, a maximum path length of 4 was settled upon in their study.

More recently, Rego et al. (2009b) developed a specialized ejection chain algorithm for the QAP, drawing on a proposal sketched in Glover (1991), that affords additional advances. The approach utilizes the ejection chain structure to build successively larger exchanges based upon the elements chosen in the proceeding chain. In this manner, all possible chains at each depth may not be considered for a given permutation. However, this process allows the method to quickly probe larger neighborhoods, with no constraints on the depths examined, by constructing these chains of moves based upon previously promising structures.

The method may be described by analogy with the node-based ejection chain model previously discussed for the VRP. In such a model facilities are associated with nodes in a graph which are to be assigned to locations. In this context the method implements a type of *multi-node exchange move*, which can be seen as a series of swap moves for the QAP. The method begins by identifying the best local move for each facility j , which constitutes removing j from its current location and relocating it in the position occupied by a facility l , which is thereby ejected. (Alternatively, the method can start by looking at each l and finding the best j to replace it.) The initialization process is completed by simply selecting initial chains based on performing a series of best 2-exchange moves. Notably, such a move corresponds to simultaneously determining the best initial node to be ejected and the best node to occupy the location of the ejected node. The chain grows by selecting a new node to be ejected by the previously ejected node. Under the natural and convenient restriction that prevents an element from being moved twice, the chain can continue to grow until all n nodes have been ejected.

By embedding this ejection chain method within a tabu search framework, strategic control over the formation of the chains can be exerted. However, the method is applied without the benefit of advanced memory strategies, except of the simplest form, in the role of “book-keeping” operations instead of in the role of performing advanced guidance. The objective is to show that even this very basic and unenhanced approach is competitive with the best strategies that instead rely extensively on metaheuristic guidance to achieve their results.

Results obtained on a standard set of 22 benchmark problems from the QAPLIB library demonstrate the capabilities of the raw ejection chain procedure and the average improvement obtained by exploring the larger neighborhoods by comparison to a traditional 2-exchange procedure and also by comparison to the leading large neighborhood approaches from the literature. Tests over 10 runs for each procedure embedded in a very simple tabu search show that the ejection chain neighborhood improved the average solution quality for 19 out of the 22 problems over its 2-exchange counterpart. Two multi-start tabu search variants are also presented, which essentially differ in the choice of the solution from which the algorithm is restarted. These enhanced variants improve the simple tabu search variant in all but 2 problem instances each, thus demonstrating the power of embedding the proposed ejection chain method within a more sophisticated local search or metaheuristic approach.

Comparisons established with two variants of the VLSN that provide the best overall solution quality of the large scale methods show that the all variants of the ejection chain algorithms significantly outperform both of these VLSN approaches. Specifically, the average solution quality for VLSN approaches over the 10 runs is 2.7% and 3.3% across all problems for each of the approaches, while the corresponding averages for the three ejection chain methods are respectively 0.73%, 0.42%, and 0.33%. With respect to averages to individual problems, the simple tabu search finds better solutions than both VLSN approaches for 17 out of the 22 problems. Moreover, the best solutions obtained by the two multi-start ejection chain approaches are better than the best solutions found by the VLSN approaches in all cases.

6 Conclusion

Important advances in local search have resulted from the development of larger neighborhoods, organized in structurally exploitable ways that are capable of exploring the solution space more extensively at each iteration. Such neighborhoods allow for a broader examination of the solution landscape and provide a greater potential to find regions of high quality solutions. Advances in this domain have particularly arisen from compound neighborhood structures, which combine simple moves to create more complex neighborhoods that can be explored to variable depths. To take advantage of the potential to find better solutions, however, careful attention must be given to managing the computational overhead involved in generating and searching compound neighborhoods. Accordingly, a number of studies have investigated strategies to combine neighborhoods efficiently, and thereby reduce the computational effort of generating solution trajectories that these neighborhoods make available.

We focus on *ejection chains* and *filter-and-fan* methods, which have become the source of significant advances in the construction of very large neighborhood structures. In addition to presenting the general framework of these methods, we elucidate the key considerations underlying their design and successful implementation. We further identify specific ejection chain and filter-and-fan algorithms that have proved effective in the solution of problems spanning the domains of facility location, routing and distribution, production scheduling, network design, resource allocation, manpower planning, and computational biology. Our purpose is to provide useful insights for developing improved algorithms in a variety of additional settings.

Finally, we briefly comment on issues that are relevant for determining when a filter-and-fan approach may be preferable to an ejection chain approach, and vice versa. Evidently, the merit of applying one method or the other depends on the application, the complexity of the problem and ultimately on the search strategy embodied in the adaptive memory process. As a rule of thumb, in settings where simple neighborhoods have proved relatively effective (at least for relatively small problem instances), methods that rely on these simple neighborhoods can very likely be enhanced by a filter-and-fan approach for more challenging applications. Conversely, in complex applications where classical neighborhoods are rather limited in their ability to explore the solution space, particularly in the case of very large problem instances, a method based on an ejection chain design is likely to prove of greater value than one based on an F&F approach. While ejection chain approaches are characteristically more powerful than filter-and-fan approaches, they are usually more difficult to implement and less flexible for being modified to handle changed problem specifications. Since advanced ejection chain methods typically involve relatively complex reference structures, they are also usually more difficult to adapt to handle new requirements and constraints. In those applications where requirements are likely to change over time, the question of the preferred method to use thus depends on the tradeoff between the value of obtaining the best possible solution and the value of being able to adapt the method to meet new conditions with a modest outlay of effort.

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