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Path relinking for the vertex separator problem

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ABSTRACT

This paper presents the first population-based path relinking algorithm for solving the NP-hard vertex separator problem in graphs. The proposed algorithm employs a dedicated relinking procedure to generate intermediate solutions between an initiating solution and a guiding solution taken from a reference set of elite solutions (population) and uses a fast tabu search procedure to improve some selected intermediate solutions. Special care is taken to ensure the diversity of the reference set. Dedicated data structures based on bucket sorting are employed to ensure a high computational efficiency. The proposed algorithm is assessed on four sets of 365 benchmark instances with up to 20,000 vertices, and shows highly comparative results compared to the state-of-the-art methods in the literature. Specifically, we report improved best solutions (new upper bounds) for 67 instances which can serve as reference values for assessment of other algorithms for the problem.

1. Introduction

Given an undirected graph G (which may be disconnected) with a vertex set $V = \{v_1, \ldots, v_n\}$ where each vertex v_i is associated with an non-negative weight w_i and an unweighted edge set E, the vertex separator problem (VSP) is to partition V into three disjoint subsets A, B and C, where A and B are non-empty, such that the total weight of vertices in C is minimized subject to two constraints: (i) there is no edge between A and B and (ii) the cardinality of A and B does not exceed a given positive integer b. Set C is called the separator of G while A and B are called the shores of the separator. Formally, VSP is formulated as follows.

$$\min \sum_{i\in C} w_i \tag{1}$$

$$\text{subject to}\quad C = V \setminus (A \cup B),\ (A \times B) \cap E = \emptyset, A \cap B = \emptyset \tag{2}$$

$$\max\{|A|, |B|\} \leq b \tag{3}$$

$$A \neq \emptyset, B \neq \emptyset, A, B, C \subset V \tag{4}$$

where constraint (2) ensures that no edge exists for any pair of vertices between shores A and B and constraint (3) requires both A and B contain no more than b vertices. A separator C is considered as balanced if $\max\{|A|, |B|\} \leq 2|V|/3$.

One of the main and first applications of the VSP concerns sparse matrix re-orderings (George & Liu, 1981). Other applications include, for instance, detection of brittle nodes in telecommunication networks (Biha & Meurs, 2011), identification of the minimal separator in the divide-and-conquer based graph algorithms (Evrendilek, 2008; Lipton & Tarjan, 1979) as well as finding protein conformation in bioinformatics (Fu & Chen, 2006). From the point view of computational complexity, the VSP is known to be NP-hard for general graphs (Bui & Jones, 1992) and even for planar graphs (Fukuyama, 2006).

As general solution methods, Leighton (1983) presented an approximation algorithm based on a linear relaxation technique and achieved an approximation ratio of $O(\log n)$. Feige, Hajiaghayi, and Lee (2008) improved this result to $O(\sqrt{\log n})$ by utilizing a semidefinite relaxation method.

There are several exact algorithms, which are able to solve instances with up to a few hundred of vertices. In 2005, de Souza and Balas (2005) designed a branch-and-cut algorithm which explores valid polyhedral inequalities obtained in Balas and de Souza (2005) and conducted extensive computational experiments. In 2011, de Souza and Cavalcante (2011) proposed a hybrid algorithm that combines Lagrangian relaxation with cutting plane techniques. Computational results showed that the hybrid al-

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gorithm outperforms the best exact algorithm available. In 2011, Biha and Meurs (2011) presented an exact approach based on a new class of valid inequalities and performed comparisons with the algorithm in de Souza and Balas (2005).

In addition to the above approximation and exact approaches, heuristic and metaheuristic algorithms have been devised to obtain good quality solutions for large VSP instances in reasonable computing times. We summarize the state-of-the-art heuristic algorithms in the literature as follows.

In 2013, Benlic and Hao (2013) presented the breakout local search (BLS) algorithm which combines a local search procedure with an adaptive perturbation procedure. The local search procedure uses a dedicated move operator to transform the current solution to a neighbor solution. This is achieved by displacing a vertex v from the separator C to the shore subset A or B, followed by displacing all the adjacent vertices of v from the opposite shore subset to the separator C. The perturbation procedure employs an adaptive mechanism to apply either a directed perturbation or a random perturbation to escape local optimum traps and direct the search toward unexplored areas. Experimental results on benchmark instances with up to 3000 vertices demonstrated the effectiveness of the BLS method.

In 2014, Sánchez-Oro, Mladenović, and Duarte (2014) introduced several variable neighborhood search (VNS) algorithms, which alternate between a local search phase and a shaking phase. Two initial solution constructive procedures (random and greedy) are used to generate seeding solutions. The local search phase relies on three types of basic moves and two combined moves to attain a local optimum. A variable neighborhood descent procedure is then used to further improve the encountered solution with the two combined neighborhoods. The shaking phase carries out random perturbations to produce new starting feasible solutions. Experiments on benchmark instances with up to 1000 vertices showed the effectiveness of the VNS algorithms.

In 2015, Hager and Hungerford (2015) proposed a continuous optimization approach. The VSP problem is first formulated as a continuous bilinear quadratic program, which is then solved by a multilevel algorithm. Following the general multilevel graph approach, the proposed algorithm is composed of three phases including 1) a coarsening phase that hierarchically coarsens a graph into a sequence of smaller graphs; 2) a refinement phase that finds an initial solution to the graph in the coarsest level; and 3) an uncoarsening phase that projects the solution of the lower-level graph to its upper level graph. Both hill climbing and Fiduccia–Mattheyses heuristics are used to solve each hierarchy of graphs. Experiments showed that this approach outperforms the general graph partitioning package METIS in terms of solution quality for graphs with 1000 to 5000 vertices, but is outperformed by the BLS method (Benlic & Hao, 2013).

Recently, the population-based path relinking framework (Glover, 1998; Glover & Laguna, 1997) has attracted much attention in combinatorial optimization and intelligent problem solving. The approach has shown outstanding performances in solving a number of challenging decision and optimization problems in various settings, such as unconstrained binary quadratic optimization (Wang, Lü, Glover, & Hao, 2012), flow shop sequencing and scheduling (Costa, Goldbarg, & Goldbarg, 2012; Peng, Lü, & Cheng, 2015; Zeng, Basseur, & Hao, 2013), clustering (Martins de Oliveira, Nogueira Lorena, Chaves, & Mauri, 2014), web services composition (Parejo, Segura, Fernandez, & Ruiz-Cortés, 2014), frequency assignment (Lai & Hao, 2015) and quadratic multiple knapsack (Chen, Hao, & Glover, 2016). PR has also been combined with other metaheuristics such as genetic algorithms (Vallada & Ruiz, 2010), scatter search (González, Oddi, Rasconi, & Varela, 2015) and GRASP (Mestria, Ochi, & Martins, 2013) to solve several difficult combinatorial problems.

In this work, we are interested in advancing the state-of-the-art of solving the VSP with heuristics. For this purpose, we propose the first population-based path relinking algorithm for the VSP (named PR-VSP). We identify the main contributions of this work as follows.

- The proposed PR-VSP algorithm is the first adaptation of the general evolutionary path-relinking framework to the NP-hard vertex separator problem. To ensure its search efficiency, PR-VSP combines a fast solution improvement procedure with a dedicated path relinking method. The solution improvement procedure relies on two complementary neighborhood search operators to visit promising candidate solutions while the relinking method employs a distanced-based strategy to generate new solutions. Additionally, special care is taken to ensure the diversity of the reference set (or population) of elite solutions. Dedicated data structures based on bucket sorting are employed to ensure a high computational efficiency.
- The performance of the proposed algorithm is assessed on four sets of 365 benchmark instances (with up to 20,000 vertices) commonly used in the literature and compared with state-of-the-art VSP algorithms. The computational results show that PR-VSP competes very favorably compared to the current best performing algorithms in terms of solution quality and computing efficiency. Specifically, the proposed algorithm finds new best solutions (updated upper bounds) for 67 instances and matches previous best solutions for all but one instance. The new upper bounds are particularly useful for assessment of other VSP algorithms.

The reminder of the paper is organized as follows. Section 2 presents the general scheme and each component of the proposed PR-VSP. Section 3 is dedicated to experimental results and comparisons with state-of-the-art algorithms in the literature. Concluding remarks are given in Section 4.

2. The proposed path relinking algorithm for VSP

Path relinking is a population-based general framework which was originally proposed for enhancing the tabu search method (Glover, 1998; Glover & Laguna, 1997). Like other general metaheuristics, when applying such a method to a particular problem, it is necessary and indispensable to make a number of specific adaptations to the problem under consideration (Wang & Punnen, 2017; Wang, Wu, & Glover, 2017). In this section, we first expose the main scheme of the proposed algorithm and then explain each specific component.

2.1. Main scheme

Algorithm 1 shows the general scheme of the PR-VSP algorithm. It first creates a reference set *RefSet* consisting of a set of elite (feasible) solutions $\{S_1, S_2, \ldots, S_p\}$ and constructs a set *PairSet* composed of indexes of all pairwise solutions in *RefSet* (See Algorithm 2, Section 2.3). Then, for each pair of solutions (S_i and S_j), a relinking method is utilized to build a solution path (i.e., a sequence of intermediate solutions) that connects the initiating solution where the path starts from (say S_i) and the guiding solution where the path ends (say S_j) (see Section 2.5). By interchanging the initiating and guiding solutions, another path is built in the same way. A solution selection method (see Section 2.6) is then applied to pick one or multiple solutions from the path for further improvement by the iterated tabu search method (see Section 2.4). The improved solution is then used to update *RefSet, PairSet* and the best solution found S^* (see Section 2.3). When *Pairset* becomes empty, the algorithm re-initializes *RefSet* and then