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A three-phase search approach for the quadratic minimum spanning tree problem

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ABSTRACT

Given an undirected graph with costs associated with each edge as well as each pair of edges, the quadratic minimum spanning tree problem (QMSTP) consists of determining a spanning tree of minimum cost. QMSTP is useful to model many real-life network design applications. We propose a three-phase search approach named TPS for solving QMSTP, which organizes the search process into three distinctive phases which are iterated: (1) a descent neighborhood search phase using two move operators to reach a local optimum from a given starting solution, (2) a local optima exploring phase to discover nearby local optima within a given regional area, and (3) a perturbation-based diversification phase to jump out of the current regional search area. TPS also introduces a pre-estimation criterion to significantly improve the efficiency of neighborhood evaluation, and develops a new swap-vertex neighborhood (as well as a swap-vertex based perturbation operator) which prove to be quite powerful for solving a series of special instances with particular structures. Computational experiments based on 7 sets of 659 popular benchmarks show that TPS produces highly competitive results compared to the best performing approaches in the literature. TPS discovers improved best known results (new upper bounds) for 33 open instances and matches the best known results for all the remaining instances. Critical elements and parameters of the TPS algorithm are analyzed to understand its behavior.

1. Introduction

Network design is an extremely challenging task in numerous resource distribution systems (e.g., transportation, electricity, telecommunication, and computer networks). Many of these systems can conveniently be modeled as some variants of the spanning or Steiner tree problem (STP). In this paper, we focus on the *quadratic minimum spanning tree problem* (*QMSTP*) which has broad practical applications. Let $G=(V,E)$ be a connected undirected graph with $|V|=n$ vertices and $|E|=m$ edges. Let $c: E\rightarrow\mathbb{R}$ be a linear cost function for the set of edges and $q: E\times E\rightarrow\mathbb{R}$ be a quadratic cost function to weigh each pair of edges (without loss of generality, assume $q_{ee}=0$ for all $e\in E$). QMSTP requires to determine a spanning tree $T=(V,X)$, so as to minimize its total cost $F(T)$, i.e., the sum of the linear costs plus the quadratic costs. Naturally, as in Cordone and Passeri (2012), this problem can be formulated as follows:

$$\text{Minimize } F(T)=\sum_{e\in E} c_e x_e+\sum_{e\in E}\sum_{f\in E} q_{ef} x_e x_f, \tag{1}$$

$$\text{subject to} \sum_{e\in E} x_e = n-1, \tag{2}$$

$$\sum_{e\in E(S)} x_e \le |S|-1, \quad \forall\ S\subset V \text{ with } |S|\ge 3, \tag{3}$$

$$x_e\in\{0,1\}, \quad \forall\ e\in E, \tag{4}$$

where $x_e=1$ if edge e belongs to the solution, $x_e=0$ otherwise. S is any possible subset of V (with $|S|\ge 3$) and $E(S)$ denotes the set of edges with both end vertices in S. Eq. (2) requires that the final solution contains $n-1$ edges and Eq. (3) ensures that no cycle exists in the solution. These two constraints together guarantee that the obtained solution is necessarily a spanning tree.

As an extension of the classical *minimum spanning tree problem* (*MST*) in graphs, QMSTP has various practical applications in network design problems, where the linear function models the cost to build or use edges, while the quadratic function models interference costs between pairs of edges. For example, in transportation, telecommunication or oil supply networks, the linear

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function represents the costs for building each road, communication link or pipe, and the quadratic function represents the extra costs needed for transferring from one road (link, pipe) to another one. Normally, the interference costs are limited to pairs of adjacent edges (which share a common vertex) (Maia et al., 2013, 2014; Pereira et al., 2013b, 2015), but in some special cases, the interference costs also exist between any pair of edges. As discussed in Assad and Xu (1992), Öncan and Punnen (2010), and Palubeckis et al. (2010), QMSTP has several equivalent formulations such as the stochastic minimum spanning tree problem, the quadratic assignment problem, and the unconstrained binary quadratic optimization problem.

During the last two decades, QMSTP has been extensively investigated and many exact and heuristic approaches have been proposed. Since QMSTP is $\mathcal{NP}$-hard and difficult to approximate (Xu, 1995), exact methods are often applied only to solve very small instances. For larger instances, heuristics are preferred to obtain feasible solutions within a reasonable time.

As for exact methods, Assad and Xu (1992) and Xu (1995) propose a Lagrangian branch-and-bound (B&B) method. Öncan and Punnen (2010) combine the Lagrangian relaxation scheme with an extended formulation of valid inequalities to obtain tighter bounds. Cordone and Passeri (2012) improve the Lagrangian B&B procedure in Assad and Xu (1992). Pereira et al. (2013a) introduce a 0-1 programming formulation based on the reformulation–linearization technique and derive an effective Lagrangian relaxation. Using the resulting strong lower bounds and other formulations, they develop two effective parallel B&B algorithms able to solve optimally problem instances with up to 50 vertices. Recently, based on reduced cost computation, Rostami and Malucelli (2014) combine a reformulation scheme with new mixed 0-1 linear formulations and report lower bounds on hundreds of instances with up to 50 vertices. Exact algorithms are also proposed for solving other closely related QMSTP variants. Buchheim and Klein (2013, 2014) propose a B&B approach for QMSTP with one quadratic term in the objective function, of which the polyhedral descriptions are completed in Fischer and Fischer (2013). Pereira et al. (2013b) introduce several exact approaches (brand-and-cut, branch-and-cut-and-price), to obtain strong lower bounds for QMSTP with adjacency costs, for which the interference costs are limited to adjacent edges.

On the other hand, to handle large QMSTP instances, heuristics become the main approaches to obtain good near-optimal solutions within a reasonable time. For example, two greedy algorithms are proposed in Assad and Xu (1992), Xu (1984), and Xu (1995). Several genetic algorithms are implemented by Zhou and Gen (1998) and tested on instances with up to 50 vertices. Another evolutionary algorithm is proposed for a fuzzy variant of QMSTP (Gao and Lu, 2005), using the Prüfer number to encode a spanning tree. Soak et al. (2005, 2006) report remarkable results with an evolutionary algorithm using an edge-window-decoder strategy. In addition to these early methods, even more heuristics have been proposed in recent years, mostly based on neighborhood search. For example, the Tabu Thresholding algorithm (Öncan and Punnen, 2010) alternatively performs local search and random moves. In Palubeckis et al. (2010), an iterated tabu search (ITS) is proposed and compared to a multi-start simulated annealing algorithm and a hybrid genetic algorithm, showing that ITS performs the best. An artificial bee colony algorithm is developed in Sundar and Singh (2010). Cordone and Passeri (2012) adopt a novel data structure and updating technique to reduce the amortized time of neighborhood exploration from $O(mn^2)$ to $O(mn)$, based on which they further propose a tabu search (TS) algorithm and report a number of improved results over previous best known results. Recently, Lozano et al. (2013) propose an iterated greedy (IG) and a strategic oscillation (SO) heuristic, and combine them with the ITS (Palubeckis et al., 2010) algorithm to obtain a powerful hybrid algorithm named HSII. In addition, for the QMSTP variant only with adjacency costs, Maia et al. develop a Pareto local search (Maia et al., 2013) as well as several evolutionary algorithms (Maia et al., 2014).

In this work, we propose a three-phase search approach named TPS for effectively solving QMSTP, whose main contributions are as follows.

- From the perspective of algorithm design, the proposed TPS approach consists of three distinctive and sequential search phases which are iterated: a descent-based neighborhood search phase (to reach a local optimum from a given starting solution), a local optima exploring phase (to discover more nearby local optima within a given regional area), and a perturbation-based diversification phase (to jump out of the current search area and move to unexplored new areas). At a high abstraction level, TPS shares similar ideas with other popular search frameworks such as iterated local search (Lourenco et al., 2003), reactive tabu search (Bastos and Ribeiro, 2002; Cerulli et al., 2005) and breakout local search (Benlic and Hao, 2013a, 2013b; Fu and Hao, 2014). Still the proposed approach promotes the idea of a clear separation of the search process into three distinctive phases which are iterated, each phase focusing on a well-specified goal with dedicated strategies and mechanisms. The proposed TPS approach also includes two original search strategies designed for QMSTP. The first one is a pre-estimation criterion, which boosts the efficiency of local search by discarding a large number of hopeless neighboring solutions (so as to avoid useless computations). The second one is a new swap-vertex neighborhood, which complements the conventional swap-edge neighborhood and proves to be particularly useful for tackling the challenging and special QMSTP instances transformed from the *Quadratic Assignment Problem* (*QAP*).
- From the perspective of computational results, TPS yields highly competitive results with respect to the best known results and best performing algorithms (tested on 7 sets of 659 benchmarks). Respectively, for the 630 conventional instances, TPS (using the same parameter setting) improves within comparative time the best known results (new upper bounds) on 30 instances and matches easily the best known results for all the remaining instances only except three cases (for which TPS also finds improved best known results within the same cutoff time by simply tuning some parameters). For the set of the 29 instances transformed from QAP which are known to be extremely challenging for existing QMSTP algorithms, TPS consistently attains the known optimal values within very short time.

In the rest of the paper, we describe the proposed approach (Section 2), show extensive computational results on the benchmark instances (Sections 3) and study several key ingredients of the algorithm (Section 4). Conclusions are drawn in Section 5, followed by a parameter analysis in the Appendix.

2. A three-phase search approach for QMSTP

2.1. General framework

The proposed three-phase search approach TPS for QMSTP is outlined in Algorithm 1, which is composed of several subroutines. Starting from an initial solution (generated by *Init_Solution*), the first search phase, ensured by *Descent_Neighborhood_Search*, employs a descent-based neighborhood search procedure to attain