

Lower Bounds for the Quadratic Minimum Spanning Tree Problem Based on Reduced Cost Computation

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Abstract

The Minimum Spanning Tree Problem (MSTP) is one of the most known combinatorial optimization problems. It concerns the determination of a minimum edge-cost subgraph spanning all the vertices of a given connected graph. The Quadratic Minimum Spanning Tree Problem (QMSTP) is a variant of the MSTP whose cost considers also the interaction between every pair of edges of the tree. In this paper we review different strategies found in the literature to compute a lower bound for the QMSTP and develop new bounds based on a reformulation scheme and some new mixed 0-1 linear formulations that result from a reformulationlinearization technique (RLT). The new bounds take advantage of an efficient way to retrieve dual information from the MSTP reduced cost computation. We compare the new bounds with the other bounding procedures in terms of both overall strength and computational effort. Computational experiments indicate that the dual-ascent procedure applied to the new RLT formulation provides the best bounds at the price of increased computational effort, while the bound obtained using the reformulation scheme seems to tradeoff between the bound tightness and computational effort.

Keywords: Quadratic minimum spanning tree problem, Lagrangian relaxation, Reformulation-linearization technique, Lower bound, Dual-ascent approach, Reduced costs.

1. Introduction

Given an undirected graph $G = (V, E)$, with $|V| = n$ and $|E| = m$, a matrix of quadratic costs C with $C_{ef} \geq 0$, $\forall e, f \in E$, and linear costs $d_e \geq 0$, $\forall e \in E$, the quadratic minimum spanning tree problem (QMSTP) consists of finding a spanning tree $T \in G$ with minimum overall cost $\sum_{e,f \in T} C_{ef} + \sum_{e \in T} d_e$.

The QMSTP has been used to model many applications arising in transportation, telecommunication, and energy networks, where linear costs account for the use or construction of edges while the quadratic costs represent the interference between the edges [1, 2]. When the

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interference refers only to pairs of adjacent edges the problem is named adjacent QMSTP (AQMSTP). Both the general QMSTP and the AQMSTP are NP-hard as proved in [1].

Many exact and heuristic algorithms have been proposed for solving both the QMSTP and the AQMSTP. Assad and Xu in [1] proposed a lower bounding procedure and two heuristic approaches. They also described the branch-and-bound algorithm based on a linearized formulation. Öncan and Punnen [3] introduced a Lagrangian relaxation procedure to obtain an improved lower bound and an efficient local search algorithm. Cordone and Passeri [4] have developed two heuristics and an exact approach. Buchheim and Klein [5] proposed complete polyhedral descriptions of the QMSTP with one quadratic term and provide an improved version of the standard linearization by means of cutting planes. Perrira et al. [6] proposed some new formulations using a particular partitioning of the spanning trees, and provided a new mixed binary formulation for the problem by applying the first level of the reformulation-linearization technique. The most effective heuristic approaches for the QMSTP can be found in [2], [7], [8], and [9].

Lower bounds constitute a fundamental component of the branch-and-bound technique, and are a basic tool for the evaluation of the quality of the solutions obtained from heuristic algorithms. There are several branch-and-bound based solution methods proposed in the literature for solving the QMSTP [1, 4, 6]. In practice, the lack of efficiently computable, tight lower bounds for the QMSTP can be key factor in the problems difficulty. In the other hand, the bounding procedure used in branch-and-bound algorithms must tradeoff between tightness and computational efficiency. The first lower bounding procedure for the QMSTP, proposed by Assad and Xu in [1] iteratively applies an adaptation of the Gilmore-Lawler procedure, originally proposed for the Quadratic Assignment Problem [10, 11], to a sequence of equivalent QMSTPs. Öncan and Punnen in [3] introduced an extended formulation based on the addition of two sets of valid inequalities to the linearized formulation of [1]. Their lower bounding approach applies a Lagrangian relaxation where the Gilmore-Lawler procedure is used to solve the resulting Lagrangian subproblem. Pereira et al. [6] proposed a new mixed binary formulation for the problem and developed a Lagrangian relaxation approach to obtain a linear programming based lower bound.

The main contribution of this paper consists in obtaining lower bounds for the QMSTP using dual information retrieved from the MSTP reduced costs. In order to find a common framework for description of the individual bounds we review and analyze different bounding procedures proposed in the literature and compare them in terms of continuous relaxation of an Mixed Integer Linear Programming problem (MILP). We describe new bounds for the problem by considering a reformulation of the problem based on dual information retrieved from the continuous relaxation of the MILP. The basic idea is to solve the continuous relaxation of the given MILP, and use the reduced costs as the objective coefficients of the reformulated problem. Moreover, for generating superior bounds, we develop a mixed 0-1 linear formulation based on the second level of the reformulation-linearization technique and show how to handle it via a Lagrangian relaxation approach to obtain a Lagrangian function with block-diagonal structure. Since the dualized constraints are indeed much more than those in the level-1 RLT [6], finding the near-optimal dual multipliers using the classical subgradient is not viable. Therefore, using the dual information retrieved from the MSTP

reduced cost, we devise an efficient dual-ascent procedure to solve the continuous relaxation of the level-2 RLT.

The paper is organized as follows: In Section 2 we review existing lower bounds for QMSTP. In Section 3 we develop a bounding procedure based on a new reformulation scheme. In Section 4 we provide a brief discussion on the level-1 and 2 forms of QMSTP and describe our dual-ascent implementation of the level-2 RLT lower bound calculation. In Section 5 we present computational experiments conducted on different benchmarks from the literature and compare the tightness and speed of computation of the new bounding techniques with those of literature.

2. Problem formulation and lower bounds review

In order to present the mathematical formulation of the QMSTP, let us first introduce some notation used in the sequel. We denote by $E(S)$ the set of all edges with both endpoints in S for any $S \subset V$, and $\delta(i)$ as the set of all edges incident in node i . We define the binary variable x_e to indicate the presence of edge $e \in E$ in the optimal spanning tree. The QMSTP has the following Integer formulation:

$$\begin{aligned} \text{QMSTP: } \min \quad & \sum_{\substack{e,f \in E \\ e \neq f}} C_{ef} x_e x_f + \sum_{e \in E} d_e x_e \\ \text{s.t. } \quad & \sum_{e \in E} x_e = n - 1 & (1) \\ & \sum_{e \in E(S)} x_e \leq |S| - 1 & \forall \emptyset \neq S \subset V & (2) \\ & x_e \text{ integer} & \forall e \in E. & (3) \end{aligned}$$

where the objective function considers the linear cost of the selected edges and also the interaction costs between pairs of edges. Constraints (2) are the subtour elimination constraints and ensure that no subgraph induced by the nonempty subset $S \subset V$ contains a cycle. These subtour elimination constraints together with the cardinality constraint (1) guarantee the connectivity of the induced subgraph. Constraints (1) to (3) define the set of spanning trees in G and thereafter is denoted by X , i.e.,

$$X = \{x \geq 0 : (1), (2), (3)\}.$$

2.1. Gilmore-Lawler type bound

The Gilmore-Lawler procedure, shortly denoted by GL, is one of the most popular approach to find a lower bound for the Quadratic Assignment Problem(QAP). The GL procedure was proposed by Gilmore [10] and Lawler [11] in the context of QAP and can be adapted to many other quadratic 0 – 1 problems [12, 13]. The popularity of this approach for computing lower bounds of the linearly constrained quadratic 0 – 1 problems stems from the fact that it is computationally inexpensive.

For each edge e , potentially in the solution, we consider the best cumulation providing the minimum interaction cost with e . Let P_e be such a subproblem for a given edge $e \in E$:

$$P_e : \quad z_e = \min \left\{ \sum_{\substack{f \in E \\ f \neq e}} C_{ef} x_f : x \in X, x_e = 1 \right\} \quad \forall e \in E. \quad (4)$$

The value z_e is the best quadratic contribution to the QMSTP objective function where edge e is in the solution. Once z_e has been computed for each $e \in E$, the GL type bound is given by the solution of the following MSTP:

$$LB_{GL} = \min \left\{ \sum_{e \in E} (z_e + d_e) x_e : x \in X \right\}. \quad (5)$$

Although the GL bound that we just described is a pure combinatorial bound of the QMSTP, it can also be obtained in the terms of a linear programming. More precisely, consider the following MILP formulation where the decision variables y_{ef} equal to 1 if and only if both edges e and f are present in the solution of the problem:

$$\begin{aligned} \text{P:} \quad & \min \quad \sum_{\substack{e, f \in E \\ e \neq f}} C_{ef} y_{ef} + \sum_{e \in E} d_e x_e \\ & \text{s.t.} \quad \sum_{f \in E} y_{ef} = (n-1)x_e \quad \forall e \in E \end{aligned} \quad (6)$$

$$\sum_{f \in E(S)} y_{ef} \leq (|S| - 1)x_e \quad \forall \emptyset \neq S \subset V, e \in E \quad (7)$$

$$y_{ee} = x_e \quad \forall e \in E \quad (8)$$

$$y_{ef} \geq 0 \quad \forall e, f \in E \quad (9)$$

$$x \in X.$$

Constraints (6) guarantee that whenever an edge $e \in E$ is selected, the total number of selected edges interacting with e must be equal to $(n-1)$, including e itself. Overall, constraints (6) to (9) enforce $y_{e_1e}, \dots, y_{e_me}$ to be a spanning tree containing e , in case $x_e = 1$, or to be the null vector, in case $x_e = 0$.

Let us consider now the lower bound computations taking advantage of the MILP formulation introduced above. Consider the continuous relaxation of problem P (CP) by replacing the boolean constraints on variable x by nonnegativity constraint. The problem CP is computationally interesting since, its optimal objective value gives the GL bound as stated in the following theorem.

Theorem 1. *The continuous relaxation of problem P gives the GL bound.*

Proof. Let λ , μ_S , α_e , and γ_{Se} denote the dual variables corresponding to constraints (1), (2), (6), and (7), respectively. Consider the dual of CP

$$\begin{aligned} \text{DCP: } \max \quad & -\lambda(n-1) - \sum_{S \subset V} \mu_S(|S|-1) \\ \text{s.t.} \quad & -\lambda - \sum_{\substack{S \subset V: \\ e \in E(S)}} \mu_S + (n-1)\alpha_e + \sum_{S \subset V} (|S|-1)\gamma_{Se} \leq d_e \quad \forall e \in E \quad (10) \end{aligned}$$

$$-\alpha_e - \sum_{\substack{S \subset V: \\ f \in E(S)}} \gamma_{Se} \leq C_{ef} \quad \forall e, f \in E \quad (11)$$

$$\begin{aligned} \gamma_{Se} &\geq 0 & \forall S \subset V, e \in E \quad (12) \\ \mu_S &\geq 0 & \forall S \subset V. \end{aligned}$$

Considering constraints (10), one can maximize the objective function by solving the following m independent subproblems; one for each $e \in E$:

$$\text{Sub}_e : \quad \bar{z}_e = \max \left\{ -(n-1)\alpha_e - \sum_{S \subset V} (|S|-1)\gamma_{Se} : (11), (12) \right\}. \quad (13)$$

For each $e \in E$, subproblem Sub_e is precisely the dual of the subproblem (4) used in the GL bound. Thus $\bar{z}_e = z_e$, and DCP can be rewritten as follows:

$$\begin{aligned} \text{DCP} \quad \max \quad & -\lambda(n-1) - \sum_{S \subset V} \mu_S(|S|-1) \\ \text{s.t.} \quad & -\lambda - \sum_{\substack{S \subset V: \\ e \in E(S)}} \mu_S \leq d_e + z_e \quad \forall e \in E \\ & \mu_S \geq 0 \quad \forall S \subset V. \end{aligned}$$

which is exactly the dual of the final MSTP (5) of the GL bound. \square

Theorem 1 shows that the optimal solution of problem CP can be computed by solving m MSTP containing a fixed edge e , and a single MSTP. Although the LB_{GL} provides a lower bound for the QMSTP that can be computed very efficiently, as in the QAP case, the obtained bounds are not so close to the optimal solution values even for small size instances.

2.2. Assad and Xu bound

In order to improve the GL bound for the QMSTP, Assad and Xu in [1] proposed a method that generates a monotonic sequence of lower bounds. Their method relies on an equivalent reformulation of the QMSTP with coefficients C'_{ef} and d'_e where:

$$d'_e = d_e - (n-2)\theta_e \quad \forall e \in E, \quad \text{and} \quad C'_{ef} = C_{ef} + \theta_f \quad \forall e, f \in E. \quad (14)$$

The authors proved that, for any value of vector θ , transformation (14) defines an equivalent QMSTP, i.e., for each $x \in X$:

$$\sum_{\substack{e,f \in E \\ e \neq f}} C'_{ef} x_e x_f + \sum_{e \in E} d'_e x_e = \sum_{\substack{e,f \in E \\ e \neq f}} C_{ef} x_e x_f + \sum_{e \in E} d_e x_e.$$

Although the optimum of the QMSTP is independent of vector θ , the approximated linear cost d'_e depends on θ . Therefore, a better choice of θ yields a tighter bound.

For a given θ , Assad and Xu apply the GL procedure to compute the following lower bound:

$$LB_{AX}(\theta) = \min \left\{ \sum_{e \in E} (z_e(\theta) + c'_e) x_e : x \in X \right\},$$

where

$$z_e(\theta) = \min \left\{ \sum_{\substack{f \in E \\ f \neq e}} C'_{ef} x_f : x_e = 1 \text{ and } x \in X \right\} \quad \forall e \in E.$$

Observe that $LB_{AX}(\theta)$ is a piecewise concave linear function, and for $\theta = 0$ it gives the GL bound. To find the best value of parameter θ the authors provide a leveling procedure to find an ε -optimal solution. More precisely, by updating $\theta_e^{i+1} = \theta_e^i + \frac{1}{n-1} z_e(\theta^i)$ at each iteration i , the $LB_{AX}(\theta)$ is iteratively improved until the stopping criterion $\max_e \{z_e(\theta^i)\} - \min_e \{z_e(\theta^i)\} < \varepsilon/(n-1)$ is satisfied.

We now turn to problem CP and review the AX bound in the context of linear programming. To this end, consider problem P and add the following set of constraints to the formulation

$$\sum_{e \in E} y_{ef} = (n-1)x_f \quad \forall f \in E \tag{15}$$

denoting the resulting formulation as QAX. Assad and Xu showed that QAX and QMSTP are equivalent. The following theorem shows the relationship between the AX bounds and the continuous relaxation of QAX.

Theorem 2. *The continuous relaxation of problem QAX gives the AX bound.*

Proof. The relaxation of (15) in QAX formulation using Lagrangian multipliers θ yields the Lagrangian dual:

$$LD : \quad \max_{\theta \in R^m} L(\theta)$$

where

$$LR(\theta) : \quad L(\theta) = \min \left\{ \sum_{\substack{e,f \in E \\ e \neq f}} (C_{ef} + \theta_f) y_{ef} + \sum_{e \in E} (d_e - (n-2)\theta_e) x_e : x \in X, (6) - (9) \right\}.$$

Since $LR(\theta)$ satisfies the integrality property, the optimal solution value of problem LD is equal to the optimal solution value of the continuous relaxation of problem QAX. On the other hand, according to Theorem 1, the value of $L(\theta)$ is equal to the GL bound of problem $LR(\theta)$. This completes the proof. \square

2.3. Öncan and Punnen bound

In [3] the authors proposed an extended formulation for the QMSTP based on the addition of the following two sets of valid inequalities to QAX:

$$\sum_{e \in \delta(i)} y_{ef} \geq x_f \quad \forall i \in V, f \in E \quad (16)$$

$$\sum_{f \in \delta(i)} y_{ef} \geq x_e \quad \forall i \in V, e \in E \quad (17)$$

The formulation is presented below as problem QOP:

$$\text{QOP: } \min \left\{ \sum_{\substack{e, f \in E \\ e \neq f}} C_{ef} y_{ef} + \sum_{e \in E} d_e x_e : x \in X, (6) - (9), (16), (17) \right\}.$$

Consider now the Lagrangian relaxation of (16) with multipliers λ_{if} . The Lagrangian function has the following form:

$$L(\lambda) = \min \left\{ \sum_{e, f \in E} C''_{ef} y_{ef} + \sum_{e \in E} d''_e x_e : x \in X, (6) - (9), (17) \right\}$$

where

$$C''_{ef} = C_{ef} - \sum_{\substack{i \in V: \\ e \in \delta(i)}} \lambda_{if} \quad \forall e, f \in E, e \neq f \quad (18)$$

$$d''_e = d_e + \sum_{i \in V} \lambda_{ie} \quad \forall e \in E. \quad (19)$$

To compute the Lagrangian function for a given λ , the authors use the decomposition approach presented in Theorem 1. In so doing, they first sequentially fix one edge at a time and find the minimum spanning tree containing it, then they solve a MSTP with the optimal objective values of the subproblems as edge weights.

It should be noted that the actual formula used in [3] for computing coefficients C'' is

$$C''_{ef} = C_{ef} - \lambda_{if} \quad \forall e, f \in E, i \in V.$$

which is not correct. However, the general form of the Lagrangian function and consequently the decomposition procedure is still correct. Our computational experiments (see section 5) show that in spite of the correct decomposition structure with easily solvable subproblems, the produced bounds are not significantly stronger than the AX bounds and in some benchmark instances are even worse.

3. Bounds based on a new reformulation

In order to develop a new bound for the QMSTP, we consider a modified problem based on dual information retrieved from the solution of the CP. The basic idea is to solve CP, and then use the reduced costs as the coefficients of a reformulation adapting the approach proposed in [14, 15] for the QAP. To this end, we introduce the following problem transformation:

$$\begin{cases} \tilde{C}_{ef} = C_{ef} + \alpha_e + \sum_{\substack{S \subset V: \\ f \in E(S)}} \gamma_{Se} + \delta_{ef} + \theta_f & \forall e, f \in E \\ \tilde{d}_e = d_e - (n-1)\alpha_e - \sum_{S \subset V} (|S|-1)\gamma_{Se} - (n-2)\theta_e & \forall e \in E. \end{cases} \quad (20)$$

where $\alpha_e, e \in E$, $\theta_f, f \in E$, δ_{ef} , for $e, f \in E$, are vectors of real parameters, and γ_{Se} , for $e \in E, S \subset V$ is a vector of nonnegative real parameters. This transformation, in general, does not provide a reformulation of the QMSTP for any value of parameters α, θ, δ , and γ , but for some particular values it guarantees the definition of an equivalent QMSTP. In the following we present the general framework of our reformulation scheme.

3.1. Reformulation framework

For any given value of θ^0 , we initialize the reformulation process by setting $\alpha = \gamma = \delta = 0$, and $\theta = \theta^0$. Noting that this parameter setting guarantees that the transformation (20) provides a reformulation for the QMSTP as proved in [1]. Next, we apply the GL procedure to obtain a the lower bound. More precisely, we sequentially consider the following m subproblems $SP(e)$, $e \in E$:

$$\begin{aligned} SP(e) : \quad z(e) = \min \sum_{f \in E} \tilde{C}_{ef} y_{ef} \\ \text{s.t.} \quad \sum_{f \in E} y_{ef} = (n-1) \end{aligned} \quad (21)$$

$$\begin{aligned} \sum_{f \in E(S)} y_{ef} &\leq |S| - 1 & \forall \emptyset \neq S \subset V & \quad (22) \\ y_{ef} &\geq 0 & \forall f \in E & \\ y_{ee} &= 1. & & \end{aligned}$$

The solution of the following minimum spanning tree problem gives the GL bound for the transformed problem:

$$W' = \left\{ \sum_e \tilde{d}_e x_e : x \in X \right\}.$$

Upon solving $SP(e)$, for all $e \in E$, we retrieve the dual solutions α'_e and γ'_{Se} corresponding to constraints (21) and (22), respectively, and modify parameters α , and γ as

$$\begin{aligned} \alpha_e &= \alpha'_e \quad \forall e \in E, \\ \gamma_{Se} &= \gamma'_{Se} \quad \forall e \in E, S \subset V. \end{aligned}$$

Moreover, we define δ_{ef} for all $e, f \in \text{ord}(E)$, and set $\delta_{fe} = -\delta_{ef}$ for all $e, f \in \text{ord}(E)$, where $\text{ord}(E) = \{e = (i, j), f = (k, l) \in E : i < k \text{ or } i = k, j < l\}$.

With the parameter setting just described we have the following:

Theorem 3. *For any value of θ and any value of δ with $\delta_{fe} = -\delta_{ef}$, $\forall e, f \in \text{ord}(E)$, if $\alpha_e = \alpha'_e$, $e \in E$ and $\gamma_{Se} = \gamma'_{Se}$, $e \in E, S \subset V$, the transformation (20) provides a reformulation of the QMSTP.*

Proof. Consider problem QAX with the following extra constraints:

$$y_{ef} = y_{fe} \quad \forall e, f \in \text{ord}(E), \quad (23)$$

Associate Lagrangian multipliers α_e , θ_f , and δ_{ef} with constraints (6), (15), and (23), respectively, and nonnegative Lagrange multipliers γ_{Se} with constraints (7). The Lagrangian function can be computed by solving the following MILP:

MP($\alpha, \theta, \delta, \gamma$):

$$\begin{aligned} \min \quad & \sum_{\substack{e, f \in E \\ e \neq f}} C_{ef} y_{ef} + \sum_{e \in E} d_e x_e + \sum_{\substack{e, f \in E \\ e \neq f}} \delta_{ef} y_{ef} + \sum_{f \in E} \theta_f \left[\sum_{\substack{e \in E \\ e \neq f}} y_{ef} - (n-2)x_f \right] \\ & + \sum_{e \in E} \alpha_e \left[\sum_{\substack{f \in E \\ f \neq e}} y_{ef} - (n-2)x_e \right] + \sum_{e \in E} \sum_{\emptyset \subset S \subset V} \gamma_{Se} \left[\sum_{f \in E(S)} y_{ef} - (|S|-1)x_e \right] \\ \text{s.t.} \quad & (6) - (9) \\ & x \in X. \end{aligned}$$

For any feasible solution (x, y) and any value of the multipliers α_e , and θ_f , the terms $\sum_f \theta_f [\sum_{e \in E} y_{ef} - (n-2)x_f]$ and $\sum_e \alpha_e [\sum_{f \in E} y_{ef} - (n-2)x_e]$ are all zero. Moreover, for each $e \in E$ and $S \subset V$ complementary slackness properties imply $\sum_{e \in E} \sum_{\emptyset \subset S \subset V} \gamma_{Se} [\sum_{f \in E(S)} y_{ef} - (|S|-1)x_e] = 0$. Therefore, the objective function of MP($\alpha, \theta, \delta, \gamma$) reduces to

$$\begin{aligned} \min \quad & \sum_{\substack{e, f \in E \\ e \neq f}} (C_{ef} + \delta_{ef}) y_{ef} + \sum_{e \in E} d_e x_e = \\ \min \quad & \sum_{e, f \in \text{ord}(E)} (C_{ef} + \delta_{ef}) y_{ef} + \sum_{e, f \notin \text{ord}(E)} (C_{fe} - \delta_{ef}) y_{fe} + \sum_{e \in E} d_e x_e. \end{aligned} \quad (24)$$

Since the optimum of (24) achieved if $y_{ef} = y_{fe}$, it is simplified as

$$\min \quad \sum_{e, f \in \text{ord}(E)} (C_{ef}) y_{ef} + \sum_{e, f \notin \text{ord}(E)} (C_{fe}) y_{fe} + \sum_{e \in E} d_e x_e.$$

and proof is completed. \square

Let us make some observations concerning the way we can choose the multipliers in (20).

Observation 1. The $MP(\alpha, \theta, \delta, \gamma)$ formulation contains an exponential number of constraints with respect to the number of nodes. Therefore, explicitly keeping track of the dual values for (22) is not practical. However, for any given value of θ and δ , transformation (20) can be interpreted by considering the meaning of reduced costs in (11), and the optimal value of subproblem $SP(e)$. More precisely, we can simplify the transformation (20) as

$$\begin{cases} \tilde{C}_{ef} = r\tilde{C}_{ef} + \delta_{ef} + \theta_f & \forall e, f \in E \\ \tilde{d}_e = d_e + z(e) - (n-2)\theta_e & \forall e \in E. \end{cases} \quad (25)$$

where $r\tilde{C}_{ef}$ is the reduced cost of edge f with respect to the optimal spanning tree containing the fixed edge e . In this case, the reduced cost $r\tilde{C}_{ef}$ can be computed without using the dual variables α and γ . More specifically, the reduced cost $r\tilde{C}_{ef}$ of any edge f not in the minimum spanning tree containing the fixed edge e is the difference between the cost of f and the largest cost of any edge, different from e , in the cycle induced by f . Note that the reduced costs computed this way are obviously non negative.

Observation 2. In order to develop a procedure to find the optimal dual multipliers δ , we can split the costs between symmetrical entries of \tilde{C} so as to maximize the value of W' . Using this idea, it is not necessary to explicitly find the value of the multipliers δ_{ef} in each iteration of the dual ascent algorithm. In fact one can adjust the coefficient \tilde{C}_{ef} on variables y_{ef} every time multiples of (23) are placed into the objective function. More precisely, for any $e, f \in \text{ord}(E)$, we can increase \tilde{C}_{ef} by the same quantity we decrease \tilde{C}_{fe} .

Observation 3. By stopping the procedure at the first iteration, with $\theta = 0$, the value of W' gives the GL bound. To obtain tighter lower bounds we can maximize the function W' to obtain the best value of θ for example through subgradient techniques. However, we follow the idea of Assad and Xu to update the parameter θ . More precisely, we propose the following two update rules:

$$\theta_e^{i+1} = \frac{1}{(n-2)^{1/2}}\theta_e^i + \frac{1}{(n-2)^{3/2}}(\tilde{d}_e + r\tilde{d}_e) \quad \forall e \in E \quad (26)$$

$$\theta_e^{i+1} = \frac{1}{n-2}\tilde{d}_e \quad \forall e \in E. \quad (27)$$

where $r\tilde{d}_e$ for all $e \in E$ is the reduced cost of edge e with respect to the optimal spanning tree. The first choice of updating θ does not guarantee a monotonically increasing sequence of lower bounds, while for the second choice our computational experiments show that it yields a monotonic sequence of lower bounds.

4. Reformulation-linearization technique applied to the QMSTP

The Reformulation-linearization technique (RLT), that was introduced in [16, 17] for general zero-one polynomial programs, transforms the problem into a mixed 0-1 linear program via two basic steps of *reformulation* and *linearization*. In the reformulation step, the

constraints are multiplied by the binary variables and their complements to construct redundant nonlinear constraints while in the linearization step, the objective and constraints of the reformulated problem are linearized by substituting a continuous variable for each distinct nonlinear term. Depending on how many times this process is applied, different levels of RLT can be obtained. In this section we concern ourselves with the level-1 and level-2 of the RLT representations of the QMSTP.

4.1. Level-1 RLT for- the QMSTP

The level-1 RLT representation of the QMSTP proposed by Perrira et al. [6] applies two sets of operations. First, each constraint defining X is multiplied by each of the m variables x_e . All such quadratic constraints are included in the formulation. Note that when a variable x_e in a given constraint is multiplied by x_f the resulting product is expressed as $x_e x_f$ in that order. The linearization step makes the substitution of $y_{ef} = x_e x_f$ for all $e, f \in E$, and imposes the restrictions $y_{ef} = y_{fe}$ for all $e, f \in \text{ord}(E)$, to rewrite the problem as the MILP below:

$$\begin{aligned} \text{QRLT1: } \quad & \min \quad \sum_{\substack{e, f \in E \\ e \neq f}} C_{ef} y_{ef} + \sum_{e \in E} d_e x_e \\ & \text{s.t.} \quad (6), (7), (8), (9), (23) \\ & \quad x \in X. \end{aligned}$$

Observe that QRLT1 is exactly the same as problem P with the addition of constraints (23). However, the continuous relaxation of QRLT1 (CRLT1) provides a lower bound at least as large as the continuous relaxations of QAX (CAX) and QOP (COP) as proved in [6]. In fact the authors showed that the feasible region to CRLT1 (P_{RLT1}) is contained within the feasible region to CAX (P_{AX}) and COP (P_{OP}), i.e,

$$P_{AX} \supseteq P_{OP} \supseteq P_{RLT1}. \quad (28)$$

A natural question concerning the relation in (28) is whether these inclusions are strict or not. In the following we show that $P_{OP} \supset P_{RLT1}$. To show the tight inclusion, consider a graph $G = (V, E)$ with $V = \{a, b, c, d\}$ and $E = \{e_1, e_2, e_3, e_4\}$ where $e_1 = \{a, b\}$, $e_2 = \{b, c\}$, $e_3 = \{b, d\}$, and $e_4 = \{c, d\}$. Suppose that the linear cost d_i for any $e_i \in E$ is equal to zero, and the quadratic costs C_{ij} of edges $e_i, e_j \in E$ is also equal to zero except for (e_1, e_2) and (e_4, e_1) which $C_{12} = C_{41} = 1$. Consider the point (\bar{x}, \bar{y}) with $\bar{x}_1 = 1, \bar{x}_2 = \bar{x}_3 = \bar{x}_4 = \frac{2}{3}$, $\bar{y}_{13} = \bar{y}_{14} = \bar{y}_{21} = \bar{y}_{31} = \bar{y}_{42} = 1, \bar{y}_{24} = \bar{y}_{32} = \bar{y}_{43} = \frac{1}{3}$ and all other $\bar{y}_{ij} = 0$ with $i \neq j$. This point is a feasible and optimal solution with objective value 0 for problem COP, but it is not feasible for CRLT1, as $1 = \bar{y}_{21} \neq \bar{y}_{12} = 0$. For the given objective function coefficients, the point (\hat{x}, \hat{y}) with $\hat{x}_1 = \hat{x}_3 = \hat{x}_4 = 1, \hat{x}_2 = 0, \hat{y}_{13} = \hat{y}_{14} = \hat{y}_{31} = \hat{y}_{34} = \hat{y}_{41} = \hat{y}_{43} = 1$ and $\hat{y}_{ij} = 0$ for all other $i \neq j$, with objective value of 1 is in fact the optimal solution for problem CRLT1. Thus we have the following:

Proposition 4.

$$P_{AX} \supseteq P_{OP} \supset P_{RLT1}.$$

In order to solve the CRLT1, the authors proposed constructing a Lagrangian dual by placing constraints (23) into the objective function and applied the GL procedure to solve the lagrangian function. They used subgradient method to compute an optimal (or near-optimal) set of Lagrangian multipliers.

4.2. Level-2 RLT for the QMSTP

Based on the success of level-1 RLT representation to gain tighter bounds for the QMSTP and also due to the block-diagonal structure of the problem which lends to efficient solution methods, we turn attention to the level-2 representation of the problem. We first present the level-2 RLT formulation of the problem and then show how to handle it via a Lagrangian relaxation approach to obtain a Lagrangian function with block-diagonal structure. Since the dualized constraints are indeed much more than those in the level-1 RLT, finding the near-optimal dual multipliers using the classical subgradient is not viable. Therefore, using the dual information retrieved from the MSTP reduced cost computation, we devise an efficient dual-ascent procedure to solve the continuous relaxation of the level-2 RLT.

The level-2 RLT representation of QMSTP can be obtained in the same way as the level-1 RLT via the following reformulation and linearization steps.

Reformulation: Multiply each constraints defining X by each binary variable x_e , $e \in E$, and also by each pair-wise product of variables $x_e x_f$, $e, f \in E$. Add these new restrictions to the problem formulation. When a variable x_e is multiplied by x_f , the resulting product is expressed as $x_e x_f$, and when it is multiplied by $x_f x_h$, the resulting product is expressed as $x_e x_f x_h$, preserving the order in both cases.

Linearization: Linearize the resulting problem by substituting, $x_e x_f$ and $x_e x_f x_h$ with continuous variables y_{ef} and u_{efh} , respectively. Enforce the equality $y_{ef} = y_{fe}$ for all $e, f \in E$, and also enforce the equalities $u_{efh} = u_{ehf} = u_{fhe} = u_{fhe} = u_{hef} = u_{hfe}$ for all $e, f, h \in E$. For convenience we set $u_{eeef} = u_{eefe} = u_{feee} = y_{fe}$ for all $e, f \in E$ and $y_{ee} = x_e$ for all $e \in E$.

The resulting formulation is presented below as problem QRLT2 where the coefficients

D_{efh} found in the objective function are all zero.

$$\begin{aligned}
\text{QRLT2: } \min \quad & \sum_{e,f,h \in E} D_{efh} u_{efh} + \sum_{\substack{e,f \in E \\ e \neq f}} C_{ef} y_{ef} + \sum_{e \in E} d_e x_e \\
& \sum_{f \in E} u_{ehf} = (n-1) y_{ef} \quad \forall e, h \in E \quad (29) \\
& \sum_{f \in E(S)} u_{ehf} \leq (|S| - 1) y_{ef} \quad \forall \emptyset \neq S \subset V, e, h \in E \quad (30) \\
& u_{eeh} = u_{eh e} = u_{hee} = y_{he} \quad \forall e, h \in E \quad (31) \\
& u_{efh} = u_{ehf} = u_{feh} = u_{fhe} = u_{hef} = u_{hfe} \quad \forall e, f, h \in E \quad (32) \\
& u_{efh} \geq 0 \quad \forall e, f, h \in E \quad (33) \\
& (6), (7), (8), (9), (23) \quad (34) \\
& x \in X.
\end{aligned}$$

Note that an optimal solution of the QRLT2 will yield an optimal solution also for the QMSTP problem. However, if the binary restrictions on variables x are relaxed in QRLT2, the problem is no longer equivalent to QMSTP, providing a lower bound.

4.2.1. Lagrangian Relaxation Scheme of QRLT2

In order to solve the continuous relaxation of QRLT2 efficiently, we apply a Lagrangian relaxation to constraints (23) and (32). Let \bar{D}_{efh} , \bar{C}_{ef} and \bar{d}_e denote the adjusted values for D_{efh} , C_{ef} and d_e respectively, after placing constraints (23) and (32) into the objective function. The resulting Lagrangian relaxation is:

$$K + \min \left\{ \sum_{e,f,h \in E} \bar{D}_{efh} u_{efh} + \sum_{\substack{e,f \in E \\ e \neq f}} \bar{C}_{ef} y_{ef} + \sum_{e \in E} \bar{d}_e x_e : x \in X, (29), (30), (31), (33), (34) \right\}, \quad (35)$$

where K is a scalar equal to 0.

To solve the Lagrangian function (35) we introduce the following subproblems. For any two edges $e, f \in E, e \neq f$, let φ_{ef} denote the cost of the optimal spanning tree containing the two fixed edges e, f , and for any edge $e \in E$, let ρ_e denotes the optimal spanning tree containing the fixed edge e ; i.e.,

$$\varphi_{ef} = \min \left\{ \sum_h \bar{D}_{efh} u_{efh} : \mathbf{u}_{ef} \in X, u_{efe} = 1, u_{eff} = 1 \right\}, \quad (36)$$

$$\rho_e = \min \left\{ \sum_f (\bar{C}_{ef} + \varphi_{ef}) y_{ef} : \mathbf{y}_e \in X, y_{ee} = 1 \right\}. \quad (37)$$

The following theorem formally shows the decomposition framework of (35).

Theorem 5. *An optimal solution of problem (35) can be obtained by solving the following minimum spanning tree problem*

$$K + \min \left\{ \sum_e (\bar{d}_e + \rho_e) x_e : x \in X \right\}. \quad (38)$$

Proof. The proof is a trivial extension of the proof of Theorem 1. \square

In the following we present a dual-ascent algorithm similar to that used in [18] for the RLT2 representation of the QAP. The most important part of the algorithm is to use the meaning of reduced costs to readjusting \bar{D} , \bar{C} and \bar{d} . The main steps of our dual-ascent algorithm are summarized as follows:

1. Initialization.
Set $\bar{D}_{efh} = 0$ for all $e, f, h \in E$, $\bar{C}_{ef} = C_{ef}$ for all $e, f \in E$, $\bar{d}_e = d_e$ for all $e \in E$, $K = 0$, and an iteration counter $I = 0$.
2. Spreading \bar{d} on \bar{C} .
For each $e \in E$, spread the coefficient \bar{d}_e on coefficients \bar{C}_{ef} for all $f \in E, f \neq e$; i.e., $\bar{C}_{ef} = \bar{C}_{ef} + \frac{\bar{d}_e}{n-2}$. Then update \bar{d}_e to 0 for each $e \in E$.
3. Spreading \bar{C} on \bar{D} .
For each $e, f \in E, e \neq f$, spread the coefficient \bar{C}_{ef} on coefficients \bar{D}_{efh} for all $h \in E, h \neq e, f$; i.e., $\bar{D}_{efh} = \bar{D}_{efh} + \frac{\bar{C}_{ef}}{n-3}$. Then update \bar{C}_{ef} to 0 for each $e, f \in E, e \neq f$.
4. Solving the Lagrangian relaxation problem.
Use Theorem 5 to solve (35) as follows:
 - 4 – a) For a selected $e, f \in E, e \neq f$, change coefficients $\bar{D}_{efh} = (\bar{D}_{efh} + \bar{D}_{ehf} + \bar{D}_{feh} + \bar{D}_{fhe} + \bar{D}_{hef} + \bar{D}_{hfe})/6$ for each $h \in E, h \neq e, f$. Solve subproblem (36) and compute the reduced cost of edge h with respect to the optimal spanning tree containing the fixed edges e, f . The reduced cost $\bar{r}\bar{D}_{efh}$ of any edge h not in the minimum spanning tree containing the fixed edges e, f , is the difference between the cost of h and the largest cost of any edge, different from edges e, f , in the cycle induced by h . Note that if the cycle contains only h and the two fixed edges e, f , then the reduced cost of h set to infinity. Set $\bar{D}_{efh} = \bar{r}\bar{D}_{efh}$ and increase \bar{C}_{ef} by φ_{ef} .
 - 4 – b) For a selected $e \in E$, change the coefficients $\bar{C}_{ef} = (\bar{C}_{ef} + \bar{C}_{fe})/2$ for each $f \in E, f \neq e$. Solve subproblem (37) and compute the reduced cost of edge f with respect to the optimal spanning tree containing the fixed edges e . The reduced cost $\bar{r}\bar{C}_{ef}$ of any edge f not in the minimum spanning tree containing the fixed edge e , is the difference between the cost of f and the largest cost of any edge, different from edges e , in the cycle induced by f . Set $\bar{C}_{ef} = \bar{r}\bar{C}_{ef}$ and increase \bar{d}_e by ρ_e .
 - 4 – c) Solve problem (38) and compute the reduced cost of edge e with respect to the optimal spanning tree, readjusting \bar{d}_e and increasing the scalar K by the weight of the minimum spanning tree.

4. If $I \geq \text{MaxIteration}$, stop; otherwise set $I = I + 1$ and return to 2.

In our implementation, each spanning tree problem is solved with Prim's algorithm [19]. Moreover, we start steps 4 – a , and 4 – b with edges having reduced costs equal to zero, to increase the possibility of obtaining a tight lower bound.

5. Computational experiments

In this section we present our computational experiments on the lower bound computations for the QMSTP. We implemented the algorithms in C++ language and run on an Intel Xeon CPU E5335 (2 quad core CPUs 2GH). In the following we first present the test instances and provide the comparison of the lower bonding approaches in details.

5.1. Test instances

We considered the benchmark sets CP and OP introduced in [4] and [3], respectively. The OP consists of three classes of random instances denoted as OPSYM, OPVSYM, and OPESYM with size ranging from $n = 6$ to $n = 18$, $n = 20$, $n = 30$, and $n = 50$. This benchmark consists of 450 instances of complete graphs with n vertices and $m = n(n - 1)/2$ edges. For each problem size, 10 random instances have been generated. The CP consists of four classes of random instances denoted as CP1, CP2, CP3, and CP4 with size $n \in \{10, 15, 20, 25, 30, 35, 40, 45, 50\}$. This benchmark consists of 108 instances with different densities $d \in \{33\%, 67\%, 100\%\}$. These two benchmarks have been generated as follows:

1. OPSYM: The linear and the quadratic costs are chosen at random according to uniformly distributed from the sets $\{1, \dots, 100\}$ and $\{1, \dots, 20\}$, respectively.
2. OPVSYM: The linear costs are uniformly distributed at random in $\{1, \dots, 10000\}$ while the quadratic costs C_{ef} are obtained associating to the vertices random values uniformly distributed in $\{1, \dots, 10\}$ and multiplying the four values associated to the end vertices of edges e and f , i.e., for two edges $e_p = (1, 2)$ and $e_f = (3, 4)$ the value of C_{ef} is computed by multiplying the weight of vertices 1, 2, 3, and 4.
4. OPESYM: The vertices uniformly have spread at random in a rectangle with coordinates $(0, 0)$, $(0, 100)$, $(100, 0)$ and $(100, 100)$. The linear costs are chosen as the Euclidean distances between the end vertices of each edge, while the quadratic costs are selected as the Euclidean distances between the midpoints of the edges.
5. CP1: The linear and the quadratic costs are chosen at random according to uniformly distributed from the set $\{1, \dots, 10\}$.
6. CP2: The linear and the quadratic costs are chosen at random according to uniformly distributed from the sets $\{1, \dots, 10\}$ and $\{1, \dots, 100\}$, respectively.
7. CP3: The linear and the quadratic costs are chosen at random according to uniformly distributed from the sets $\{1, \dots, 100\}$ and $\{1, \dots, 10\}$, respectively.

Table 1: Comparison of different lower bounding approaches on TestSet OPvSYM.

Instance			Gap(%)						CPU Time					
n	d(%)	Ub	AX	OP	RLT1	MR	NMR	RLT2	AX	OP	RLT1	MR	NMR	RLT2
6	100	16273.9	1.2	4.8	0.0	0.8	1.8	0.0	0	0	0	0	0	0
7	100	19625.7	1.0	5.33	0.0	1.1	2.2	0.0	0	0	0	0	0	0
8	100	27039.4	2.0	4.65	0.0	1.5	1.4	0.0	0	0	0	0	0	0
9	100	22769.9	0.7	2.6	0.0	1.1	1.1	0.0	0	0	0	0	0	0
10	100	25743.8	0.9	6.1	0.0	2.1	2.0	0.0	0	0	0	0	0	0
11	100	29325.6	1.0	4.5	0.0	2.1	1.6	0.0	0	0	0	0	0	0
12	100	32577.8	0.7	3.5	0.0	1.2	1.1	0.0	0	0	0	0	0	1
13	100	40488.5	1.0	3.6	0.0	1.1	1.0	0.0	0	0	0	0	0	2
14	100	44240.4	0.6	2.2	0.0	1.1	1.0	0.0	0	0	0	0	1	5
15	100	50821.6	0.7	2.3	0.0	1.1	0.9	0.0	0	1	1	0	0	7
16	100	41940.2	1.1	2.1	0.0	2.3	2.2	0.0	0	2	2	0	0	10
17	100	41819.0	1.0	1.2	0.0	0.8	0.7	0.0	0	2	2	0	0	12
18	100	46130.2	1.3	2.0	0.0	1.5	1.3	0.0	0	3	3	0	0	24
20	100	55326.2	0.9	1.8	0.0	1.1	1.0	0.0	0	5	7	0	0	42
30	100	78999.9	0.5	0.7	0.0	1.1	1.0	0.0	0	23	23	1	1	445
50	100	165419.6	0.5	0.3	0.0	0.5	0.4	-	2	366	371	17	18	-

CP4. The linear and the quadratic costs are chosen at random according to uniformly distributed from the set $\{1, \dots, 100\}$.

5.2. Lower bound computation

We compare the lower bounds effectiveness and computational efficiency using six alternative approaches discussed in this paper. Due to the tradeoff between bound strength and CPU execution time we terminated the dual-ascent algorithms for RLT2 in 20 iterations for $n < 30$, and 10 iterations for $n \geq 30$. Moreover, due to the exceeded memory limit we are not able to solve the RLT2 for instances with size $n \geq 40$. In subgradient implementation, we allow 1500 iterations with an initial step size of 2.

Tables 1 to 3 present the percent gap between the lower bounds and the objective value of the best known solutions, and CPU execution times of using different approaches for OPvSYM, OPESYM and OPSYM, respectively. Each row of the Tables 1 to 3 gives the average values of the respective 10 randomly generated test instances. Tables 4 to 7 report the results for CP1 to CP4 in terms of the gap and CPU execution times. In all tables the first three columns indicate the problem size (n), the density (d), and the objective value of the best known solutions (Ub) obtained from [4]. The next six columns from left to right, give the percent gaps obtained using the Assad and Xu's procedure (AX), the revised form of the Öncan and Punnen Lagrangian relaxation approach by considering the correct formula (18) and (19) (OP), the subgradient implementation of QRLT1 (RLT1), the Monotonic Reformulation (MR) scheme, the Non Monotonic Reformulation (NMR) scheme, and the dual-ascent implementation of QRLT2 (RLT2). The CPU execution times of each approach are given in the last six columns of the tables. The formula we used to compute the percent gaps is $100 \times (Ub - Lb)/Lb$, where Lb stands for the value of the lower bound.

Table 2: Comparison of different lower bounding approaches on TestSet OPEsym.

Instance			Gap(%)						CPU Time					
n	d(%)	Ub	AX	OP	RLT1	MR	NMR	RLT2	AX	OP	RLT1	MR	NMR	RLT2
6	100	541.2	2.9	3.0	0.4	2.6	3.2	0.5	0	0	0	0	0	0
7	100	783.7	4.8	4.7	0.3	4.5	4.2	1.2	0	0	0	0	0	0
8	100	1020.1	5.2	4.4	0.4	5.7	5.3	1.9	0	0	0	0	0	0
9	100	1356	6.5	5.6	0.6	5.5	4.8	2.2	0	0	0	0	0	0
10	100	1427.1	6.7	3.5	0.5	5.7	5.2	2.3	0	0	0	0	0	0
11	100	1545.1	6.4	6.0	0.3	5.6	4.7	2.4	0	0	0	0	0	0
12	100	1901.6	8.0	6.5	0.4	6.7	5.5	2.8	0	0	1	0	0	2
13	100	2175.3	7.9	6.8	0.3	6.6	5.7	2.9	0	0	1	0	0	4
14	100	2527.9	8.2	6.8	0.2	6.2	5.4	2.9	0	1	2	0	0	6
15	100	2588.8	8.2	7.8	0.4	6.5	5.6	2.9	0	1	3	0	0	11
16	100	2980.1	9.2	8.6	0.6	7.6	6.4	3.3	0	1	4	0	0	19
17	100	3372.2	9.8	8.2	0.9	7.8	6.9	3.7	0	2	5	0	0	24
18	100	3569.0	10.7	8.7	0.5	7.8	6.8	3.9	0	3	6	0	0	34
30	100	8056.7	13.2	12.1	1.7	11.0	9.6	6.3	1	21	59	4	9	493
50	100	15788.8	14.9	13.7	1.91	12.1	10.5	-	9	392	658	37	93	-

Table 3: Comparison of different lower bounding approaches on TestSet OPSym.

Instance			Gap(%)						CPU Time					
n	d(%)	Ub	AX	OP	RLT1	MR	NMR	RLT2	AX	OP	RLT1	MR	NMR	RLT2
6	100	258.4	13.2	25.6	1.92	14.8	13.1	2551.4	0	0	0	0	0	0
7	100	326.8	24.3	38.1	5.3	22.1	19.0	2.9	0	0	0	0	0	0
8	100	438.5	24.2	39.5	9.7	25.7	22.5	5.8	0	0	0	0	0	0
9	100	534.9	31.5	44.2	14.7	33.9	28.3	7.7	0	0	0	0	0	0
10	100	653.9	41.4	57.9	23.4	45.5	39.3	11.89	0	0	0	0	0	1
11	100	785.9	55.5	71.8	34.5	57.8	51.3	17.6	0	0	1	0	0	2
12	100	918.5	64.9	84.4	42.0	69.5	60.5	21.6	0	0	1	0	0	3
13	100	1067.1	75.9	92.2	51.0	79.9	71.9	25.7	0	0	2	0	0	5
14	100	1249.8	82.0	98.4	56.4	85.0	77.1	29.0	0	1	2	0	0	8
15	100	1390.2	101.2	118.9	70.4	104.8	94.6	34.7	0	1	3	0	0	12
16	100	1629.3	115.4	134.7	83.7	119.6	110.6	28.2	0	2	4	0	0	20
17	100	1823.8	123.2	142.0	89.6	127.1	116.5	44.9	0	2	5	0	0	26
18	100	2981	137.3	157.3	103.2	142.5	131.8	49.2	0	3	6	0	0	37
20	100	2572.7	167.9	189.5	127.1	173.2	160.3	59.9	0	8	10	0	0	70
30	100	6015.9	329.9	356.3	261.5	332.2	315.7	111.6	0	32	59	2	6	503
50	100	17616.9	774.2	793.2	618.1	719.9	699.6	-	3	584	749	37	76	-

Table 4: Comparison of different lower bounding approaches on TestSet CP1.

Instance			Gap(%)							CPU Time					
n	d(%)	Ub	AX	OP	RLT1	MR	NMR	RLT2	AX	OP	RLT1	MR	NMR	RLT2	
10	33	350	12.2	7.4	0.0	5.1	5.1	1.7	0	1	1	0	0	1	
10	67	255	49.1	44.9	25.6	42.5	37.1	12.8	0	1	1	0	0	1	
10	100	239	67.1	64.8	48.4	64.8	60.4	20.1	0.0	1	1	0	0	1	
Ave.		281.3	42.8	39.1	24.6	37.4	32.5	11.5	0.0	1.0	1.0	0.0	0.0	1.0	
15	33	745	46.6	41.1	28.4	42.2	38.2	16.8	0	2	30	0	0	13	
15	67	659	95.0	86.7	71.2	87.8	82.0	34.8	0	2	3	0	0	13	
15	100	620	112.3	105.3	93.2	104.6	102.6	40.0	0	2	3	0	0	13	
Ave.		674.6	84.6	77.7	64.2	78.2	74.2	30.5	0.0	2.0	3.0	0.0	0.0	13.0	
20	33	1379	76.3	69.2	55.3	71.3	65.6	30.5	0	7	10	0	1	78	
20	67	1252	132.3	120.8	107.6	126.8	120.1	48.5	0	6	10	0	1	82	
20	100	1174	154.7	141.1	131.6	145.6	141.1	59.1	0	8	10	0	1	78	
Ave.		1268.3	121.1	110.3	98.1	114.5	108.9	46.0	0.0	7.0	10.0	0.0	1.0	79.3	
25	33	2185	95.8	83.5	70.1	87.1	82.1	37.0	0	15	26	1	1	328	
25	67	2023	167.6	153.5	142.3	157.7	152.9	63.2	0	18	27	1	1	334	
25	100	1943	190.4	176.8	170.2	182.4	178.8	78.1	0	18	28	1	1	332	
Ave.		2050.3	151.2	137.9	127.5	142.4	137.9	59.4	0.0	17.0	27.0	1.0	1.0	331.3	
30	33	3205	124.1	111.4	98.1	115.2	110.7	49.1	0	33	54	3	3	544	
30	67	2998	193.1	176.5	168.1	182.5	177.8	78.3	0	42	61	3	3	521	
30	100	2874	208.3	195.3	191.4	201.5	199.1	92.2	0	46	68	3	3	491	
Ave.		3025.6	175.1	166.1	152.5	166.4	162.5	73.2	0.0	40.3	61.0	3.0	3.0	518.6	
35	33	4474	149.6	134.2	122.1	139.7	134.9	59.1	1	74	111	8	8	1475	
35	67	4147	211.5	196.0	190.4	200.2	198.1	87.8	1	95	118	6	8	1393	
35	100	4000	222.5	210.8	206.8	216.9	214.9	104.8	1	92	143	6	8	1393	
Ave.		4207.0	194.5	180.3	174.7	185.5	182.6	83.9	1.0	87.0	124.0	6.7	8.0	1420.3	
40	33	5945	173.3	155.4	143.8	162.1	156.8	-	1	142	200	15	16	-	
40	67	5567	229.6	214.7	210.0	220.6	217.7	-	1	163	244	12	12	-	
40	100	5368	235.7	225.5	222.1	231.1	229.7	-	1	189	268	14	18	-	
Ave.		5626.6	212.8	198.5	191.9	204.6	201.4	-	1.0	164.6	237.3	13.6	15.3	-	
45	33	7521	188.9	170.8	161.2	177.1	172.1	-	2	279	329	21	26	-	
45	67	7161	241.4	228.6	225.2	235.1	232.3	-	2	307	395	22	33	-	
45	100	6944	244.7	236.2	234.5	241.2	239.7	-	2	351	489	24	37	-	
Ave.		7208.6	225.0	211.8	206.9	217.8	214.7	-	2.0	312.3	404.3	22.3	32.0	-	
50	33	9393	207.9	188.3	179.7	194.8	190.0	-	2	501	534	36	51	-	
50	67	8958	251.2	239.4	236.8	245.6	243.6	-	3	563	712	42	60	-	
50	100	8713	252.1	243.9	243.4	248.6	247.5	-	3	649	835	46	66	-	
Ave.		9021.3	237.1	223.8	219.9	229.6	227.0	-	2.6	571.0	693.6	41.3	59.0	-	

As we can observe in tables 1 to 3, the bounds obtained by NMR are almost always stronger than the AX, MR, and OP bounds for all three data sets, but still weaker than the RLT1 and RLT2. For the OPVSYM, which seems to be the easiest test set among the OP instances, the RLT1 and RLT2 almost always give the optimal solutions with more CPU execution times. For this data set, the AX, MR, NMR and OP approaches provide tight bounds with short execution times with the exception of OP whose computational times for instances with $n = 50$ are high. For the OPESYM, which seems to be more difficult than the OPVSYM, the best approach is the RLT1 and the worst one is the AX. For this data set NMR provides good bounds in reasonable times, and always outperform the AX, MR and OP. The RLT2 provides the bounds slightly worse than RLT1 and requires more computational effort. For the OPSYM which seems to be the most difficult data set amongst the OP test set, the RLT2 provides lower bounds that are significantly stronger than those provided by the other approaches (especially those by RLT1.) For this test set, the bound obtained by NMR are still stronger than the AX, MR, and OP. Note that, the revised form of the Öncan and Punnen Lagrangian relaxation approach does not always yield tighter lower bound values for all the data sets than the ones obtained by the Assad and Xu’s leveling procedure, as claimed in their paper [3].

The results of comparing different lower bounding approaches for the CP data set are given in Tables 4 to 7. For all four CP data sets, the RLT2 outperforms the other approaches in terms of the bound tightness, but it always needs more computational effort. After the RLT2, the RLT1 is the one that provides the best bounds. Considering the significant gaps obtained for these data set, we can conclude that the NMR, OP, and RLT1 almost provide the same bounds, but NMR outperforms the other two in terms of execution times. In order to give a better explanation of the comparison we reported the average results over the 12 different instance of each dimension in Table 8. Overall, the table indicates that the dual-ascent strategy applied for RLT2 provides a significant improvement over all the other approaches reducing the gaps between the linear programming and the best known integer solution values. For the size $n = 35$, which was the biggest size that we could solved by RLT2, the overall gap reduction of the RLT2 over the AX is 68%, while the overall gap reduction of RLT1, NMR, OP, and MR over the AX are 17%, 9.3%, 8%, and 6.6%, respectively. From these results we can conclude that the RLT2 yields the tightest bound but in the cost of increased CPU execution time. Moreover, the NMR seems to be a good candidate when the tradeoff between the bounds tightness and the CPU execution times matters.

6. Conclusion

In this paper we proposed a reformulation for the QMSTP based on dual information retrieved from the continuous relaxation of an MILP. We reviewed and analyzed the Gilmore-Lawler type bound, the Assad and Xu reformulation scheme, and the Lagrangian relaxation of Öncan and Punnen, and compared them in terms of continuous relaxation of the proposed MILP. To improve the bounds for the QMSTP, we develop a mixed 0-1 linear formulation based on using the second level of the reformulation-linearization technique and devised

Table 5: Comparison of different lower bounding approaches on TestSet 2.

Instance			Gap(%)						CPU Time					
n	d(%)	Ub	AX	OP	RLT1	MR	NMR	RLT2	AX	OP	RLT1	MR	NMR	RLT2
10	33	3122	17.2	9.2	0.0	7.2	7.3	2.5	0	1	1	0	0	1
10	67	2042	91.7	81.3	45.9	78.1	67.5	19.4	0	1	1	0	0	1
10	100	1815	137.2	127.1	93.7	125.7	116.1	31.1	0	1	1	0	0	1
Ave.		2326.3	82.0	72.5	46.5	70.3	63.6	17.6	0.0	1.0	1.0	0.0	0.0	1.0
15	33	6539	67.9	59.1	39.6	59.5	54.2	22.7	0	2	3	0	0	13
15	67	5573	170.1	148.0	115.2	146.1	140.0	48.2	0	2	3	0	0	13
15	100	5184	243.5	222.9	183.3	225.2	210.9	60.2	0	2	3	0	0	13
Ave.		5765.3	160.5	143.3	112.7	143.6	135.0	43.7	0.0	2.0	3.0	0.0	0.0	13.0
20	33	12425	113.2	100.7	76.6	106.4	93.7	40.4	0	6	10	0	1	81
20	67	10893	247.4	218.4	185.4	225.7	214.1	65.7	0	7	10	0	1	83
20	100	10215	356.0	313.0	271.7	321.9	307.4	87.7	0	7	9	0	1	83
Ave.		11177.6	238.8	210.7	177.9	217.6	204.9	64.4	0.0	6.7	9.7	0.0	1.0	82.3
25	33	19976	144.4	122.5	98.4	127.5	119.2	48.4	0	16	24	1	2	326
25	67	18251	339.2	300.3	261.1	307.2	297.1	88.8	0	20	24	1	2	314
25	100	17411	504.5	451.8	401.9	473.4	446.4	119.8	0	20	25	1	2	302
Ave.		11177.6	329.3	291.5	253.8	302.7	287.4	85.6	0.0	18.6	24.3	1.0	2.0	314.0
30	33	29731	198.2	174.3	146.8	184.5	171.2	65.7	0	36	54	5	6	507
30	67	27581	427.7	377.3	336.4	389.7	374.9	114.8	0	47	56	8	9	528
30	100	26146	616.7	552.5	503.5	570.5	550.4	146.1	0	50	66	6	6	490
Ave.		27819.3	414.2	368.1	328.9	381.5	365.5	108.8	0.0	44.3	58.7	6.3	7.0	508.3
35	33	42305	248.1	215.2	188.1	221.3	214.0	79.5	0	77	122	19	21	1421
35	67	38490	522.0	464.7	419.5	474.1	462.6	136.5	0	97	114	11	14	1394
35	100	36723	728.7	653.4	600.6	669.8	653.7	168.3	0	102	117	10	13	1394
Ave.		39172.7	499.3	444.2	402.3	454.7	443.2	128.1	0.0	92.0	117.6	13.3	16.0	1403.0
40	33	56237	300.4	260.4	229.6	275.0	260.3	-	1	150	214	30	40	-
40	67	51851	610.6	542.6	496.1	567.4	542.9	-	1	183	205	22	30	-
40	100	49817	861.3	774.2	717.4	798.9	775.9	-	1	192	232	22	25	-
Ave.		52635.0	590.7	525.6	480.8	546.6	526.2	-	1.0	175.0	217.0	24.7	31.7	-
45	33	70603	340.5	296.7	266.2	311.0	297.1	-	1	294	348	40	57	-
45	67	66889	691.8	618.0	570.3	639.4	619.2	-	1	341	374	34	46	-
45	100	64840	974.7	875.9	817.8	896.0	878.1	-	1	377	382	35	45	-
Ave.		67444.0	668.9	596.8	551.4	615.4	598.1	-	1.0	337.3	368.0	36.3	49.3	-
50	33	88942	394.2	345.1	310.8	363.0	345.5	-	2	516	543	80	75	-
50	67	84020	783.3	699.3	649.9	721.0	702.6	-	2	621	614	66	81	-
50	100	81858	1090.8	983.0	925.0	1008.1	987.3	-	2	611	656	51	72	-
Ave.		84940.0	756.1	675.8	628.5	697.3	678.4	-	2.0	582.7	604.3	65.7	76.0	-

Table 6: Comparison of different lower bounding approaches on TestSet CP3.

Instance			Gap(%)						CPU Time					
n	d(%)	Ub	AX	OP	RLT1	MR	NMR	RLT2	AX	OP	RLT1	MR	NMR	RLT2
10	33	646	0.6	3.1	0.0	1.8	1.8	0.0	0	1	1	0	0	1
10	67	488	11.4	22.6	0.0	14.2	10.1	2.5	0	1	1	0	0	1
10	100	426	18.9	35.2	10.3	24.2	20.6	6.2	0	1	1	0	0	1
Ave.		520.7	10.3	20.3	3.4	13.4	10.8	2.9	0.0	1.0	1.0	0.0	0.0	1.0
15	33	1236	14.0	23.9	4.7	19.4	14.8	5.1	0	2	4	0	0	13
15	67	966	25.7	37.0	13.9	32.3	24.6	9.0	0	2	4	0	0	13
15	100	975	36.1	50.4	25.0	41.3	36.5	14.8	0	2	3	0	0	13
Ave.		1059.0	25.2	37.1	14.5	31.0	25.3	9.6	0.0	2.0	3.7	0.0	0.0	13.0
20	33	1972	29.5	38.0	17.9	33.4	27.8	12.1	0	6	9	1	1	86
20	67	1792	50.9	62.7	37.1	56.6	48.8	21.9	0	6	10	1	1	80
20	100	1544	62.3	74.0	46.2	61.0	57.0	26.5	0	6	10	1	1	81
Ave.		1769.3	47.5	58.2	33.7	50.3	44.5	20.1	0.0	6.0	10.0	1.0	1.0	82.3
25	33	2976	43.7	51.9	30.0	47.3	42.3	19.6	0	14	28	1	1	323
25	67	2546	73.3	84.2	56.2	75.1	70.0	32.8	0	16	26	2	2	324
25	100	2471	93.0	104.0	75.3	88.7	85.6	42.0	0	15	28	2	2	305
Ave.		2664.3	70.0	80.0	53.8	70.3	65.9	31.4	0.0	15.0	27.3	1.7	1.7	319.3
30	33	4070	56.1	61.1	42.5	59.8	54.5	25.8	0	33	57	3	4	507
30	67	3649	95.8	104.6	77.7	94.7	89.6	45.0	0	34	66	4	5	502
30	100	3483	114.8	122.9	96.1	109.3	105.9	54.3	0	42	68	4	5	490
Ave.		3734.0	88.9	96.2	72.1	87.9	83.3	41.7	0.0	36.3	63.7	3.7	4.7	499.7
35	33	5423	78.9	84.9	61.4	84.8	76.6	37.4	0	69	125	8	12	1416
35	67	4981	116.4	126.2	98.0	112.6	109.2	55.9	0	81	126	8	12	1482
35	100	4770	138.0	144.1	117.8	130.8	127.0	66.4	0	92	146	8	11	1457
Ave.		5058.0	111.1	118.4	92.4	109.4	104.2	53.2	0.0	80.7	132.3	8.0	11.7	1451.7
40	33	6925	94.9	99.1	76.1	95.9	91.2	-	1	135	220	17	23	-
40	67	6456	133.6	140.0	113.3	127.7	123.9	-	1	152	272	19	25	-
40	100	6208	158.1	159.5	135.9	151.7	145.6	-	1	171	272	17	23	-
Ave.		6529.7	128.8	133.0	108.4	125.1	120.2	-	1.0	152.7	254.7	17.7	23.7	-
45	33	8720	108.3	111.3	89.2	110.0	103.5	-	1	285	410	35	45	-
45	67	8225	150.6	154.1	130.0	144.5	139.8	-	1	284	486	30	45	-
45	100	7827	171.9	170.0	149.9	163.6	158.7	-	1	331	502	30	45	-
Ave.		8257.3	143.6	145.1	122.7	139.3	134.0	-	1.0	300.0	466.0	31.7	45.0	-
50	33	10717	124.2	126.5	103.9	122.8	117.7	-	2	421	664	72	76	-
50	67	10100	167.9	168.6	145.5	159.5	155.2	-	2	509	816	58	81	-
50	100	9836	191.3	186.2	167.5	182.8	176.6	-	2	593	873	53	82	-
Ave.		10217.7	161.1	160.4	138.9	155.0	149.8	-	2.0	507.7	784.3	61.0	79.7	-

Table 7: Comparison of different lower bounding approaches on TestSet CP4.

Instance			Gap(%)						CPU Time					
n	d(%)	Ub	AX	OP	RLT1	MR	NMR	RLT2	AX	OP	RLT1	MR	NMR	RLT2
10	33	3486	14.3	8.7	0.0	6.1	6.0	1.8	0	1	1	0	0	1
10	67	2404	67.4	60.8	34.0	58.8	49.5	15.8	0	1	1	0	0	1
10	100	2197	93.2	91.2	66.3	87.6	83.5	26.0	0	1	1	0	0	1
Ave.		2695.7	58.3	53.5	33.4	50.8	46.3	14.5	0.0	1.0	1.0	0.0	0.0	1.0
15	33	7245	58.5	50.9	35.3	52.1	47.2	20.4	0	2	3	0	0	13
15	67	6188	130.8	119.5	92.5	119.0	111.4	42.6	0	2	3	0	0	13
15	100	5879	172.8	162.6	136.1	160.5	154.7	52.1	0	2	4	0	0	13
Ave.		6437.3	120.7	111.0	88.1	110.5	104.5	38.3	0.0	2.0	3.3	0.0	0.0	13.0
20	33	13288	98.3	88.5	67.9	90.7	82.3	36.4	0	7	10	1	1	78
20	67	11893	198.7	180.0	153.4	187.3	176.2	59.8	0	7	10	1	1	83
20	100	11101	265.2	243.3	210.6	246.5	237.7	78.5	0	8	11	1	1	83
Ave.		12094.0	187.4	170.6	143.9	174.8	165.4	58.2	0.0	7.7	10.3	1.0	1.0	81.3
25	33	21176	127.7	110.0	89.3	114.1	107.1	45.2	0	18	26	4	3	337
25	67	19207	270.5	245.8	215.1	251.9	242.3	80.3	0	18	27	2	3	325
25	100	18370	375.1	350.2	309.1	359.0	342.6	107.0	0	20	26	3	3	350
Ave.		19584.3	257.7	235.3	204.5	241.6	230.6	77.5	0.0	18.7	26.3	3.0	3.0	337.3
30	33	31077	174.3	154.6	131.9	161.6	152.4	61.2	0	37	56	5	7	537
30	67	28777	346.9	313.9	280.3	326.0	311.1	105.3	0	45	55	8	7	504
30	100	27314	465.5	433.1	391.7	442.9	427.2	131.4	0	46	61	6	6	534
Ave.		29056.0	328.9	300.5	267.9	310.1	296.9	99.3	0.0	42.7	57.3	6.3	6.7	525.0
35	33	43629	220.2	193.5	169.8	200.3	192.3	74.6	0	86	108	18	21	1393
35	67	39660	419.7	384.8	346.4	389.1	381.8	120.7	0	88	113	12	15	1394
35	100	38049	552.4	514.5	467.3	525.8	509.3	153.0	0	93	122	12	16	1394
Ave.		40446.0	397.4	364.6	327.8	371.7	361.1	116.1	0.0	89.0	114.3	14.0	17.3	1393.7
40	33	58874	274.9	241.4	214.5	254.5	241.4	-	1	158	194	40	35	-
40	67	53592	498.6	455.1	415.5	469.7	453.4	-	1	212	209	22	29	-
40	100	51229	652.5	609.1	558.1	626.6	605.2	-	1	197	232	22	28	-
Ave.		54565.0	475.3	435.2	396.1	450.2	433.3	-	1.0	189.0	211.7	28.0	30.6	-
45	33	72676	305.3	269.7	242.8	282.1	269.7	-	1	286	354	43	46	-
45	67	68737	565.0	516.9	477.6	534.1	516.7	-	1	355	369	35	52	-
45	100	66508	744.7	692.9	640.3	707.1	690.2	-	1	366	398	39	57	-
Ave.		69307.0	538.3	493.1	453.5	507.7	492.2	-	1.0	335.7	373.7	39.0	51.7	-
50	33	91009	353.4	313.4	282.9	328.2	313.4	-	2	541	582	80	75	-
50	67	86231	642.8	588.4	546.0	608.5	588.8	-	2	612	606	69	80	-
50	100	83838	838.1	781.7	726.7	796.5	779.3	-	2	657	690	69	80	-
Ave.		87026.0	611.4	561.1	518.5	577.7	560.5	-	2.0	603.3	626.0	72.7	78.3	-

Table 8: Comparison of different lower bounding approaches on TestSet CP. Each row reports the average on 12 instances

Instance		Gap(%)						CPU Time					
n	Ub	AX	OP	RLT1	MR	NMR	RLT2	AX	OP	RLT1	MR	NMR	RLT2
10	1455.8	48.3	46.3	27.0	43.0	38.7	11.6	0.0	1.0	1.0	0.0	0.0	1.0
15	3484.1	97.8	92.3	69.8	90.8	84.8	30.5	0.0	2.0	3.2	0.0	0.0	13.0
20	6577.3	148.7	137.5	113.4	139.4	131.0	47.3	0.0	6.7	10.0	1.0	1.0	81.3
25	10711.2	202.1	186.2	159.9	189.3	180.5	63.5	0.0	17.3	26.2	1.7	1.9	325.0
30	15908.7	251.8	231.5	205.4	236.5	227.1	80.8	0.0	40.9	60.2	4.8	5.3	512.9
35	22220.9	300.7	276.9	249.1	280.5	272.8	95.0	0.3	87.2	122.1	10.5	13.2	1417.2
40	29839.1	363.0	323.1	294.4	331.7	320.3	-	1.0	170.3	230.2	21.0	24.8	-
45	38054.2	394.04	361.8	333.7	370.1	359.7	-	1.3	321.3	403.0	32.3	44.5	-
50	47801.2	441.4	405.3	376.5	414.9	404.0	-	2.2	506.2	631.5	60.2	73.2	-

an efficient dual-ascent algorithm to solve the continuous relaxation of the proposed model based on reduced costs. The basic idea proposed in the paper is to use the meaning of the reduced cost to retrieve the dual information of the continuous relaxation of the MILP. In Computational experiments we compared the tightness and speed of computation of the new bounding techniques with those of literature. The results indicated that the dual-ascent procedure applied to QRLT2 provides the best bounds at the price of large computational effort, while the bound obtained by the non-monotonic reformulation scheme seems to tradeoff between the bound tightness and computational effort.

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