

# Combinatorial optimization with one quadratic term: Spanning trees and forests<sup>☆</sup>

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## ABSTRACT

The standard linearization of a binary quadratic program yields an equivalent reformulation as an integer linear program, but the resulting LP-bounds are very weak in general. We concentrate on applications where the underlying linear problem is tractable and exploit the fact that, in this case, the optimization problem is still tractable in the presence of a single quadratic term in the objective function. We propose to strengthen the standard linearization by the use of cutting planes that are derived from jointly considering each single quadratic term with the underlying combinatorial structure. We apply this idea to the quadratic minimum spanning tree and spanning forest problems and present complete polyhedral descriptions of the corresponding problems with one quadratic term, as well as efficient separation algorithms for the resulting polytopes. Computationally, we observe that the new inequalities significantly improve dual bounds with respect to the standard linearization, particularly for sparse graphs.

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## 1. Introduction

Optimization problems with a quadratic objective function and linear constraints over binary variables are usually hard to solve. This remains true in general in the special case where the underlying linear problem is polynomially solvable; even in the unconstrained case the binary optimization problem is NP-hard due to its equivalence to the Maximum-Cut problem [5].

A very common approach to binary quadratic optimization is to linearize the quadratic terms and to develop an appropriate polyhedral description of the corresponding set of feasible solutions. For reasons of complexity, one cannot expect to find a tight and polynomial sized polyhedral description. A straightforward idea is to linearize each product in the objective function independently and simply combine the result with the given linear side constraints [7]. This approach yields a correct integer programming model of the problem, but the resulting LP-relaxations lead to very weak bounds in general, so that branch-and-cut algorithms based on this simple linearization idea perform very poorly in practice. For this reason, one usually searches for stronger inequalities to tighten the description; see, e.g., [3].

In this paper, we consider another approach that, to the best of our knowledge, has not been investigated yet: we examine the problem version with only one product term in the objective function, but with all linear side constraints taken into account [2]. Any valid cutting plane for this problem will remain valid for the original problem and potentially improves over the straightforward model, since the chosen product is considered together with all side constraints. The advantage of our approach lies in the fact that there exists a polynomial time separation algorithm for the one-product problem whenever the underlying linear problem is tractable. This is guaranteed by a general result by Grötschel et al. [10], since the corresponding

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optimization problem is polynomially solvable: for this, we can solve the underlying linear problem four times, with different fixings of the two variables appearing in the chosen product. The resulting cutting planes may not be facet defining for the original problem, but they lead to a tighter polyhedral description in general.

From a practical point of view, the indirect separation approach by Grötschel et al. is too general and it does not pay off to apply it inside a branch-and-cut approach; the computational effort for generating a single cutting plane is too high. Therefore, we have a closer look at specific quadratic optimization problems in order to find valid inequalities and fast separation routines for the quadratic case, which might be inspired by the corresponding techniques in the linear case.

In this paper, we investigate our approach for the quadratic minimum spanning tree (QMST) problem and the closely related quadratic minimum spanning forest (QMSF) problem. The *linear* spanning forest problem deals with finding a cycle free spanning subgraph of minimal cost in a given underlying graph, where costs are defined edge-wise. If additionally the subgraph is required to be connected, we obtain the linear version of the spanning tree problem. The latter problem is well studied and solvable in polynomial time, e.g., by the algorithms of Prim [17] or Kruskal [12]. If additional costs arise for pairs of edges, we obtain the QMST problem, which was shown to be NP-hard in general by Assad and Xu [1]. In their work the authors also give examples for the QMST problem arising in applications related to transportation problems or communication and energy networks. Here, additional costs occur whenever two adjacent edges of different types are chosen to belong to the tree. Examples are trees with changeover and reload costs, recently studied by Galbiati et al. [8,9]. Exact and heuristic algorithms for QMST have been presented by Cordone and Passeri [4], Öncan and Punnen [15], and very recently by Pereira et al. [16], who apply the reformulation–linearization technique (RLT) combined with Lagrangian relaxation. More heuristic approaches are discussed in [22,21,14]. Special cases of QMST have been shown to be tractable, e.g., the case of a multiplicative objective function with positive factors [18].

In contrast to the QMST, the quadratic minimum *forest* problem has received little attention in the literature so far. Lee and Leung [13] define the polytope corresponding to the linearized QMSF as the *Boolean Quadric Forest Polytope* and classify several facet classes. For some of these classes, they develop polynomial time separation algorithms. Note that many variants of the linear spanning forest problem have been considered in the literature, e.g., the number of connected components or the degree of vertices may be bounded. In this paper, we do not consider any such restriction but optimize over the set of all spanning forests in the given graph.

Following our general approach outlined above, we devise complete polyhedral descriptions of the spanning forest problem and the spanning tree problem with one quadratic term. It turns out that, beyond the well-known subtour elimination constraints for the linear case and the standard linearization constraints, only one additional exponential-size class of facet-defining inequalities is needed for the complete description. The shape of these constraints depends on whether the two edges involved in the quadratic term share a vertex or not; in both cases they are closely related to the subtour elimination constraints. In particular, we present exact and efficient separation algorithms based on the separation algorithm for subtour elimination constraints.

Turning back to the general QMSF and QMST problems, this separation algorithm can be applied to each quadratic term independently. We evaluate the strength of the resulting relaxation by computational experiments, integrating the new separation algorithm into a branch-and-bound scheme. Our experiments show that the new cutting planes significantly improve over the standard linearization in terms of dual bounds, particularly for sparse graphs.

Based on our approach, Fischer and Fischer [6] recently published an alternative proof for one of our results that devises a complete polyhedral description of the spanning tree problem with one quadratic term. For showing optimality of a given tree with respect to this linear description, both proofs construct a corresponding dual solution. While we construct the dual solution directly, distinguishing the four possible assignments of the two product variables, Fischer and Fischer start from a dual optimal solution obtained by ignoring the quadratic term and adapt this solution appropriately. However, they do not discuss separation algorithms and, in particular, they do not evaluate the approach experimentally.

This paper is organized as follows. In Section 2, we introduce the basic notation needed throughout the paper. Sections 3 and 4 present our polyhedral results for QMSF and QMST with one quadratic term. The corresponding separation problem is addressed in Section 5, whereas Section 6 contains the results of an experimental evaluation. Section 7 concludes.

## 2. Preliminaries

Throughout this paper, we assume that  $G = (V, E)$  is a complete undirected graph. A *spanning forest*  $F$  is a cycle free subgraph of  $G$  with  $V(F) = V$ . In a weighted graph, the cost of a spanning forest is the sum of edge weights  $c_e$  over all edges  $e \in E(F)$ . If additional costs  $q_{ef}$  arise for each pair of different edges  $e, f \in E$  contained in the forest, we have a *quadratic minimum spanning forest problem* (QMSF). In a very natural way, QMSF can be formulated as an integer program with linear constraints and a quadratic objective function:

$$\begin{aligned}
 (\text{QIP}_{\text{QMSF}}) \quad & \min \sum_{e \in E} c_e x_e + \sum_{\substack{e, f \in E \\ e \neq f}} q_{ef} x_e x_f \\
 \text{s.t.} \quad & \sum_{e \in E(G[S])} x_e \leq |S| - 1 \quad \forall \emptyset \neq S \subseteq V \\
 & x_e \in \{0, 1\} \quad \forall e \in E.
 \end{aligned} \tag{1}$$

Here  $G[S]$  denotes the subgraph of  $G$  induced by the vertices in  $S$  and  $E(G[S])$  denotes its edge set. The subtour elimination constraints (1) ensure that no subgraph induced by  $S$  contains a cycle.

To get rid of the quadratic terms in the objective function, we linearize all products  $x_e x_f$  by introducing artificial binary variables  $y_{ef}$  and link them to the original variables using the following additional linear inequalities:

$$y_{ef} \leq x_e, x_f \quad \forall e, f \in E \quad (2)$$

$$y_{ef} \geq x_e + x_f - 1 \quad \forall e, f \in E. \quad (3)$$

The  $x$ -entries of all feasible solutions of the linearized problem (QIP<sub>QMSF</sub>) model exactly the incidence vectors of all spanning forests, and due to the binary constraints, the value of every  $y_{ef}$  is exactly the product of  $x_e$  and  $x_f$  by (2) and (3).

In the following, we denote the convex hull of all incidence vectors of spanning forests by  $P^{lin}$ , while  $P^{ql}$  is the convex hull of all feasible vectors of the linearized quadratic problem, i.e., of all binary vectors  $(x, y)$  satisfying (1)–(3). While it is well-known that the inequalities (1) yield a complete polyhedral description of  $P^{lin}$ , the inequalities (1)–(3) do not suffice to describe  $P^{ql}$  completely. Moreover, while all inequalities (1) are facet-defining for  $P^{lin}$ , this does not remain true for  $P^{ql}$ . We will see that both negative statements concerning  $P^{ql}$  hold true even in the case of a single product term in the objective function.

When considering a quadratic objective function with a single product term, we have to distinguish between two cases. In the first case, the product term consists of variables corresponding to two adjacent edges. Throughout the paper, we denote these edges by  $e_1 := \{u, v\}$  and  $e_2 := \{v, w\}$  and the product of their variables is called a *connected monomial*. The corresponding problem is denoted by QMSF<sup>c</sup> in the following. In the second case, the edges of the product variables are non-adjacent in the graph, therefore, the edges are  $e_1 := \{u, v\}$  and  $e_2 := \{w, z\}$  with pairwise distinct vertices  $u, v, w, z \in V$ . In this case, we refer to a *disconnected monomial* and denote the problem by QMSF<sup>d</sup>. Whenever the context leads to the correct association, we shortly denote the linearization variable  $y_{e_1 e_2}$  by  $y$ .

Our aim is thus to investigate the polytope corresponding to QMSF<sup>c</sup>, defined as

$$P_F^c := \text{conv} \{ (x, y) \in \{0, 1\}^{|E|+1} \mid x \text{ satisfies (1) and } y = x_{\{u,v\}} x_{\{v,w\}} \}$$

and the polytope corresponding to QMSF<sup>d</sup>, defined as

$$P_F^d := \text{conv} \{ (x, y) \in \{0, 1\}^{|E|+1} \mid x \text{ satisfies (1) and } y = x_{\{u,v\}} x_{\{w,z\}} \}.$$

A *spanning tree*  $T$  is a connected spanning forest. In a similar vein to the QMSF, the *quadratic minimum spanning tree problem* (QMST) can be formulated as an integer program by adding the cardinality constraint

$$\sum_{e \in E} x_e = |V| - 1 \quad (4)$$

to (QIP<sub>QMSF</sub>), which in combination with the subtour elimination constraints (1) guarantees connectivity. Considering the QMST with one single product term we analogously define the polytopes corresponding to QMST<sup>c</sup> and QMST<sup>d</sup>, i.e., the spanning tree polytopes with one linearized connected, respectively disconnected monomial:

$$P_T^c := \text{conv} \{ (x, y) \in \{0, 1\}^{|E|+1} \mid x \text{ satisfies (1), (4) and } y = x_{\{u,v\}} x_{\{v,w\}} \}$$

$$P_T^d := \text{conv} \{ (x, y) \in \{0, 1\}^{|E|+1} \mid x \text{ satisfies (1), (4) and } y = x_{\{u,v\}} x_{\{w,z\}} \}.$$

By definition, we have  $P_T^c \subseteq P_F^c$  and  $P_T^d \subseteq P_F^d$ . In the following two sections, we devise complete polyhedral descriptions of all four polytopes.

### 3. Complete polyhedral descriptions for spanning forests

In the following we assume  $|V| \geq 4$ . The dimension of the (linear) spanning forest polytope  $P^{lin}$  is  $|E|$ . Clearly, the additional linearization variable  $y$  increases the dimension by at most one. In fact, we have

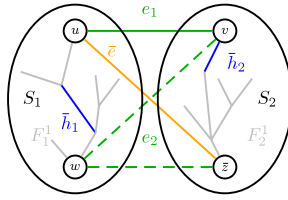
#### Theorem 3.1.

$$\dim(P_F^c) = \dim(P_F^d) = \dim(P^{lin}) + 1 = |E| + 1.$$

**Proof.** For each of the two polytopes  $P_F^c$  and  $P_F^d$  we list  $|E| + 2$  feasible and affinely independent vectors.

Let  $\bar{z} \in V \setminus \{u, v, w\}$  be an arbitrary but fixed vertex in the connected case and  $\bar{z} = z$  in the disconnected case. Let  $S_1$  be a set of vertices containing both  $u$  and  $w$ , but neither  $v$  nor  $\bar{z}$ . Define  $S_2 := V \setminus S_1$  and  $\bar{e} := \{u, \bar{z}\}$ . Choose  $r_1 := |E(G[S_1])|$  forests  $F_1^1, \dots, F_{r_1}^1$  on the subgraphs induced by the set of vertices  $G[S_1]$  and  $r_2 := |E(G[S_2])|$  forests  $F_1^2, \dots, F_{r_2}^2$  on the subgraph induced by  $G[S_2]$  whose incidence vectors are pairwise affinely independent. Let  $\bar{h}_1 \in F_1^1$  and  $\bar{h}_2 \in F_1^2$  be fixed edges in the paths in  $F_1^1$  from  $u$  to  $w$  and in  $F_1^2$  from  $v$  to  $\bar{z}$ , respectively; see Fig. 1 for an illustration.

The  $x$ -components of all vectors constructed below are incidence vectors of forests, whereas the  $y$ -entry is determined by  $y = x_{e_1} x_{e_2}$ . The incidence vectors of the forests  $F$  listed in 1–7 are affinely independent, as every new vector violates some (trivial) equation which all former vectors satisfy. Here, the  $y$ -variable in the corresponding incidence vector is always set



**Fig. 1.** Illustration of the fixed forests and edges. The dashed lines represent the two different cases for edge  $e_2$ : in the connected case,  $e_2$  is the edge from vertex  $w$  to vertex  $v$ ; in the disconnected case,  $e_2$  connects  $w$  and  $z$ .

to zero, since not both product edges  $e_1$  and  $e_2$  belong to  $F$ . The incidence vector of the forest in 8 is affinely independent, as  $y = 1$  since  $e_1, e_2 \in F$ .

1.  $F = F_1^1 \cup F_2^1$ .
2.  $F = F_1^1 \cup F_2^1 \cup \{\bar{e}\}$ .
3.  $F = F_1^i \cup F_2^1 \cup \{\bar{e}\}$  for all  $i = 2, \dots, r_1$ .
4.  $F = F_1^1 \cup F_2^i \cup \{\bar{e}\}$  for all  $i = 2, \dots, r_2$ .
5.  $F = F_1^1 \cup F_2^1 \cup \{e\}$  for all edges  $e \in \delta(S_1)$  with  $e \neq \bar{e}$ .
6.  $F = F_1^1 \cup (F_2^1 \setminus \{h_2\}) \cup \{e_1, \bar{e}\}$ .
7.  $F = (F_1^1 \setminus \{h_1\}) \cup F_2^1 \cup \{e_2, \bar{e}\}$ .
8.  $F = (F_1^1 \setminus \{h_1\}) \cup F_2^1 \cup \{e_1, e_2\}$ .

We obtain a total number of

$$2 + (r_1 - 1) + (r_2 - 1) + (|S_1| |S_2| - 1) + 3 = |E(G[S_1])| + |E(G[S_2])| + |\delta(S_1)| + 2 = |E| + 2$$

affinely independent vectors in  $P_F^c$  and  $P_F^d$ , respectively. Therefore, the corresponding polytopes are of dimension  $|E| + 1$ .  $\square$

The following results introduce one class of facet-defining inequalities for each of the polytopes  $P_F^c$  and  $P_F^d$ , respectively. Both strengthen the subtour elimination constraints (1); we call them *quadratic subtour elimination constraints* in the following.

**Theorem 3.2.** Let  $S_1 \subset V$  be a set of vertices with  $u, w \in S_1$  and  $v \in V \setminus S_1$ . Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + y \leq |S_1| - 1 \quad (5)$$

is valid and induces a facet of  $P_F^c$ .

**Proof.** If  $y = 0$ , inequality (5) is obviously valid as it agrees with a subtour elimination constraint (1). Validity in case  $y = 1$  also follows from the subtour elimination constraints by rewriting

$$\sum_{e \in E(G[S_1])} x_e = \sum_{e \in E(G[S_1 \cup \{v\}])} x_e - \sum_{\substack{e = \{v, s\} \\ s \in S_1}} x_e.$$

By (1) the middle sum is at most  $|S_1 \cup \{v\}| - 1 = |S_1|$ , while the right sum subtracts at least a value of 2 since  $x_{e_1} = x_{e_2} = 1$  due to  $y = 1$ . Combined and with the addition of  $y = 1$ , we obtain a value of at most  $|S_1| - 1$  for the left hand side of (5).

Consider a fixed vertex set  $S_1$  with  $u, w \in S_1$  and  $v \in V \setminus S_1 =: S_2$ . To prove the facet-defining property, we show that the dimension of the face induced by inequality (5) equals  $|E|$ . Similar to the proof of Theorem 3.1 we construct  $|E| + 1$  valid and affinely independent vectors satisfying (5) with equality.

$|S_2| \geq 2$ : As in the proof of Theorem 3.1, define the forests  $F_1^i$  and  $F_2^i$  and the edges  $\bar{e}$ ,  $\bar{h}_1$  and  $\bar{h}_2$ . Then all  $|E| + 1$  vectors defined in 1–6 and 8 satisfy  $\sum_{e \in E(G[S_1])} x_e + y = |S_1| - 1$ .

$|S_2| = 1$ : Define  $\bar{f} := \{\bar{z}, v\}$  for a fixed vertex  $\bar{z} \neq u, v, w$ . Since  $S_2 = \{v\}$ , we have  $\bar{f} \in \delta(S_1)$ . Again, choose  $r_1 := |E(G[S_1])| = |E| - (|V| - 1)$  forests  $F_1^1, \dots, F_1^{r_1}$  with affinely independent incidence vectors on the subgraph induced by  $G[S_1]$  and let  $\bar{h}_1$  be an edge in the cycle of  $F_1^1 \cup \{e_1, e_2\}$ . The reasoning for affine independence is as before, with  $y = 1$  only in case 5:

1.  $F = F_1^1$ .
2.  $F = F_1^1 \cup \{\bar{f}\}$ .
3.  $F = F_1^i \cup \{\bar{f}\}$  for  $i = 2, \dots, r_1$ .

4.  $F = F_1^1 \cup \{f\}$  for all edges  $f \in \delta(S_1)$  with  $f \neq \bar{f}$ .

5.  $F = (F_1^1 \setminus \{\bar{h}_1\}) \cup \{e_1, e_2\}$ .

We therefore have  $2 + (r_1 - 1) + (|V| - 2) + 1 = |E| + 1$  affinely independent vectors being tight in (5).

In summary, for all cases of  $S_1 \subset V$  with  $u, w \in S_1$  and  $v \in V \setminus S_1$ , the dimension of the induced face is  $|E|$ , showing that it is a facet of  $P_F^c$ .  $\square$

**Theorem 3.3.** Let  $S_1, S_2 \subset V$  be disjoint subsets of vertices such that both edges  $e_1$  and  $e_2$  have exactly one end vertex in  $S_1$  and one end vertex in  $S_2$ . Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + \sum_{e \in E(G[S_2])} x_e + y \leq |S_1| + |S_2| - 2 \quad (6)$$

is valid and induces a facet of  $P_F^d$ .

**Proof.** In case of  $y = 0$ , the inequality is obviously valid since it is the sum of two subtour elimination constraints. In the case of  $y = 1$ , we rewrite

$$\sum_{e \in E(G[S_1])} x_e + \sum_{e \in E(G[S_2])} x_e = \sum_{e \in E(G[S_1 \cup S_2])} x_e - \sum_{\substack{e = \{s_1, s_2\} \\ s_1 \in S_1, s_2 \in S_2}} x_e$$

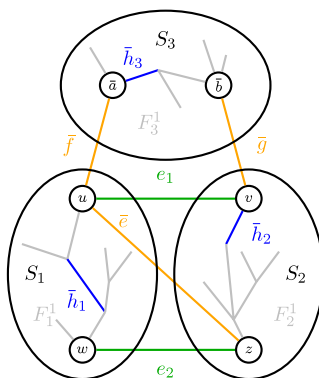
and due to (1) and with the same arguments as in the proof for Theorem 3.2, inequality (6) follows.

For the proof of the facet-defining property, assume without loss of generality  $u, w \in S_1$  and  $v, z \in S_2$ . We again construct  $|E| + 1$  affinely independent vectors satisfying (6) with equality. We distinguish by the number of vertices in  $S_3 := V \setminus (S_1 \cup S_2)$ .

$|S_3| = 0$  : As in the proof of Theorem 3.1, define spanning forests  $F_1^i$  and  $F_2^i$  on the subgraphs induced by  $G[S_1]$  and  $G[S_2]$ , respectively, and consider the edge  $\bar{e} := \{u, z\}$ . Let  $\bar{h}_1 \in F_1^1$ ,  $\bar{h}_2 \in F_2^1$  again be edges in the paths in  $F_1^1$  from  $u$  to  $w$  and in  $F_2^1$  from  $v$  to  $z$ , respectively. Now the  $|E|$  vectors 1–5 and 8 of the proof of Theorem 3.1 satisfy (6) with equality. The missing affinely independent vector can be chosen as the incidence vector corresponding to the forest  $F_1^1 \cup (F_2^1 \setminus \bar{h}_2) \cup \{e_1, e_2\}$ .

$|S_3| > 1$  : Let  $\bar{a}, \bar{b} \in S_3$ . Define the three edges  $\bar{e} := \{u, z\}$ ,  $\bar{f} := \{u, \bar{a}\}$  and  $\bar{g} := \{v, \bar{b}\}$  connecting the vertex sets  $S_1, S_2$  and  $S_1, S_3$  and  $S_2, S_3$ , respectively. Again consider  $r_j := |E(G[S_j])|$  affinely independent incidence vectors of spanning forests  $F_j^1, \dots, F_j^{r_j}$  on the subgraphs of  $G[S_j]$ , for  $j = 1, 2, 3$ , and let the edges  $\bar{h}_1 \in F_1^1$  and  $\bar{h}_2 \in F_2^1$  be in the cycle in  $F_1^1 \cup F_2^1 \cup \{e_1, e_2\}$ , and further let  $\bar{h}_3 \in F_3^1$  be an edge in the cycle in  $F_1^1 \cup F_2^1 \cup F_3^1 \cup \{\bar{e}, \bar{f}, \bar{g}\}$ .

We again construct  $|E| + 1$  affinely independent vectors with appropriate  $y$ -value, which are tight in inequality (6).



1.  $F = F_1^1 \cup F_2^1$ .
2.  $F = F_1^1 \cup F_2^1 \cup F_3^1 \cup \{\bar{e}, \bar{f}\}$ .
3.  $F = F_1^1 \cup F_2^1 \cup F_3^1 \cup \{\bar{f}, \bar{g}\}$ .
4.  $F = F_1^1 \cup F_2^1 \cup F_3^1 \cup \{\bar{g}, \bar{e}\}$ .
5.  $F = F_1^i \cup F_2^1 \cup F_3^1 \cup \{\bar{e}, \bar{f}\}$  for  $i = 2, \dots, r_1$ .
6.  $F = F_1^1 \cup F_2^i \cup F_3^1 \cup \{\bar{e}, \bar{f}\}$  for  $i = 2, \dots, r_2$ .
7.  $F = F_1^1 \cup F_2^1 \cup F_3^i \cup \{\bar{e}, \bar{f}\}$  for  $i = 2, \dots, r_3$ .
8.  $F = F_1^1 \cup F_2^1 \cup F_3^1 \cup \{\bar{e}, f\}$  for all edges  $f \neq \bar{f}$  with exactly one end vertex in  $S_1$  and one end vertex in  $S_3$ .
9.  $F = F_1^1 \cup F_2^1 \cup F_3^1 \cup \{\bar{f}, g\}$  for all edges  $g \neq \bar{g}$  with exactly one end vertex in  $S_2$  and one end vertex in  $S_3$ .

10.  $F = F_1^1 \cup F_2^1 \cup F_3^1 \cup \{\bar{g}, e\}$  for all edges  $e \neq \bar{e}$  with exactly one end vertex in  $S_1$  and one end vertex in  $S_2$ .
11.  $F = F_1^1 \cup F_2^1 \cup (F_3^1 \setminus \{\bar{h}_3\}) \cup \{\bar{e}, \bar{f}, \bar{g}\}$ .
12.  $F = F_1^1 \cup (F_2^1 \setminus \{\bar{h}_2\}) \cup F_3^1 \cup \{e_1, e_2, \bar{f}\}$ .
13.  $F = (F_1^1 \setminus \{\bar{h}_1\}) \cup F_2^1 \cup F_3^1 \cup \{e_1, e_2, \bar{f}\}$ .

Summing up, we obtain  $|E| + 1$  affinely independent vectors being tight in (6).

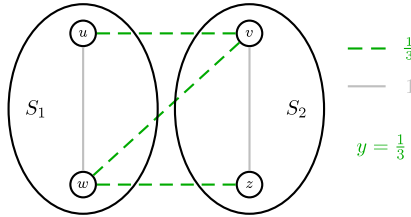
$|S_3| = 1$ : The only forest in  $S_3$  is the empty forest, therefore set  $F_3^1 = \emptyset$  and consider the same forests as before except the ones in 7 and 9 which do not exist. In total they sum up to  $|E| + 1$  forests again.

For each case of the disjoint vertex sets  $S_1$  and  $S_2$  with the required properties for the vertices  $u, v, w$  and  $z$ , the face induced by inequality (6) has dimension  $|E|$  and therefore is a facet of  $P_F^d$ .  $\square$

The two new classes of inequalities (5) and (6) lead to tighter descriptions of the polytopes  $P_F^c$  and  $P_F^d$ , respectively, as they take the influence of the product variable into account. The following example on four vertices shows that both classes of inequalities indeed cut off infeasible vectors which are feasible in the linearized and relaxed problem (QIP<sub>QMSF</sub>).

**Example 3.4.** Consider the fractional solution illustrated below, with non-zero values on the edge variables  $x_{\{u,w\}} = 1$ ,  $x_{\{v,z\}} = 1$ ,  $x_{\{u,v\}} = x_{\{v,w\}} = x_{\{w,z\}} = 1/3$ , and the value  $y = 1/3$  for the product variable.

This solution is feasible for the subtour elimination constraints (1) and satisfies (2) and (3), i.e., the inequalities of the standard linearization. However, the quadratic subtour elimination constraints (5) and (6) are both violated for the subset  $S_1$  and the subsets  $S_1$  and  $S_2$ , respectively.



Theorems 3.2 and 3.3 show that the quadratic subtour elimination constraints are needed in any complete polyhedral description of  $P_F^c$  and  $P_F^d$ , respectively. In the following, we show that they also suffice to describe these polyhedra completely, together with (1)–(3). However, we first consider the case of a nonnegative weight on the product variable, where it turns out that quadratic subtour elimination constraints are not needed.

**Proposition 3.5.** Let  $q_{e_1 e_2} \geq 0$ . Then the linear program

$$\begin{aligned}
 (LP^{\geq 0}) \quad & \min \sum_{e \in E} c_e x_e + q_{e_1 e_2} y \\
 \text{s.t.} \quad & \sum_{e \in E(G[S])} x_e \leq |S| - 1 \quad \forall \emptyset \neq S \subset V \\
 & y \leq x_{e_1}, x_{e_2} \\
 & y \geq x_{e_1} + x_{e_2} - 1 \\
 & x, y \geq 0
 \end{aligned}$$

has an integer optimal solution.

**Proof.** Let  $(x^*, y^*)$  be an optimal integer solution of  $(LP^{\geq 0})$ , so that  $x^*$  is the incidence vector of a spanning forest  $F^*$  and  $y^* = x_{e_1}^* x_{e_2}^*$ . It suffices to exhibit a feasible solution  $z^*$  of the dual of  $(LP^{\geq 0})$  such that  $(x^*, y^*)$  and  $z^*$  satisfy the complementary slackness conditions. Our construction uses a similar argumentative structure as given in the proof for a complete description of the spanning tree polytope given in [11], Theorem 6.12.

As  $F^*$  is a minimal spanning forest, for each of its edges the optimality criterion

$$c_e \leq 0 \quad \text{for } e \in E(F^*) \quad (7)$$

is satisfied, since edges with positive costs are not considered in an optimal solution, and for all edges not contained in the forest we have the optimality criteria

$$c_e \geq \begin{cases} c_f & \forall e \notin E(F^*) \text{ leading to a cycle } \mathcal{C}_e \text{ in } F^* \cup \{e\} \text{ and } \forall f \in \mathcal{C}_e \\ 0 & \forall e \notin E(F^*) \text{ otherwise} \end{cases} \quad (8)$$

as otherwise the insertion of  $e$ , eventually with a removal of  $f$ , would yield a better feasible solution.

In order to set up the dual problem, we introduce a dual variable  $z_S$  for each set  $\emptyset \neq S \subseteq V$ . Additionally, three variables  $z_1, z_2$  and  $z_{12}$  are needed for the linearization inequalities. We obtain

$$\begin{aligned}
 (\text{DP}^{\geq 0}) \quad & \max \quad - \sum_{\emptyset \neq S \subseteq V} (|S| - 1) z_S - z_{12} \\
 \text{s.t.} \quad & - \sum_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S \leq c_e \quad \forall e \in E \setminus \{e_1, e_2\} \\
 & - \sum_{\substack{S \subseteq V \\ e_1 \in E(G[S])}} z_S + z_1 - z_{12} \leq c_{e_1} \\
 & - \sum_{\substack{S \subseteq V \\ e_2 \in E(G[S])}} z_S + z_2 - z_{12} \leq c_{e_2} \\
 & -z_1 - z_2 + z_{12} \leq q_{e_1 e_2} \\
 & z_S, z_1, z_2, z_{12} \geq 0 \quad \forall \emptyset \neq S \subseteq V.
 \end{aligned}$$

We first assume that none of the edges  $e_1$  and  $e_2$  belongs to  $F^*$ , so that  $y^* = 0$ . Our construction of  $z^*$  starts as in the proof given in [11]: let the edges  $E(F^*) = \{f_1, \dots, f_{m-1}\}$  of the optimal spanning forest  $F^*$  be sorted by ascending costs, i.e.  $c_{f_1} \leq \dots \leq c_{f_{m-1}}$ . For  $k = 1, \dots, m-1$ , let  $S_k \subseteq V$  be the connected component of the subgraph  $(V, \{f_1, \dots, f_k\})$  containing edge  $f_k$ . Now for  $k \leq m-2$ , we assign  $z_{S_k}^* := c_{f_l} - c_{f_k}$ , where  $l$  is the first index greater than  $k$  for which  $f_l \cap S_k \neq \emptyset$ . Additionally, we set  $z_{S_{m-1}}^* := -c_{f_{m-1}}$  and  $z_S^* := 0$  for all  $S \notin \{S_1, \dots, S_{m-1}\}$ . Note that by this construction we have  $z_S \geq 0$  for all  $S \subseteq V$  due to the ascending sorting and due to (7). Finally, we assign  $z_1^* := 0, z_2^* := 0$  and  $z_{12}^* := 0$ . If the end vertices of an edge  $e$  are in the same connected component of  $F^*$ , this construction yields

$$- \sum_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S = c_{f_i},$$

see [11], where  $i$  is the smallest index with  $e \subseteq S_i$ . If otherwise the end vertices are in different connected components of  $F^*$ , we have

$$- \sum_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S = 0.$$

The solution  $z^*$  is thus dual feasible by (8). Moreover, the dual constraint corresponding to an edge  $e$  is satisfied with equality whenever  $x_e^* > 0$ , whereas  $z_S^* > 0$  implies that the corresponding subtour elimination constraint is tight. In summary, the complementary slackness conditions are satisfied by  $(x^*, y^*)$  and  $z^*$ .

Now let only one of the product edges, say  $e_1$ , be contained in  $F^*$ , i.e.  $x_{e_1}^* = 1, x_{e_2}^* = 0$  and thus  $y^* = 0$ . Then, the optimality criterion (7) still holds, but if insertion of  $e_2$  leads to a cycle  $C_{e_2}$ , the corresponding inequalities (8) are no longer valid for  $e_2$  and  $f \in C_{e_2}$  but only the weaker optimality criterion

$$c_{e_2} + q_{e_1 e_2} \geq c_f \quad \forall f \in C_{e_2} \setminus \{e_1\}. \quad (9)$$

We construct  $z^*$  analogously but define  $z_1^* := q_{e_1 e_2}$  and  $z_{12}^* := q_{e_1 e_2}$ ; thus  $z_1^*, z_{12}^* \geq 0$ . For all edges  $e \neq e_1, e_2$  the complementary slackness constraints are satisfied by (8) and the same arguments as before. For edge  $e_1$  we have equality in the dual problem by  $z_1^* = z_{12}^*$  and  $x_{e_1}^* > 0$ ; in particular, we obtain complementary slackness. Furthermore, if the insertion of  $e_2$  leads to a cycle, the left hand side of the inequality corresponding to  $e_2$  equals  $c_{f_i} - q_{e_1 e_2}$  which in turn is not greater than  $c_{e_2}$  due to optimality criterion (9). Otherwise, the left hand side equals  $-q_{e_1 e_2} \leq 0$  such that complementary slackness is satisfied by optimality criterion (8). Finally,  $-z_1^* - z_2^* + z_{12}^* = 0 \leq q_{e_1 e_2}$  proves dual feasibility of  $z^*$ .

It thus remains to consider the case that  $F^*$  contains both  $e_1$  and  $e_2$ . Then, the optimality criterion (7) does not hold for  $e_1, e_2$  but we have

$$c_{e_1} + q_{e_1 e_2} \leq 0 \quad \text{and} \quad c_{e_2} + q_{e_1 e_2} \leq 0, \quad (10)$$

since otherwise removing one of these edges would increase the solution value. In this case we change the entire construction of the dual solution by considering a modified objective function

$$\tilde{c}_e := \begin{cases} c_e & \text{if } e \in E \setminus \{e_1, e_2\} \\ c_{e_1} + q_{e_1 e_2} & \text{if } e = e_1 \\ c_{e_2} + q_{e_1 e_2} & \text{if } e = e_2 \end{cases}$$

and by recomputing the basic dual solution  $z^*$  according to this new cost function  $\tilde{c}$  instead of  $c$ . Note that  $\tilde{c}_{e_1}, \tilde{c}_{e_2} \leq 0$  because of (10). Moreover, we set  $z_{12}^* := q_{e_1 e_2}$  in this case. Again, this solution turns out to be dual feasible and complementary slackness conditions corresponding to all  $x_e^* > 0$  as well as to all  $z_S^* > 0$  are satisfied. The additional complementary slackness condition resulting from  $y^* > 0$  is  $z_{12}^* = q_{e_1 e_2}$  and hence satisfied by definition.  $\square$



The modified objective function  $\tilde{c}$ , used in the last case of the preceding proof, is motivated by the following reasoning: if the optimal forest contains both edges  $e_1$  and  $e_2$ , then removing one of these edges not only decreases the objective function by the linear weight  $c_{e_1}$  or  $c_{e_2}$ , but also by the product weight  $q_{e_1 e_2}$ , as the variable  $y$  switches to zero as well in this case. The linear optimality criterion (8) can thus be extended to  $\tilde{c}$ .

Proposition 3.5 shows that quadratic subtour elimination constraints are not needed if the objective function coefficient of the single product term is nonnegative. Nevertheless, for general objective functions, Example 3.4 shows that the quadratic subtour elimination constraints lead to a tighter description of the corresponding polytope. In fact, we can show that they even yield a complete polyhedral description of  $P_F^c$  and  $P_F^d$ , respectively.

### Theorem 3.6.

$$P_F^c = \{(x, y) \in [0, 1]^{|E|+1} \mid (x, y) \text{ satisfies (1), (2), (3) and (5)}\}.$$

**Proof.** All constraints (1), (2), (3), and (5) are valid for  $P_F^c$ , it thus remains to show that they yield a complete polyhedral description of  $P_F^c$ . As in the proof of Proposition 3.5, we use duality. The primal problem reads

$$\begin{aligned} \text{(LP)} \quad & \min \sum_{e \in E} c_e x_e + q_{e_1 e_2} y \\ \text{s.t.} \quad & \sum_{e \in E(G[S])} x_e + y \leq |S| - 1 \quad \text{for } \emptyset \neq S \subset V \text{ with } u, w \in S, v \notin S \\ & \sum_{e \in E(G[S])} x_e \leq |S| - 1 \quad \text{for } S \subseteq V \text{ else} \\ & y \leq x_{e_1}, x_{e_2} \\ & y \geq x_{e_1} + x_{e_2} - 1 \\ & x, y \geq 0. \end{aligned}$$

Again, we introduce a dual variable  $z_S$  for each  $\emptyset \neq S \subseteq V$  and one variable each for the three linearization inequalities, denoted by  $z_1, z_2$  and  $z_{12}$ . The dual then turns out to be

$$\begin{aligned} \text{(DP)} \quad & \max - \sum_{\emptyset \neq S \subseteq V} (|S| - 1) z_S - z_{12} \\ \text{s.t.} \quad & - \sum_{\substack{S \subseteq V \\ e \in E(G[S])}} z_S \leq c_e \quad \text{for } e \in E \setminus \{e_1, e_2\} \quad \text{(d1)} \\ & - \sum_{\substack{S \subseteq V \\ e_1 \in E(G[S])}} z_S + z_1 - z_{12} \leq c_{e_1} \quad \text{(d2)} \\ & - \sum_{\substack{S \subseteq V \\ e_2 \in E(G[S])}} z_S + z_2 - z_{12} \leq c_{e_2} \quad \text{(d3)} \\ & - \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S - z_1 - z_2 + z_{12} \leq q_{e_1 e_2} \quad \text{(d4)} \\ & z_S, z_1, z_2, z_{12} \geq 0 \quad \text{for } \emptyset \neq S \subseteq V. \end{aligned}$$

Let  $(x^*, y^*)$  be an optimal integer solution of (LP), so that  $x^*$  is the incidence vector of a spanning forest  $F^*$  and  $y^* = x_{e_1}^* x_{e_2}^*$ . As in the proof of Proposition 3.5, we sort the forest edges  $E(F^*) = \{f_1, \dots, f_{m-1}\}$  by ascending costs, construct the connected components  $S_k$  and define the corresponding basic dual solution  $z^*$ , to be modified in the following. Note that again optimality criteria (7) and (8) hold such that  $S_k \geq 0$  and the dual constraint (d1) follows as in the linear case by construction. Moreover we can assume  $q_{e_1 e_2} < 0$  by Proposition 3.5.

As the spanning forest  $F^*$  can either contain or not contain the edges  $e_1$  and  $e_2$ , we split up the construction of the dual solution into four cases two of which are symmetric.

$x_{e_1}^* = x_{e_2}^* = y^* = 0$ , i.e. none of the edges  $e_1$  and  $e_2$  belong to  $F^*$ .

Initially, consider the case that the three vertices  $u, v$  and  $w$  are connected in  $F^*$ . Let  $r$  be the smallest index with  $|S_r \cap \{u, v, w\}| = 2$  and  $t$  the smallest index with  $\{u, v, w\} \subseteq S_t$ . In the following, we distinguish between two cases: either  $S_r$  contains  $u$  and  $v$  (case I), or it contains  $u$  and  $w$  (case II). The case that  $S_r$  contains  $v$  and  $w$  is analogous to case I.

In both cases,  $e_1, e_2 \notin F^*$  yields the optimality criterion

$$c_{e_1} + c_{e_2} + q_{e_1 e_2} \geq c_{f_r} + c_{f_t} \quad (11)$$

as otherwise replacing  $f_r$  and  $f_t$  by  $e_1$  and  $e_2$  in  $E(F^*)$  would yield a strictly better solution than  $(x^*, y^*)$ .

Case I: We extend the basic dual solution by setting

$$z_1^* := c_{e_1} - c_{f_r}, \quad z_2^* := c_{e_2} - c_{f_t}, \quad z_{12}^* := 0.$$



This solution satisfies (d2) with equality, as

$$- \sum_{\substack{S \subseteq V \\ e_1 \in E(G[S])}} z_S^* + z_1^* - z_{12}^* = c_{f_r} + c_{e_1} - c_{f_r} = c_{e_1},$$

and equality in (d3) follows analogously. To show (d4), we use the optimality criterion (11) and the fact that  $z_S^* = 0$  for all  $S \subset V$  with  $u, w \in S, v \notin S$ . This leads to

$$- \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* - z_1^* - z_2^* + z_{12}^* = c_{f_r} - c_{e_1} + c_{f_t} - c_{e_2} \leq q_{e_1 e_2}.$$

*Case II:* As  $t$  is both minimal with  $u, v \in S_t$  and with  $v, w \in S_t$ , the first sums on the left hand sides of (d2) and (d3) both equal  $c_{f_t}$ . Adding

$$z_1^* := c_{e_1} - c_{f_t}, \quad z_2^* := c_{e_2} - c_{f_t}, \quad z_{12}^* := 0$$

to the basic dual solution, we obtain equality in both (d2) and (d3). Inequality (d4) is satisfied since

$$- \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* - z_1^* - z_2^* + z_{12}^* = c_{f_r} - c_{f_t} - z_1^* - z_2^* = c_{f_r} - c_{e_1} + c_{f_t} - c_{e_2},$$

which by optimality criterion (11) is bounded by  $q_{e_1 e_2}$ .

Now consider the case that only two of the three vertices  $u, v$  and  $w$  are connected. Then again, let  $r$  be the index with  $|S_r \cap \{u, v, w\}| = 2$  such that we have the optimality criterion

$$c_{e_1} + c_{e_2} + q_{e_1 e_2} \geq c_{f_r}. \quad (12)$$

*Case I:*  $u, v \in S_r$  results in  $c_{e_2} \geq 0$  by optimality criterion (8). We extend  $z^*$  by

$$z_1^* := c_{e_1} - c_{f_r}, \quad z_2^* := c_{e_2}, \quad z_{12}^* := 0.$$

Then, (d2) is satisfied with equality by the same arguments as before. As there is no edge in  $F^*$  connecting  $u$  or  $v$  with  $w$ , we have

$$- \sum_{\substack{S \subseteq V \\ e_1 \in E(G[S])}} z_S^* = 0 \quad \text{and} \quad - \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* = 0,$$

such that the left hand sides of (d3) and (d4) sum up to  $c_{f_r} - c_{e_1} - c_{e_2}$ . By (12), this is not greater than  $q_{e_1 e_2} \leq 0 \leq c_{e_2}$ , such that we have feasibility in both (d3) and (d4).

*Case II:*  $u, w \in S_r$  and (8) lead to  $c_{e_1}, c_{e_2} \geq 0$ . We set

$$z_1^* := c_{e_1}, \quad z_2^* := c_{e_2}, \quad z_{12}^* := 0.$$

Then, we obtain

$$- \sum_{\substack{S \subseteq V \\ e_1 \in E(G[S])}} z_S^* - z_1^* = -c_{e_1} \leq 0 \leq c_{e_1}, \quad - \sum_{\substack{S \subseteq V \\ e_2 \in E(G[S])}} z_S^* - z_2^* = -c_{e_2} \leq 0 \leq c_{e_2},$$

and with  $u, w \in S_r$

$$- \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* = c_{f_r} - c_{e_1} - c_{e_2} \leq q_{e_1 e_2}.$$

Finally, if  $u, v$  and  $w$  are in pairwise different components of  $F^*$ , we have  $c_{e_1}, c_{e_2} \geq 0$  by (8) and the optimality criterion

$$c_{e_1} + c_{e_2} + q_{e_1 e_2} \geq 0. \quad (13)$$

We again extend  $z^*$  by

$$z_1^* := c_{e_1}, \quad z_2^* := c_{e_2}, \quad z_{12}^* := 0$$

such that (d2) and (d3) are satisfied as in case II directly above and we have

$$- \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* = 0 - c_{e_1} - c_{e_2} \leq q_{e_1 e_2}$$

due to (13).

We have thus constructed a dual feasible solution in all cases of  $e_1, e_2 \notin F^*$ . The complementary slackness conditions for  $x_e^* > 0$  and  $z_S^* > 0$  are satisfied as in the linear case, while the remaining ones are satisfied by the construction of  $z_1^*, z_2^*$  and  $z_{12}^*$ .

$x_{e_1}^* = 1, x_{e_2}^* = 0, y^* = 0$  (the case  $x_{e_1}^* = 0, x_{e_2}^* = 1, y^* = 0$  is analogous).

In this case we again make use of the optimality criteria (7)–(9) and first of all we consider the case where the vertices  $u, v$  and  $w$  are connected in  $F^*$ . Let again  $r$  be the smallest index with  $|S_r \cap \{u, v, w\}| = 2$  and  $t$  be the smallest index with  $\{u, v, w\} \subseteq S_t$ . We again distinguish between the cases where either  $u, v \in S_r$  (case I) or  $u, w \in S_r$  (case II). The case  $v, w \in S_r$  is analogous to case I.

*Case I:* We set

$$z_1^* := 0, \quad z_2^* := -q_{e_1 e_2}, \quad z_{12}^* := 0.$$

Note that  $q_{e_1 e_2} < 0$  implies  $z_2^* > 0$ . Inequality (d2) is satisfied as in the linear case. Furthermore, from (9) we derive

$$- \sum_{\substack{S \subseteq V \\ e_2 \in E(G[S])}} z_S^* + z_2^* = c_{f_t} - q_{e_1 e_2} \leq c_{e_2};$$

this shows (d3). Constraint (d4) is trivially satisfied in case I, since  $z_S^* = 0$  for all sets  $S$  with  $u, w \in S, v \notin S$ .

*Case II:* We set

$$z_1^* := 0, \quad z_2^* := c_{e_2} - c_{e_1}, \quad z_{12}^* := 0.$$

Note that (7) and (8) guarantee  $z_2^* \geq 0$ . Inequality (d2) is satisfied as in the linear case. Being in case II, we have  $f_t = e_1$ , so that we obtain equality in (d3)

$$- \sum_{\substack{S \subseteq V \\ e_2 \in E(G[S])}} z_S^* + z_2^* = c_{f_t} + c_{e_2} - c_{e_1} = c_{e_2}$$

and feasibility in (d4), since

$$- \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* - z_1^* - z_2^* + z_{12}^* = c_{f_r} - c_{f_t} - c_{e_2} + c_{e_1} = c_{f_r} - c_{e_2} \leq q_{e_1 e_2}$$

due to (9), as  $f_r \in \mathcal{C}_{e_2}$ .

Now consider the case that  $w$  is not connected with  $u$  and  $v$ . Then we obtain the additional optimality criterion

$$c_{e_2} + q_{e_1 e_2} \geq 0 \tag{14}$$

and set

$$z_1^* := 0, \quad z_2^* := -q_{e_1 e_2}, \quad z_{12}^* := 0.$$

By the same arguments as in case I we obtain feasibility in (d2) and (d4), furthermore, the left hand side of (d3) equals  $-q_{e_1 e_2}$  which is not greater than  $c_{e_2}$  due to (14).

In all cases, the complementary slackness conditions for  $x_e^* > 0$  and  $z_S^* > 0$  are satisfied as in the linear case, observing  $z_1^* = 0$  and  $z_{12}^* = 0$  for equality in (d2). The remaining complementary slackness conditions are satisfied by construction.

$x_{e_1}^* = x_{e_2}^* = y^* = 1$ , i.e. both  $e_1, e_2 \in F^*$ .

Let  $F'$  be a minimal linear spanning forest subject to the cost function  $c$ , where we may assume  $E(F^*) \setminus E(F') \subseteq \{e_1, e_2\}$ . Define the sets  $S_k$  and the basic solution  $z^*$  as before, but based on the forest  $F'$  instead of  $F^*$ . Let  $r$  be the smallest index with  $|S_r \cap \{u, v, w\}| = 2$  and let  $t$  be the smallest index with  $\{u, v, w\} \subseteq S_t$ . We again distinguish between the two cases that either  $S_r$  contains  $u$  and  $v$  (case I), or it contains  $u$  and  $w$  (case II). The case that  $S_r$  contains  $v$  and  $w$  is analogous to case I.

In both cases, we obtain (d1) as in the linear case. Moreover, we can derive

$$c_{f_r} + c_{f_t} \geq c_{e_1} + c_{e_2} + q_{e_1 e_2} \tag{15}$$

from the optimality of  $F^*$ , as otherwise the forest  $F'$  would yield a better solution of (LP) than  $F^*$ . Note that we do not exclude that  $e_1$  or  $e_2$  agree with  $f_r$  or  $f_t$ .

*Case I:* We extend  $z^*$  by setting

$$z_1^* := c_{e_1} - c_{f_r}, \quad z_2^* := c_{e_2} - c_{f_t}, \quad z_{12}^* := 0, \quad z_{\{u, w\}}^* := -q_{e_1 e_2} - z_1^* - z_2^*.$$

Optimality of  $F'$  yields  $z_1^* \geq 0$  and  $z_2^* \geq 0$ , while  $z_{\{u, w\}}^* \geq 0$  follows from (15). We now obtain equality in both (d2) and (d3), as

$$- \sum_{\substack{S \subseteq V \\ e_1 \in E(G[S])}} z_S^* + z_1^* - z_{12}^* = c_{f_r} + c_{e_1} - c_{f_r} = c_{e_1}$$

and

$$- \sum_{\substack{S \subseteq V \\ e_2 \in E(G[S])}} z_S^* + z_2^* - z_{12}^* = c_{f_t} + c_{e_2} - c_{f_t} = c_{e_2}.$$

Equality in (d4) also follows, since

$$\sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* = z_{\{u, w\}}^*$$

in case I and hence

$$- \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* - z_1^* - z_2^* + z_{12}^* = q_{e_1 e_2} + z_1^* + z_2^* - z_1^* - z_2^* = q_{e_1 e_2}.$$

*Case II:* We extend  $z^*$  by setting

$$z_1^* := c_{e_1} - c_{f_t}, \quad z_2^* := c_{e_2} - c_{f_t}, \quad z_{12}^* := 0, \quad z_{\{u, w\}}^* := -q_{e_1 e_2} - z_1^* - z_2^*.$$

Note that  $z_1^* \geq 0$ , as we are in case II. Moreover, we have  $z_2^* \geq 0$  by optimality of  $T'$ , and  $z_{\{u, w\}}^* \geq 0$  as

$$-q_{e_1 e_2} - c_{e_1} + c_{f_t} - c_{e_2} + c_{f_t} \geq -q_{e_1 e_2} - c_{e_1} + c_{f_t} - c_{e_2} + c_{f_t} \geq 0$$

by  $c_{f_t} \geq c_{f_r}$  and (15). Insertion into (d2)–(d4) yields equality:

$$\begin{aligned} - \sum_{\substack{S \subseteq V \\ e_1 \in E(G[S])}} z_S^* + z_1^* - z_{12}^* &= c_{f_t} + c_{e_1} - c_{f_t} = c_{e_1}, \\ - \sum_{\substack{S \subseteq V \\ e_2 \in E(G[S])}} z_S^* + z_2^* - z_{12}^* &= c_{f_t} + c_{e_2} - c_{f_t} = c_{e_2}, \\ - \sum_{\substack{S \subseteq V \\ u, w \in S, v \notin S}} z_S^* - z_1^* - z_2^* + z_{12}^* &= q_{e_1 e_2} + z_1^* + z_2^* - z_1^* - z_2^* = q_{e_1 e_2}. \end{aligned}$$

In both cases, the complementary slackness conditions are satisfied, noting that equality in (d2)–(d4) holds as required by  $x_{e_1}^* = x_{e_2}^* = y^* = 1$ , and that setting  $z_{\{u, w\}}^* > 0$  does not violate the complementary slackness conditions, since the subtour elimination constraint for  $S = \{u, w\}$  is satisfied with equality. Moreover, setting  $z_{\{u, w\}}^* > 0$  increases the slack only in (d1) and only for edge  $\{u, w\}$ , in which case equality is not required.  $\square$

The above proof shows that the constraint  $y \geq x_{e_1} + x_{e_2} - 1$ , corresponding to the dual variable  $z_{12}^*$ , is only needed in the case  $q_{e_1 e_2} \geq 0$ , which was addressed in Proposition 3.5.

### Theorem 3.7.

$$P_F^d = \{(x, y) \in [0, 1]^{|E|+1} \mid (x, y) \text{ satisfies (1), (2), (3) and (6)}\}.$$

**Proof.** Analogous to the proof of Theorem 3.6.  $\square$

To conclude this section, we remark that these results cannot easily be generalized to the case of matroid polytopes, as one might be tempted to believe, considering that the forests in  $G$  form the independent sets of the graphic matroid of  $G$ . E.g., for the uniform matroid, one can show that the convex hull of the linearized problem with one quadratic term has an exponential number of facets, while the corresponding polytope in the linear case has a compact polyhedral description. In particular, it is not possible in general to obtain a polyhedral description of the one-product case by adding  $y$  to the left hand side of facets of the linear case.

## 4. Complete polyhedral descriptions for spanning trees

It is well-known that a complete polyhedral description of the spanning tree problem in the linear case is given by nonnegativity and the constraints (1) and (4), i.e., by adding the cardinality constraint (4) to the complete description of the spanning forest polytope. In fact, we will show that even our polyhedral results obtained for the spanning forest problem with one quadratic term can be carried over to the spanning tree problem with one quadratic term.

First of all, we can derive the dimension of the polytopes in the spanning tree case from Theorem 3.1, since all incidence vectors constructed in the corresponding proof remain feasible, except for the first one.

**Corollary 4.1.**

$$\dim(P_T^c) = \dim(P_T^d) = |E|.$$

Furthermore, the quadratic subtour elimination constraints remain facet defining in both cases.

**Corollary 4.2.** (a) Let  $S_1 \subset V$  be a set of vertices with  $u, w \in S_1$  and  $v \in V \setminus S_1$ . Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + y \leq |S_1| - 1$$

is valid and induces a facet of  $P_T^c$ .

(b) Let  $S_1, S_2 \subset V$  be disjoint subsets of vertices such that both edges  $\{u, v\}$  and  $\{w, z\}$  have exactly one end vertex in  $S_1$  and one end vertex in  $S_2$ . Then the inequality

$$\sum_{e \in E(G[S_1])} x_e + \sum_{e \in E(G[S_2])} x_e + y \leq |S_1| + |S_2| - 2$$

is valid and induces a facet of  $P_T^d$ .

**Proof.** Validity of (5) follows by  $P_T^c \subset P_F^c$  and  $P_T^d \subset P_F^d$ , i.e., each valid inequality for the quadratic spanning forest polytope remains valid for the quadratic spanning tree polytope. For the facet-inducing property, consider the incidence vectors of Theorem 3.2 in case (a) and of Theorem 3.3 in case (b). All these vectors except the first one of each case also satisfy the cardinality constraint (4). Without these first vectors we result in  $|E|$  feasible and affinely independent vectors in each case.  $\square$

In the spanning forest case, the main result of Section 3 states that the quadratic subtour elimination constraints yield a complete description of the spanning forest polytope with one quadratic term, when added to the well-known polyhedral description of the linear case and the standard linearization constraints. The same statement remains true for spanning trees, which is a direct consequence of the following observation.

**Lemma 4.3.** (a)  $P_T^c$  is a face of  $P_F^c$ .

(b)  $P_T^d$  is a face of  $P_F^d$ .

**Proof.** By the subtour elimination constraints (1), one direction of the cardinality constraint (4) is valid for both polytopes  $P_F^c$  and  $P_F^d$ , so that (4) induces a face in both polytopes. In particular, the intersection of both  $P_F^c$  and  $P_F^d$  with (4) is an integer polytope and hence by definition agrees with  $P_T^c$  and  $P_T^d$ , respectively.  $\square$

Using Lemma 4.3, we derive the following results from Proposition 3.5 and Theorems 3.6 and 3.7, respectively.

**Corollary 4.4.** Let  $q_{e_1 e_2} \geq 0$ . Then the linear program

$$\begin{aligned} \min \quad & \sum_{e \in E} c_e x_e + q_{e_1 e_2} y \\ \text{s.t.} \quad & \sum_{e \in E} x_e = |V| - 1 \\ & \sum_{e \in E(G[S])} x_e \leq |S| - 1 \quad \forall \emptyset \neq S \subset V \\ & y \leq x_{e_1}, x_{e_2} \\ & y \geq x_{e_1} + x_{e_2} - 1 \\ & x, y \geq 0 \end{aligned}$$

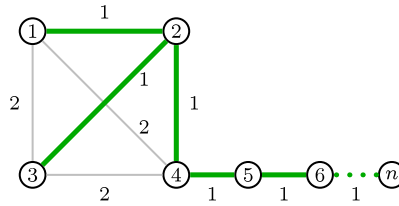
has an integer optimal solution.

**Corollary 4.5.** (a)  $P_T^c = \{(x, y) \in [0, 1]^{|E|+1} \mid (x, y) \text{ satisfies (1), (2), (3), (4), and (5)}\}$ .

(b)  $P_T^d = \{(x, y) \in [0, 1]^{|E|+1} \mid (x, y) \text{ satisfies (1), (2), (3), (4), and (6)}\}$ .

One might wonder whether the result of Corollary 4.4 also holds in the case of more than one quadratic term. The following example shows that for the spanning tree case this is not true in general even in the case of a fixed number of quadratic terms, even if the corresponding optimization problem is still tractable in this case.

**Example 4.6.** Consider the graph  $K_n = (V, E)$ . The costs of single edges are indicated in the illustration on the right; the omitted edges are assigned a cost value large enough to ensure that they never appear in any optimal solution. Quadratic costs  $q_{ef}$  are only given for the products of edges in the subgraph induced by  $T := \{1, 2, 3, 4\}$ ; they are set to 2.



The optimal integral solution of

$$\begin{aligned}
 \min \quad & \sum_{e \in E} c_e x_e + \sum_{\{e,f\} \in E(G[T])} q_{ef} y_{ef} \\
 \text{s.t.} \quad & \sum_{e \in E} x_e = |V| - 1 \\
 & \sum_{e \in E(G[S])} x_e \leq |S| - 1 \quad \text{for } \emptyset \neq S \subset V \\
 & y \leq x_{e_1}, x_{e_2} \quad \text{for } e, f \in E(G[T]) \\
 & y \geq x_{e_1} + x_{e_2} - 1 \quad \text{for } e, f \in E(G[T]) \\
 & x, y \geq 0
 \end{aligned}$$

is the vector  $(x^*, y^*)$  with  $x^*$  being the incidence vector of the spanning tree given by the highlighted edge set  $\{\{1, 2\}, \{2, 3\}, \{2, 4\}, \{4, 5\}, \{5, 6\}, \dots, \{n-1, n\}\}$  and  $y^*$  being the corresponding linearization vector, with an objective value of  $n + 5$ . However,  $(x^*, y^*)$  is not optimal for the LP relaxation stated above, as there exists a feasible solution with lower objective value  $n + \frac{7}{3}$ , given as follows:

- $x_{\{1,2\}} = x_{\{1,3\}} = x_{\{1,4\}} = \frac{1}{3}$ ,
- $x_{\{2,3\}} = x_{\{2,4\}} = x_{\{3,4\}} = \frac{2}{3}$ ,
- $x_{\{4,5\}} = x_{\{5,6\}} = \dots = x_{\{n-1,n\}} = 1$ ,
- $y_{\{2,3\}\{2,4\}} = y_{\{2,3\}\{3,4\}} = y_{\{2,4\}\{3,4\}} = \frac{1}{3}$ ,
- $x_e = 0$  and  $y_{ef} = 0$  otherwise.

## 5. Separation routines

All three classes of subtour elimination constraints (1), (5) and (6) are of exponential size, so that these inequalities cannot be separated by enumeration. Therefore, to use these inequalities within a cutting plane approach, a polynomial time separation routine is required. For (1), a well-known separation algorithm is based on a minimal cut algorithm. For the sake of clarity and completeness, we shortly review the concept of this separation routine. Details of the reformulations can be found in [19].

### Separation of linear subtour elimination constraints

Let  $x^* \in [0, 1]^{|E|}$ . For  $i \in V$  define  $d_i := 2 - \sum_{e \in \delta(i)} x_e^*$  and rewrite

$$\begin{aligned}
 \sum_{e \in E(G[S])} x_e^* - |S| &= -\frac{1}{2} \left( \sum_{e \in \delta(S)} x_e^* + \sum_{i \in S} d_i \right) \\
 &= -\frac{1}{2} \left( \underbrace{\left( \sum_{e \in \delta(S)} x_e^* + \sum_{\substack{i \in S \\ d_i > 0}} d_i - \sum_{\substack{i \in V \setminus S \\ d_i < 0}} d_i \right)}_{=: f(S)} + \underbrace{\sum_{\substack{i \in V \\ d_i < 0}} d_i}_{=: \kappa} \right).
 \end{aligned}$$

Now there exists a violated subtour elimination constraint, corresponding to some set  $S$ , if and only if there exists a nonempty set  $S \subseteq V$  with

$$\sum_{e \in E(G[S])} x_e^* - |S| > -1. \quad (16)$$

As  $\kappa$  is a constant, this can be decided by minimizing  $f(S)$  over all  $\emptyset \neq S \subseteq V$ . For this purpose, construct a directed network  $G' := (V', E', c)$ : double all edges of  $G$ , direct them reversely and set capacities  $c_{(i,j)} = c_{(j,i)} = x_{\{i,j\}}^*$ . Add two vertices  $s$  and  $t$  with directed edges from  $s$  to  $i$  if  $d_i > 0$  and from  $i$  to  $t$  if  $d_i < 0$ . Set the capacities on these edges to  $c_{[s,i]} = d_i$

and  $c_{[i,t]} = -d_i$ . Then,

$$f(S) = \sum_{e \in \delta_{E'}^{\text{in}}(S \cup \{t\})} c_e,$$

which is the value of a cut set in  $G'$  containing  $t$  and which is to minimize. As  $S$  must not be empty, for each vertex  $i \in V$  a minimal cut has to be computed with  $i$  being linked to  $t$  by setting  $c_{[i,t]} = \infty$ . This in turn leads to  $|V|$  maximal flow problems. Each of the corresponding  $|V|$  sets satisfying (16) yields a violated subtour elimination constraint. If no such set satisfies (16), then  $x^*$  is valid for (1).

### Separation of quadratic subtour elimination constraints

#### Connected case:

For the separation of constraints (5) we propose a highly analogous algorithm. Again, the values  $d_i$  and the network are defined and, with appropriate fixings, a maximal  $s$ – $t$ -flow is calculated. There are only two differences to consider. The first one is the additional  $y$ -term, i.e., a vector  $(x^*, y^*) \in [0, 1]^{|E|+1}$  violates an inequality of type (5) if there exists a set  $S_1$  with

$$\sum_{e \in E(G[S_1])} x_e^* - |S_1| > -1 - y^*. \quad (17)$$

Second, only those subsets  $S_1$  including the vertices  $u$  and  $w$  but excluding vertex  $v$  are feasible. Therefore, we set infinite capacities on the edges  $\{u, t\}$ ,  $\{w, t\}$  and  $\{s, v\}$ . As a result, only a single maximal  $s$ – $t$ -flow has to be computed, since the cut cannot be empty in this context. Afterwards, it has to be checked whether the subset  $S_1$  on the  $t$ -side of the corresponding cut satisfies inequality (17).

#### Disconnected case:

The separation of constraints (6) is slightly more complicated. We can rewrite (6) as

$$\sum_{e \in E(G[S_1])} x_e^* - |S_1| + \sum_{e \in E(G[S_2])} x_e^* - |S_2| \leq -2 - y^*.$$

This in turn is equivalent to

$$4 + 2y^* + 2\kappa \leq \sum_{e \in \delta_{E'}^{\text{in}}(S_1 \cup \{t\})} c_e + \sum_{e \in \delta_{E'}^{\text{in}}(S_2 \cup \{t\})} c_e.$$

The requirement that  $e_1$  and  $e_2$  have to connect  $S_1$  and  $S_2$  leads to four cases out of which we describe the case  $u, w \in S_1$  and  $v, z \in S_2$ ; the other cases can be handled analogously. As in the former separation routines, we define  $d_i$  and the network with capacities, set infinite costs on the edges  $\{u, t\}$ ,  $\{w, t\}$ ,  $\{s, v\}$  and  $\{s, z\}$  and calculate the minimal cut set  $S_1$  containing  $t$ . In a second step, we go for the same but invert the linkings to  $s$  and  $t$  and calculate the minimal cut set  $S_2$  containing  $t$ . The combination of  $S_1$  and  $S_2$  is used to check inequality (6) for violation. Although this approach does not necessarily lead to disjoint sets  $S_1$  and  $S_2$ , the separation routine is correct, as the inequality remains valid for non-disjoint sets  $S_1$  and  $S_2$ .

In all cases, the proposed separation algorithms can be implemented to run in polynomial time, as at most eight maximum  $s$ – $t$ -flows have to be calculated.

## 6. Experimental results

In the previous sections, we could derive complete polyhedral descriptions and efficient separation algorithms for the polytopes obtained from adding and linearizing a single quadratic term to the spanning forest or spanning tree problem. Our ultimate motivation, however, is to solve the problem in the case where more or all quadratic terms are present in the objective function. Since all inequalities obtained in the case of a single quadratic term remain valid in this setting, we can apply our results to each quadratic term individually, one after another, and thus obtain a separation algorithm for the general QMSF and QMST problems.

Our aim in the following is to determine the impact of such a separation algorithm in terms of the bound improvement. Therefore, we implemented the devised separation algorithms and embedded them into the branch-and-cut software SCIL [20]. We considered the basic problem formulation using Constraints (1)–(3) where the subtour elimination constraints were separated dynamically and no further reformulation was applied (called *stdlin* in the following). For comparison, we then separated the quadratic subtour elimination constraints (5) and (6) for each of the appearing products (*qsec*). As it turns out that the constraints (6) often do not lead to a significant improvement, and since in many application we only have connected quadratic terms in the objective function, we also consider the separation approach only using the constraints (5), denoted by *qsec<sup>c</sup>*.

We tested random graphs generated as in [4]. For a given number  $n$  and a given density  $d$ , we produce a random graph with  $n$  vertices and  $\lfloor \binom{n}{2} d \rfloor$  edges. All edges obtain random integer coefficients in the range  $\{1, \dots, 10\}$ . We consider instances where either all possible products of variables have non-zero coefficients or where only connected products are present. All non-zero quadratic coefficients are chosen either from  $\{-100, \dots, -1\}$  or  $\{1, \dots, 100\}$ .

**Table 1**

Results for spanning forests with negative coefficients on connected terms; each line reports averages over ten random instances.

Vertices	Density	sep	# subs	# LPs	cputime	septime	rootgap
10	20%	stdlin	1.00	2.00	0.00	0.00	0.00%
		+qsec <sup>c</sup>	1.00	2.00	0.00	0.00	0.00%
	30%	stdlin	20.40	23.10	0.01	0.00	31.01%
		+qsec <sup>c</sup>	8.20	12.70	0.01	0.00	17.30%
	40%	stdlin	62.60	63.90	0.05	0.00	47.73%
		+qsec <sup>c</sup>	26.20	34.00	0.05	0.01	41.06%
	50%	stdlin	308.20	284.50	0.35	0.01	69.61%
		+qsec <sup>c</sup>	128.20	149.70	0.41	0.07	63.25%
	12	stdlin	7.20	8.30	0.00	0.00	12.65%
		+qsec <sup>c</sup>	3.20	5.30	0.00	0.00	4.75%
		stdlin	64.20	62.70	0.04	0.00	38.71%
		+qsec <sup>c</sup>	27.40	33.80	0.04	0.01	31.52%
		stdlin	358.20	317.20	0.45	0.04	57.46%
		+qsec <sup>c</sup>	112.80	141.60	0.38	0.08	52.26%
		stdlin	1473.80	1396.90	3.90	0.16	72.68%
		+qsec <sup>c</sup>	606.40	683.00	3.64	0.68	68.58%
	14	stdlin	22.40	26.30	0.01	0.00	19.53%
		+qsec <sup>c</sup>	8.00	12.50	0.01	0.00	11.74%
		stdlin	328.40	327.40	0.47	0.04	47.30%
		+qsec <sup>c</sup>	124.00	155.70	0.41	0.10	40.87%
		stdlin	3138.20	3126.90	8.81	0.52	71.56%
		+qsec <sup>c</sup>	1102.20	1331.10	7.42	1.42	68.66%
		stdlin	9921.80	9340.20	59.57	2.09	72.08%
		+qsec <sup>c</sup>	3864.00	4022.80	59.43	8.63	70.13%
	16	stdlin	90.80	90.20	0.08	0.01	24.95%
		+qsec <sup>c</sup>	27.00	38.20	0.05	0.01	15.92%
		stdlin	3472.80	3348.40	8.51	0.65	64.03%
		+qsec <sup>c</sup>	977.60	1333.90	5.93	1.25	59.05%
		stdlin	20 305.20	20 690.90	139.12	5.06	72.46%
		+qsec <sup>c</sup>	7327.00	8708.60	124.09	17.76	69.64%
		stdlin	94 662.60	92 729.60	1673.11	25.54	81.54%
		+qsec <sup>c</sup>	31 323.40	34 508.20	1402.86	125.14	79.53%
	18	stdlin	289.40	277.40	0.46	0.05	31.92%
		+qsec <sup>c</sup>	82.00	109.20	0.28	0.07	26.02%
		stdlin	5760.00	6283.50	30.13	1.64	48.52%
		+qsec <sup>c</sup>	2132.00	2685.50	22.34	5.12	44.89%
	20	stdlin	1056.40	1072.80	2.58	0.26	38.32%
		+qsec <sup>c</sup>	318.40	431.80	1.62	0.53	33.12%
		stdlin	130 753.40	138 239.90	2582.81	50.28	67.01%
		+qsec <sup>c</sup>	38 619.40	47 254.30	935.33	151.21	63.67%

All experiments were carried out on Intel Xeon E5-2670 processors, running at 2.60 GHz with 64 GB of RAM. All computing times are stated in cpu seconds. We are mostly interested in the root gaps obtained (*rootgap*), computed as

$$\frac{OPT - rootDB}{|OPT|},$$

i.e. the relative difference between the optimal solution (*OPT*) and the dual bound (*rootDB*) in the root node of the branch and bound tree, and in the number of subproblems that have to be enumerated to solve the instance to optimality (*# subs*). These two values indicate the strength of the additional cutting planes. Moreover, we report the time needed for separation (*septime*), the total time needed to solve the instance to optimality (*cputime*), and the total number of LPs to be solved (*# LPs*). All lines in the following tables report average results over 10 random instances.

We start by considering the spanning forest problem. As the case of positive coefficients of the quadratic terms is trivial then, we consider only instances with quadratic coefficients in  $\{-100, \dots, -1\}$ . When only connected product terms are present in the original instance, as is the case for typical applications involving reload or changeover costs, we obtain the results summarized in Table 1. The results show that the new inequalities can improve the root gap significantly with respect to the standard linearization for instances on sparse graphs. For denser graphs, the improvement in the root gap is much smaller, but the number of subproblems to be enumerated is still decreased significantly, showing that the new inequalities are effective in deeper levels of the enumeration tree. Nevertheless, the separation time remains small compared to the total time. In summary, this results in a decrease of computational times for all instances considered.



**Table 2**

Results for spanning forests with negative coefficients on all terms; each line reports averages over ten random instances.

Vertices	Density	sep	# subs	# LPs	cputime	septime	rootgap
10	20%	stdlin	1.00	2.00	0.00	0.00	0.00%
		+qsec <sup>c</sup>	1.00	2.00	0.00	0.00	0.00%
		+qsec	1.00	2.00	0.00	0.00	0.00%
	30%	stdlin	65.40	56.90	0.07	0.01	31.49%
		+qsec <sup>c</sup>	42.00	40.90	0.07	0.01	23.70%
		+qsec	33.40	37.80	0.10	0.02	23.33%
	40%	stdlin	767.60	683.50	1.67	0.05	72.10%
		+qsec <sup>c</sup>	494.00	482.60	1.59	0.09	68.85%
		+qsec	465.60	481.20	2.69	0.43	68.85%
	50%	stdlin	6690.80	6569.40	37.33	0.48	123.55%
		+qsec <sup>c</sup>	4153.00	4410.30	32.03	1.28	118.88%
		+qsec	3780.20	4204.50	53.00	6.12	118.88%
12	20%	stdlin	8.80	11.00	0.01	0.00	4.55%
		+qsec <sup>c</sup>	4.60	6.40	0.01	0.00	1.72%
		+qsec	2.60	4.50	0.01	0.00	1.34%
	30%	stdlin	941.20	865.80	3.11	0.06	55.32%
		+qsec <sup>c</sup>	635.80	634.50	2.84	0.14	51.32%
		+qsec	570.00	615.40	4.59	0.87	51.29%
	40%	stdlin	20 128.00	19 650.60	179.53	1.97	101.70%
		+qsec <sup>c</sup>	12 729.00	13 399.10	155.41	5.21	98.44%
		+qsec	11 191.40	12 627.90	244.01	29.83	98.44%
14	20%	stdlin	126.20	121.20	0.30	0.01	19.99%
		+qsec <sup>c</sup>	90.20	77.60	0.27	0.01	15.84%
		+qsec	66.40	71.30	0.42	0.12	15.12%
	30%	stdlin	23 322.20	22 434.80	241.62	2.73	77.96%
		+qsec <sup>c</sup>	15 781.00	15 969.10	212.94	6.77	74.17%
		+qsec	13 288.80	15 035.90	336.70	45.75	74.15%
16	20%	stdlin	1858.40	1691.80	10.98	0.23	36.53%
		+qsec <sup>c</sup>	1194.60	1116.70	8.77	0.39	32.23%
		+qsec	1026.80	1102.60	14.69	3.73	31.92%
18	20%	stdlin	64 032.60	61 917.50	1126.54	10.80	57.08%
		+qsec <sup>c</sup>	43 881.40	45 018.20	1069.21	23.64	54.72%
		+qsec	40 006.40	43 786.40	1763.52	233.87	54.64%

When considering instances with all quadratic terms having non-zero coefficients, our results are weaker in general, see Table 2. While the root gaps are only slightly improved, the number of subproblems can still be decreased by adding both inequalities for the connected and the disconnected quadratic terms. However, while the former also lead to a slight improvement in terms of computational times, the latter lead to longer times due to the higher computational effort of separation. Also the gap improvement obtained by adding the latter inequalities is very small even for sparse instances, which suggests that the constraints of type (5) are much more effective in practice than those of type (6).

We next investigate quadratic spanning trees. Then also the case of positive quadratic coefficients is non-trivial. However, by Corollary 4.4, we cannot expect to obtain any improvement in this case by adding constraints of type (5) or (6). For this reason, we reformulate the cardinality constraint (4) in a quadratic fashion: we add the constraint

$$\sum_{e,f \in E, e \neq f} y_{ef} = \binom{|V| - 1}{2} \quad (18)$$

to our linear problem formulation. This constraint fixes the sum of all product variables, so that the signs of the corresponding coefficients become irrelevant. Note that this additional constraint has a positive impact on bounds even if added to the standard linearization. Whenever adding (18) to our model, we denote this by *qref* in our tables.

In Tables 3 and 4, we state the results for the cases of negative and positive quadratic coefficients, respectively. The results in the first case turn out to be much better than those obtained for QMSF. However, this improvement is apparent in all methods and partly due to the reformulation *qref*. Indeed, when comparing different methods, the relative behavior is very similar to the QMSF case. Comparing positive and negative coefficients, it turns out that the latter case is slightly easier to solve than the former, but the difference is comparably small.

To conclude, we also tested our approach on the original instances of Cordone and Passeri [4]. For given  $n = 10, 15, 20$  and given density  $d = 33, 67, 100$ , we have coefficient ranges  $\{1, \dots, 10\}$  or  $\{1, \dots, 100\}$  for linear and quadratic variables in each combination, leading to four different instances per row. Results are given in Table 5. As mentioned above, our method cannot achieve the same computational times as the approach presented in [4]. However, just by separating our constraints (5) and the quadratic reformulation (18), we can solve 18 of these instances within the time limit of 5 h.

**Table 3**

Results for spanning trees with negative coefficients on all terms; each line reports averages over ten random instances.

Vertices	Density	sep	# subs	# LPs	cputime	septime	rootgap
10	20%	stdlin + qref	1.00	2.00	0.00	0.00	0.00%
		+qsec <sup>c</sup> + qref	1.00	2.00	0.00	0.00	0.00%
		+qsec + qref	1.00	2.00	0.00	0.00	0.00%
	30%	stdlin + qref	7.20	9.10	0.01	0.00	2.81%
		+qsec <sup>c</sup> + qref	5.40	8.40	0.03	0.00	1.79%
		+qsec + qref	5.00	8.10	0.01	0.00	1.62%
	40%	stdlin + qref	93.20	93.90	0.28	0.01	18.99%
		+qsec <sup>c</sup> + qref	75.00	85.10	0.31	0.01	18.39%
		+qsec + qref	74.20	85.60	0.30	0.04	18.39%
	50%	stdlin + qref	320.00	309.00	2.01	0.03	25.48%
		+qsec <sup>c</sup> + qref	264.60	300.80	1.78	0.08	24.57%
		+qsec + qref	253.60	296.60	1.97	0.30	24.57%
12	20%	stdlin + qref	1.40	3.90	0.00	0.00	0.06%
		+qsec <sup>c</sup> + qref	1.00	3.20	0.00	0.00	0.00%
		+qsec + qref	1.00	3.10	0.01	0.00	0.00%
	30%	stdlin + qref	103.20	100.60	0.41	0.01	14.64%
		+qsec <sup>c</sup> + qref	80.20	81.90	0.42	0.02	13.93%
		+qsec + qref	75.80	80.20	0.45	0.09	13.86%
	40%	stdlin + qref	1041.00	934.70	9.24	0.08	25.34%
		+qsec <sup>c</sup> + qref	852.60	909.20	8.27	0.28	24.81%
		+qsec + qref	825.60	919.70	9.64	1.73	24.81%
	50%	stdlin + qref	3186.00	3088.60	68.95	0.47	27.55%
		+qsec <sup>c</sup> + qref	2636.00	3101.20	61.10	1.35	27.30%
		+qsec + qref	2707.00	3191.70	68.15	8.56	27.30%
14	20%	stdlin + qref	10.40	13.00	0.04	0.00	1.81%
		+qsec <sup>c</sup> + qref	7.60	10.10	0.04	0.00	1.38%
		+qsec + qref	7.20	10.10	0.05	0.02	1.32%
	30%	stdlin + qref	1619.20	1570.30	18.38	0.19	24.47%
		+qsec <sup>c</sup> + qref	1245.40	1344.50	15.24	0.39	23.71%
		+qsec + qref	1215.40	1353.10	17.77	3.14	23.69%
	40%	stdlin + qref	11 139.60	10 738.60	329.38	2.04	29.81%
		+qsec <sup>c</sup> + qref	9074.00	10 699.70	291.47	6.47	29.60%
		+qsec + qref	8775.20	10 628.00	328.23	44.66	29.60%
	50%	stdlin + qref	47 158.00	46 778.60	3566.61	11.04	31.87%
		+qsec <sup>c</sup> + qref	38 313.00	46 052.40	2948.17	40.41	31.77%
		+qsec + qref	37 098.40	45 462.00	3141.08	281.16	31.77%
16	20%	stdlin + qref	110.00	102.30	0.77	0.01	6.99%
		+qsec <sup>c</sup> + qref	94.60	91.30	0.75	0.03	6.41%
		+qsec + qref	81.40	87.40	0.95	0.28	6.36%
	30%	stdlin + qref	17 712.20	16 830.00	547.16	3.35	29.66%
		+qsec <sup>c</sup> + qref	14 413.40	16 305.90	474.70	9.52	29.21%
		+qsec + qref	14 446.40	16 675.70	542.13	85.00	29.21%
18	20%	stdlin + qref	3913.60	3763.10	72.69	0.66	18.61%
		+qsec <sup>c</sup> + qref	3286.00	3241.00	65.59	1.53	18.18%
		+qsec + qref	3187.20	3275.30	76.48	14.33	18.17%
20	20%	stdlin + qref	29 314.00	26 738.60	1083.51	6.87	22.90%
		+qsec <sup>c</sup> + qref	24 940.60	24 314.30	950.09	17.09	22.52%
		+qsec + qref	23 675.20	24 371.10	1095.19	184.61	22.52%

## 7. Conclusion

We propose a new polyhedral approach for quadratic combinatorial optimization problems based on the idea of considering a single product term at a time. Assuming that the underlying linear problem is tractable, the same is true for optimizing the problem with one quadratic term, and hence also the corresponding separation problem is tractable from a theoretical point of view. To make such an approach practical, one needs to consider specific underlying problems and develop concrete separation algorithms that are not based on an optimization oracle. In this article, we investigate this approach for the quadratic spanning forest problem and the quadratic spanning tree problem, presenting a complete polyhedral description and an efficient separation algorithm for the corresponding problems with one quadratic term. Computationally, we show that the resulting inequalities lead to better LP-bounds when embedded into a branch-and-cut scheme, particularly in the sparse case. Even if this approach in itself is not able to – and not meant to – compete with tailored, fully-fledged approaches to the quadratic spanning tree problem presented recently in the literature, it can be combined with any other linearization-based approach, leading to improved bounds and thus to faster computational times if applied carefully.

**Table 4**

Results for spanning trees with positive coefficients on all terms; each line reports averages over ten random instances.

Vertices	Density	sep	# subs	# LPs	cputime	septime	rootgap
10	20%	stdlin + qref	1.00	2.00	0.00	0.00	0.00%
		+qsec <sup>c</sup> + qref	1.00	2.00	0.00	0.00	0.00%
		+qsec + qref	1.00	2.00	0.00	0.00	0.00%
	30%	stdlin + qref	12.00	12.90	0.02	0.00	3.09%
		+qsec <sup>c</sup> + qref	9.60	11.10	0.02	0.00	2.68%
		+qsec + qref	8.40	11.60	0.04	0.01	2.64%
	40%	stdlin + qref	53.80	49.90	0.14	0.00	18.56%
		+qsec <sup>c</sup> + qref	45.40	49.90	0.17	0.01	17.87%
		+qsec + qref	49.00	53.10	0.22	0.04	17.87%
	50%	stdlin + qref	249.00	211.20	1.30	0.02	31.07%
		+qsec <sup>c</sup> + qref	209.00	218.40	1.23	0.04	30.64%
		+qsec + qref	199.40	223.80	1.43	0.22	30.64%
12	20%	stdlin + qref	1.20	3.10	0.00	0.00	0.03%
		+qsec <sup>c</sup> + qref	1.20	3.10	0.00	0.00	0.03%
		+qsec + qref	1.00	2.70	0.01	0.00	0.00%
	30%	stdlin + qref	83.60	73.70	0.35	0.00	14.68%
		+qsec <sup>c</sup> + qref	58.60	61.80	0.28	0.02	13.19%
		+qsec + qref	59.00	62.70	0.38	0.11	13.15%
	40%	stdlin + qref	507.20	429.00	4.11	0.06	29.55%
		+qsec <sup>c</sup> + qref	381.60	403.90	3.66	0.12	28.79%
		+qsec + qref	385.40	418.60	4.18	0.68	28.79%
	50%	stdlin + qref	2220.40	1973.30	42.57	0.24	38.30%
		+qsec <sup>c</sup> + qref	1728.40	2023.70	37.99	0.76	37.79%
		+qsec + qref	1709.80	2039.60	40.95	4.32	37.79%
14	20%	stdlin + qref	5.60	8.70	0.03	0.00	1.07%
		+qsec <sup>c</sup> + qref	5.40	7.70	0.03	0.00	0.70%
		+qsec + qref	4.80	7.90	0.05	0.01	0.64%
	30%	stdlin + qref	867.80	801.50	9.11	0.10	29.04%
		+qsec <sup>c</sup> + qref	750.40	756.10	8.30	0.24	28.37%
		+qsec + qref	713.60	774.10	9.78	1.80	28.37%
	40%	stdlin + qref	9603.60	8968.90	279.73	1.55	39.89%
		+qsec <sup>c</sup> + qref	8116.60	8924.50	246.27	4.46	39.50%
		+qsec + qref	7797.00	9071.10	265.74	27.56	39.50%
	50%	stdlin + qref	35 372.40	33 993.00	2705.89	7.08	46.05%
		+qsec <sup>c</sup> + qref	29 163.40	35 036.70	2160.54	24.29	45.82%
		+qsec + qref	28 799.60	35 463.50	2269.69	171.40	45.82%
16	20%	stdlin + qref	83.40	82.30	0.67	0.02	7.03%
		+qsec <sup>c</sup> + qref	59.80	66.60	0.55	0.02	6.32%
		+qsec + qref	56.00	65.30	0.75	0.19	6.28%
	30%	stdlin + qref	12 745.00	11 304.90	356.06	2.29	37.61%
		+qsec <sup>c</sup> + qref	10 495.20	11 130.20	318.35	5.62	36.98%
		+qsec + qref	10 602.80	11 499.10	361.48	51.18	36.98%
18	20%	stdlin + qref	1444.60	1258.70	22.37	0.27	19.43%
		+qsec <sup>c</sup> + qref	1089.00	1067.30	19.10	0.57	18.68%
		+qsec + qref	1028.20	1095.30	24.85	5.90	18.67%
20	20%	stdlin + qref	13 318.40	11 128.30	439.46	3.15	26.59%
		+qsec <sup>c</sup> + qref	10 307.60	10 218.80	366.25	7.21	25.97%
		+qsec + qref	9590.20	10 359.60	447.28	81.86	25.96%

**Table 5**

Results for instances of Cordone and Passeri [4].

Vertices	Density	sep	Solved	# subs	# LPs	cputime	septime	rootgap
10	33%	+qsec <sup>c</sup> + qref	4	4.00	5.25	0.02	0.00	1.31%
	67%	+qsec <sup>c</sup> + qref	4	867.50	922.75	12.63	0.26	34.74%
	100%	+qsec <sup>c</sup> + qref	4	2803.50	3503.75	197.79	2.06	43.96%
15	33%	+qsec <sup>c</sup> + qref	4	5432.50	6226.25	146.38	2.46	33.57%
	67%	+qsec <sup>c</sup> + qref	1	3781.00	4231.00	1075.26	7.96	21.33%
	100%	+qsec <sup>c</sup> + qref	0	–	–	–	–	–
20	33%	+qsec <sup>c</sup> + qref	1	80969.00	99098.00	16014.59	203.46	24.14%
	67%	+qsec <sup>c</sup> + qref	0	–	–	–	–	–
	100%	+qsec <sup>c</sup> + qref	0	–	–	–	–	–

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