# MINIMUM SPANNING TREES WITH NEIGHBORHOODS

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ABSTRACT. This paper studies Minimum Spanning Trees under incomplete information for its vertices. We assume that no information is available on the precise placement of vertices so that it is only known that vertices belong to some neighborhoods that are second order cone representable and distances are measured with a  $\ell_q$ -norm. Two mixed integer non linear mathematical programming formulations are presented, based on alternative representations of subtour elimination constraints. A solution scheme is also proposed, resulting from a reformulation suitable for a Benders-like decomposition, which is embedded within an exact branch-and-cut framework. Furthermore, a mathheuristic is developed, which alternates in solving convex subproblems in different solution spaces, and is able to solve larger instances. The results of extensive computational experiments are reported and analyzed.

### 1. INTRODUCTION

Nowadays Combinatorial Optimization (CO) lies in the heart of multiple applications in the field of Operations Research. Many such applications can be formulated as optimization problems defined on graphs where some particular structure is sought satisfying some optimality property. Traditionally this type of problems assumed implicitly the exact knowledge of all input elements, and, in particular, of the precise position of vertices and edges. Nevertheless, this assumption does not always hold, as uncertainty, lack of information, or some other factors may affect the relative position of the elements of the input graph. Hence, new tools are required to give adequate answers to these challenges, which have been often ignored by standard CO tools.

A matter that, in this context, has attracted the interest of researchers over the last years is the solution of certain CO problems when the exact position of the vertices of the underlying graph is not known with certainty. If probabilistic information is available, then stochastic programming tools can be used, and optimization over expected values carried out. Moreover, even under the assumption of incomplete information one could use a uniform distribution and still apply such an approach. However, the use of probabilistic information and allowing to consider all possible locations for the vertices is not always suitable. For instance, when for each point of the input graph, a unique representative associated with it must be determined. Scanning the related literature one can find papers applying both methodologies. Examples of stochastic approaches are for instance [3] or [19]. Examples of the second type of approach arise in variants of the traveling salesman problem (TSP), minimum spanning tree (MST), or facility location problems that

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deal with *demand regions* instead of *demand points* (see [1, 5, 7, 11, 24, 31, 36], to mention just a few).

A relevant common question raised by the latter class of problems is how to model and solve optimization problems on graphs when vertices are not points but regions in a given domain. The above mentioned case of the TSP, first introduced by Arkin and Hassin [1], has been addressed recently by a number of authors. It generalizes the Euclidean TSP and the group Steiner tree problem, and has applications in VLSI-design and other routing problems, in which only imprecise information of the positions of the vertices is available. Several inapproximability results and approximation algorithms have been developed for particular cases. The case of the spanning tree problem with neighborhoods (MSTN) was first addressed by Yang et al. [36], who proved that the general case of the problem in the plane is NP-hard (result also reproved by Löffler and van Kreveld in [26]), and gave several approximation algorithms and a PTAS for the particular case of disjoint unit disks in the plane. Some extensions considering the maximization of the weights are studied in Dorrigiv et. al [10]. In particular, they proved the non existence of FPTAS for MSTN, for general disjoint disks, in the planar Euclidean case. Disser et. al [9] consider the shortest path problem and the rectilinear MSTN, and give some approximability results. To the best of our knowledge, Gentilini et al [20] are the first authors to propose an exact Mixed Integer Non Linear Programming (MINLP) formulation for the TSP with neighborhoods, but we are not aware of any MINLP for the MSTN.

Our goal in this paper is to develop MINLP formulations and solution methods for the MSTN. We first present two MINLP formulations that allow to solve medium size MSTN planar and 3D Euclidean instances with up to 20 vertices, for neighborhoods of varying radii using an on-the-shelf solver. Furthermore, we develop an effective branch-and-cut strategy, based on a generalized Benders decomposition [2, 21], and compare its performance with that of the solver for the proposed formulations. For this we present an alternative formulation for the MSTN, in which the master problem consists in finding an MST with costs derived from a continuous non linear (slave) subproblem, and we develop the expression and separation of the cuts that are added in the solution algorithm. Given that both the solver (for the two MINLP formulations) and the exact branch-and-cut algorithm can be too demanding, in terms of their computing times, we have also developed an effective and efficient mathheuristic. The mathheuristic stems from the observation that the subproblems defined in the solution spaces of each of the two main sets of variables are convex (so they can be solved very efficiently); it alternates in solving subproblems in each of these solution spaces.

The paper is organized as follows. Section 2 is devoted to introduce the MSTN and to state a generic formulation. In Section 3 we present and compare two MINLP formulations for the MSTN, based on alternative representations of the spanning trees polytope. Section 4 develops the exact branch-and-cut algorithm, based on a Benders-like decomposition scheme: we define the master and the non linear subproblem, and derive the cuts and their separation. In Section 4.1 we first compare the performance of the on-the-shelf solver with the two MINLP formulations, and then we report the numerical results obtained with the exact row-generation algorithm. The mathheuristic is presented in Section 5, where we also give the

numerical results that it produces. The paper ends with some concluding remarks and our list of references.

## 2. MINIMUM SPANNING TREES WITH NEIGHBORHOODS

Let G = (V, E) be a connected undirected graph, whose vertices are embedded in  $\mathbb{R}^d$ , i.e.,  $v \in \mathbb{R}^d$  for all  $v \in V$ . Associated with each vertex  $v \in V$ , let  $\mathcal{N}_v \subseteq \mathbb{R}^d$ denote a convex set containing v in its interior. Let also  $\|\cdot\|$  denote a given norm.

Feasible solutions to the Minimum Spanning Tree with Neighborhoods (MSTN) problem consist of a set of points,  $Y^* = \{y_v \in \mathcal{N}_v \mid v \in V\}$ , together with a spanning tree  $T^*$  on the graph  $G^* = (Y^*, E^*)$ , with edge set  $E^* = \{\{y_v, y_w\} : \{v, w\} \in E\}$ . Edges lengths are given by the norm-based distance between the selected points relative to  $\|\cdot\|$ , i.e.:

$$d(y_v, y_w) = ||y_v - y_w||, \text{ for all } \{y_v, y_w\} \in E^*.$$

The overall cost of  $(Y^*, T^*)$  is therefore

$$d(T^*) = \sum_{e = \{y_v, y_w\} \in T^*} d(y_v, y_w).$$

The MSTN is to find a feasible solution,  $(Y^*, T^*)$ , of minimum total cost.

Particular cases of the MSTN have been studied in the literature for planar graphs. Disser et. al [9] studied the case when the sets  $\mathcal{N}_v$  are rectilinear neighborhoods centered at  $v \in V$ . Dorrigiv et. al [10] addressed the problem when the sets  $\mathcal{N}_v$  are disjoint Euclidean disks. Both referenced works study the complexity of the considered problems but do not attempt to develop MINLP formulations or solution methods for it.

In this paper, we consider the general case where the graph G is embedded in  $\mathbb{R}^d$ . Even if our developments can be extended to generic convex sets, we focus on the case where  $\mathcal{N}_v$  is second order cone (SOC) representable [25]. The main reason for this is that state-of-the-art solvers incorporate mixed integer non-linear implementations of SOC constraints. Such a modeling assumption could be readily overcome if on-the-shelf solvers incorporated more general tools to deal with convex sets.

Observe that SOC representable neighborhoods allow to model, as a particular case, centered balls of a given radius  $r_v$ , associated with the standard  $\ell_p$ -norm with  $p \in [1, \infty]$  in  $\mathbb{R}^d$ , that we denote by  $\|\cdot\|_p$ , i.e., neighborhoods in the form  $\mathcal{N}_v = \{x \in \mathbb{R}^d : \|x - v\|_p \leq r_v\}$ , where

$$||z||_{p} = \begin{cases} \left(\sum_{k=1}^{d} |z_{k}|^{p}\right)^{\frac{1}{p}} & \text{if } p < \infty \\ \max_{k \in \{1, \dots, d\}} |z_{k}| & \text{if } p = \infty \end{cases}$$

The reader is referred to [4] for further details on the SOC constraints that allow to represent (as intersections of second order cone and/or rotated second order cone constraints) such norm-based neighborhoods. Indeed, we can also easily handle neighborhoods defined as bounded polyhedra in  $\mathbb{R}^d$ , as well as intersections of polyhedra and balls. Hence, more sophisticated convex neighborhoods can be suitably represented or approximated using elements from the above mentioned families of sets.

Two extreme situations that can be modeled within our framework are the following. If the neighborhood for each vertex  $v \in V$  is the singleton  $\mathcal{N}_v = \{v\}$ , then MSTN becomes the classical MST problem with edge lengths given by the normbased distances between each pair of vertices. On the other hand, if the considered neighborhoods are big enough so that  $\bigcap_{v \in V} \mathcal{N}_v \neq \emptyset$ , then the problem reduces to finding a degenerate one-vertex tree and the solution to the MSTN is that vertex with cost 0.

Throughout this paper we use the following notation:

- ST<sub>G</sub> as the set of incidence vectors associated with spanning trees on G,
  i.e. ST<sub>G</sub> = {x ∈ ℝ<sup>|E|</sup><sub>⊥</sub> : x is a spanning tree on G}
- $\mathcal{Y} = \prod_{v \in V} \mathcal{N}_v$ , where  $\mathcal{N}_v$  is the neighborhood associated to vertex v, which

contains the possible sets of vertices for the spanning trees of MSTN.

Then, the MSTN can be stated as:

(MSTN) 
$$\min \sum_{e \in E} d(y_v, y_w) x_e$$
  
s.t.  $x \in ST_G, y \in \mathcal{Y}$ .

Several observations follow from the formulation above:

- (1) Fixing  $x \in ST_G$  in MSTN results in a continuous SOC problem, which is well-known to be convex [25]. On the other hand, fixing  $y \in \mathcal{Y}$  results in a standard MST problem. It is a well-known that MST admits continuous linear programming representations [14, 28]. Thus, MSTN can be seen as a biconvex optimization problem, which is neither convex nor concave [22].
- (2) Due to the expression of its objective function, MSTN is not separable, even if each of its sets of variables x and y belong to convex domains in different spaces.
- (3) Since MSTN *combines* the above two subproblems, it is suitable to be represented as a MINLP.

The following example illustrates the MSTN.

Example 2.1. Let us consider a graph with eight vertices and 14 edges, G = (V, E) embedded in  $\mathbb{R}^2$ . The graph G and an Euclidean Minimum Spanning Tree for this graph are shown in Figure 1(A).

Figure 1(B) shows the input graph together with the neighborhoods  $N_v$  associated with the vertices  $v \in V$ . The neighborhoods are (Euclidean) balls centered at the original vertices, each of them with a different radius. Figure 2 shows an optimal MSTN solution: the location of the vertex selected in each neighborhood, as well as the final spanning tree (both in gray).

Observe that the optimal spanning tree to the classical MST problem in the original input graph shown in Figure 1(A), with edges lengths given by the Euclidean distances between the initial vertices, is no longer valid for the MSTN. The reason is that the actual distances have been updated in order to consider the coordinates

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(A) Input graph G and Euclidean MST (B) Neighborhoods of the vertices. (black lines).

FIGURE 1. Data for Example 2.1.



FIGURE 2. A MSTN for the data in Example 2.1.

of the selected vertices, which are unknown beforehand. Note also that the structure of the original graph is somehow broken, since in the final solution some of the "initial" vertices are *merged* into a single one (note that the MST in Figure 2 has seven vertices while the original graph had eight). This is possible only when some of the neighborhoods have a non-empty intersection.

In Figure 3 we show an optimal solution to the MSTN in the same input graph, for a different definition of the neighborhoods. Now they are defined as boxes in the form  $\mathcal{N}_v = \{z \in \mathbb{R}^2 : |z_k - v_k| \leq r_v, k = 1, 2\}.$ 

As we see below, some of the properties of the standard MST extend to MSTN. In particular, the cut and cycle properties that allow reducing the dimensionality of MSTN by discarding edges that will not appear in an optimal solution as well as those edges that will appear in it. Before, we introduce the additional notation



FIGURE 3. A MSTN for the data in Example 2.1 for polyhedral neighborhoods.

associated with each edge  $e = \{v, w\} \in E$ .

•  $\widetilde{U}_e$  and  $\widetilde{u}_e$  respectively denote the maximum and minimum distance between any pair of points in the neighborhoods of the end-vertices of e. That is,  $\widetilde{U}_e = \max\{d(y_v, y_w) : y_v \in \mathbb{B}_r^p(v), y_w \in \mathbb{B}_r^p(w)\}$  and  $\widetilde{u}_e = \min\{d(y_v, y_w) : y_v \in \mathbb{B}_r^p(v), y_w \in \mathbb{B}_r^p(w)\}$ .

Property 1.

- (a) Let C be a cycle of G = (V, E) and  $e \in C$  such that  $\tilde{u}_e > \min_{e' \in E} \{ \tilde{U}_{e'} : e' \in C, e' \neq e \}$ . Then, e does not belong to a MSTN.
- (b) Let  $S \subset V$  and  $(S, V \setminus S) = \{e = \{v, w\} \in E \mid v \in S \text{ and } w \in V \setminus S\}$  be its associated cutset. Let  $e = \{v, w\} \in (S, V \setminus S)$  be such that  $\widetilde{U}_e < \min_{e' \in E} \{\widetilde{u}_{e'} : e' = \{v', w'\} \in E, e' \neq e, v' \in S, w' \in V \setminus S\}$ . Then, e belongs to any MSTN.

### Proof.

(a) Let C be a cycle of G = (V, E) and  $e \in C$  such that  $\widetilde{u}_e > \min_{e \in E} \{ \widetilde{U}_{e'} : e' \in C, e' \neq e \}.$ 

Suppose, there is an MSTN of G, T with  $e \in T$ . Then, for any other edge e' in the cycle C, the tree  $T' = T \cup \{e'\} \setminus \{e\}$  satisfies that:

$$d(T') \le d(T) + \widetilde{U}_{e'} - \widetilde{u}_e < d(T).$$

Thus, the cost of T' is strictly smaller than the cost of T, contradicting the optimality of T. Hence e will not appear in T.

(b) Let T be a MSTN of G with e ∉ T. Since T is a tree, the unique cycle of T ∪ {e} contains both e and the unique path in G connecting v and w, that does not contain e. Let e' the edge in such a path crossing the cut, i.e., e' = {v', w'} with v' ∈ S and w' in V\S. Then, T' = T ∪ {e}\{e'\} is a tree

and such that

$$d(T') \le d(T) + \widetilde{U}_e - \widetilde{u}_{e'} < d(T),$$

so T' has an overall distance smaller than T, contradicting its optimality. Hence e will appear in T.

## 3. MIXED INTEGER NON LINEAR PROGRAMMING FORMULATIONS

In this section we present alternative MINLP formulations for the MSTN that will be compared computationally in later sections. All formulations use the following sets of decision variables:

- Binary variables  $x_e \in \{0, 1\}, e \in E$ , to represent the edges of the spanning trees.
- Continuous variables  $y_v \in \mathcal{N}_v, v \in V$ , to represent the point selected in each neighborhood.
- Continuous variables  $u_e \ge 0$ ,  $e = \{v, w\} \in E$ , to represent the distance  $d(y_v, y_w)$  between the pairs of selected points.

Properties 1(a) and (b) can be exploited in order to reduce the number of x variables in the formulations. In particular, we only need to define variables  $x_e$  associated with edges that do not satisfy the condition 1(a). On the other hand, we can set at value 1 all variables  $x_e$  associated with edges that satisfy 1(b).

Let  $\mathcal{U} = \{ u \in \mathbb{R}^{|E|}_+ : u_e \geq d(y_v, y_w) \}$ , for all  $e = \{v, w\} \in E$ , for some  $y \in \mathcal{Y} \}$  denote implicitly the domain for the feasibility of the *u* variables. Then, a generic bilinear formulation for MSTN is

(P<sub>xu</sub>) 
$$\min \sum_{e \in E} u_e x_e$$
  
s.t.  $x \in ST_G, \ u \in U$ .

In the following we resort to McCormick's envelopes [29] for the linearization of the bilinear terms of the objective function. For this, we define an additional set of continuous decision variables  $\theta_e \geq 0$ ,  $e \in E$  to represent the products  $u_e x_e$ . Then the linearization of the generic formulation  $P_{xu}$  is:

(RL - MSTN) min 
$$\Theta = \sum_{e \in E} \theta_e$$
  
(LIN - Mc) s.t.  $\theta_e \ge u_e - \widetilde{U}_e(1 - x_e), \quad \forall e \in E,$   
 $x \in \mathcal{ST}_G, \quad u \in \mathcal{U}, \quad \theta_e \ge 0, e \in E.$ 

Furthermore, throughout we will describe the set  $\mathcal{U}$  using the set of constraints

(U<sub>1</sub>)  $||y_v - y_w|| \le u_e, \quad \forall e = \{v, w\} \in E,$ 

$$(\mathbf{U}_2) \qquad \qquad y \in \mathcal{Y},$$

which set the distance values and impose that the y points belong to the appropriate neighborhoods, respectively. Note that the above formulation (RL – MSTN) can be reinforced by adding the following valid inequalities:  $\theta_e \geq \tilde{u}_e x_e$ , for all  $e \in E$ .

The two formulations below differ from each other in the representation of subtour elimination constraints (SEC). One of them uses the classical representation of [14], which consists of a family with an exponential number of inequalities. The other one uses a compact formulation based on the well-known Miller-Tucker-Zemlin (MTZ) constraints [30]. Despite having a weaker linear programming bound than the subtour elimination representation for the classical MST problem, we use this formulation since, in practice, it has given quite good results for other problems related to spanning trees [27, 15]. Indeed, other compact representations could be used, like for instance, the one by Martin [28]. In our experience, [30] gives a good tradeoff between the number of variables it requires and the bounds it produces.

#### 3.1. MSTN formulation based on classical representation of SECs.

(SEC - MSTN) min 
$$\Theta = \sum_{e \in E} \theta_e$$
  
s.t. (LIN - Mc), (U<sub>1</sub>), (U<sub>2</sub>),  
(ST<sub>1</sub>)  $\sum x_e = |V| - 1$ ,

(ST<sub>2</sub>) 
$$\sum_{e=\{v,w\}:v,w\in S} x_e \le |S| - 1, \forall S \subset V,$$

 $e \in E$ 

(D<sub>1</sub>) 
$$u, \theta \in \mathbb{R}^{|E|}_+, y \in \mathbb{R}^{|V| \times d}, x \in \{0, 1\}^{|E|}.$$

Constraints (ST<sub>1</sub>) impose that exactly |V| - 1 edges are selected and subtours are prevented by (ST<sub>2</sub>). (D<sub>1</sub>) define the domain of the variables.

As mentioned, the number of constraints in  $(ST_2)$  is exponential on |V|, so a separation procedure (e.g. max flow - min cut) to certify whether a solution is feasible or otherwise, to provide a violated constraint, is needed to solve this formulation. This is avoided in the next formulation, which uses the MTZ compact representation of SECs [30].

3.2. **MSTN formulation based on Miller-Tucker-Zemlin.** The formulation based on the MTZ representation of SECs builds a tree rooted at an arbitrarily selected vertex where the arcs of the tree are oriented *towards* the root. In our case we set vertex 1 as the root of the trees. Associated with each edge  $\{v, w\} \in E$  we define two additional binary decision variables,  $z_{vw}$  and  $z_{wv}$ , to indicate whether or not (v, w) (resp. (w, v)) is used as a directed arc. The set of such arcs is denoted by A. As it is usual for the representation of the SEC constraints we use continuous variables  $s_v, v \in V$ , associated with the vertices. The MTZ-MSTN formulation is:

 $\Theta = \sum_{e \in E} \theta_e$ (MTZ - MSTN) min s.t.  $(LIN - Mc), (U_1), (U_2),$  $\forall e = \{u, v\} \in E,$  $(MTZ_1)$  $x_e = z_{uv} + z_{vu},$  $\sum_{(v,1)\in\delta^-(1)} z_{v1} \ge 1,$  $(MTZ_2)$  $\sum_{(v,w)\in\delta^-(u)} z_{vw} = 1,$  $\forall v \in V \backslash \{1\},$  $(MTZ_3)$  $\forall (v, w) \in A, \\ \forall u \in V \setminus \{1\}$  $|V|z_{vw} + s_v - s_w \le |V| - 1,$  $(MTZ_4)$  $s_1 = 1; 2 \le s_u \le |V|,$  $\forall u \in V \setminus \{1\},$  $(MTZ_5)$ 

(D<sub>1</sub>) 
$$u, \theta \in \mathbb{R}^{|E|}_+, y \in \mathbb{R}^{|V| \times d}, x \in \{0, 1\}^{|E|},$$

(D<sub>2</sub>)  $z \in \{0, 1\}^{|E|}, s \in \mathbb{R}^{|V|}_+.$ 

The meaning of the new constraints is as follows. Constraints  $(MTZ_1)$  relate the *edge* and *arc* decision variables. The connectivity with the root is guaranteed by  $(MTZ_2)$ - $(MTZ_3)$ . Subtours are eliminated by  $(MTZ_4)$  - $(MTZ_5)$ , where the later set appropriate bounds for the vertex variables *s*. The domain of the new variables is set by  $(D_2)$ .

As mentioned, the two formulations presented above use the *norm* constraints  $(U_1)$  and  $(U_2)$  to represent both the distance measure for the edges and the neighborhoods. As we see below both sets of constraints can also be handled by using either SOC or linear constraints. The following remarks show the explicit representation of some general cases of this type of constraints.

Remark 3.1 ( $\ell_q$ -norm representation). As shown in [4, Lemma 3], if the norm  $\|\cdot\|$  is a  $\ell_q$ -norm with  $q \in \mathbb{Q}$  and  $q = \frac{r}{s} > 1$  (with gcd(r, s) = 1), then the constraints of the form  $\|X - Y\|_q \leq Z$  as those of (U<sub>1</sub>) can be rewritten as the following set of inequalities:

The above gives a representation of  $(U_1)$  with a number of SOC inequalities that is polynomial in the dimension d and q.

*Remark* 3.2 (Polyhedral norm representation). When the norm  $\|\cdot\|$  is a polyhedral (or block) norm, a (linear) representation, much simpler than the one given in

Remark 3.1 is possible. Let  $B^*$  be the unit ball of its dual norm and  $\text{Ext}(B^*)$  the set of extreme points of  $B^*$ . The constraint  $Z \ge ||X - Y||$  is then equivalent to

$$Z \ge e^t (X - Y), \ \forall e \in \operatorname{Ext}(B^*),$$

where  $e^t$  denotes the transpose of e.

3.3. Computational comparison of the two formulations. We have performed a series of computational experiments in order to compare the performance of the two formulations SEC – MSTN and MTZ – MSTN, as well as to explore the limitations of each of them. For this we have generated several batteries of instances with different settings. We consider complete graphs with a number of vertices ranging in [5, 20], and randomly generated coordinates in  $\mathbb{R}^2$  and  $\mathbb{R}^3$  ranging in [0, 100]. Distances are measured using the Euclidean norm and Euclidean balls are used as neighborhoods of the vertices. In addition, we consider four different scenarios for generating the radii to define the neighborhoods of each vertex in a given instance:

Small size Neighborhoods (r = 1):: Radii randomly generated in [0, 5].

Small-Medium size Neighborhoods (r = 2):: Radii randomly generated in [5, 10].

Medium-Large size Neighborhoods (r = 3):: Radii randomly generated in [10, 15].

Large size Neighborhoods (r = 4):: Radii randomly generated in [15, 20].

The above four cases allow us to observe the performance of the formulations for neighborhoods of varying sizes and to analyze how these sizes affect the computation the MSTN in each case. Finally, five different instances were generated for each combination of number of vertices and radii, both in the plane and in the 3D-space. The generated data are available at bit.ly/mstneigh.

All the formulations were coded in C, and solved using Gurobi 6.5 [23] in a Mac OSX El Capitan with an Intel Core i7 processor at 3.3 GHz and 16GB of RAM. A time limit of 2 hours was set in all the experiments.

Tables 1-2 summarize the results of these experiments. In these tables the column CPU, under the heading of each formulation, reports the average computing time (in seconds) to attain optimality. Whenever the time limit of 2 hours is reached without certifying optimality, columns under GAP report the average percentage deviation of the best solution found during the exploration with respect to the lower bound at termination. Columns under #Nodes report the average number of nodes explored in the branch-and-bound search, whereas column SEC gives the average number of constraints (ST<sub>2</sub>) incorporated to formulation SEC-MSTN throughout the solution process. Finally, the last column in each block reports the percentage of instances optimally solved with each formulation.

Observe that the computing times required by SEC-MSTN are in most cases smaller than those required by MTZ-MSTN. Furthermore, some instances that could not be solved with MTZ-MSTN, were optimally solved with SEC-MSTN. In most of the cases where SEC-MSTN did not succeed, MTZ-MSTN was also not able to solve the corresponding instance. Note that, for the instances with n = 20, we only report the results for the first scenario (r = 1), since neither SEC-MSTN nor MTZ-MSTN were able to solve any of such instances for  $r \ge$ 2. We would like to highlight that, even if the 3-dimensional instances have a higher number of variables than the planar ones, the results, in terms of computing times, percentage deviations, and number of optimally solved instances are better for these instances than for the 2-dimensional ones. Observe that the difficulty of an instance is highly related to whether or not the neighborhoods have nonempty intersections; in such cases, the continuous relaxation tends to *collapse* the vertices of intersecting neighborhoods into a single one, which is not necessarily an optimal strategy. This justifies the higher difficulty of planar instances since, with uniform randomly generated points and given radii, the probability of intersection of neighborhoods is higher in case of the plane than in the space [12].

			MTZ - M	STN		SEC - MSTN				
r	n	CPU	#Nodes	GAP	%Solved	CPU	#SECs	#Nodes	GAP	%Solved
	5	0.0652	5.40		100%	0.0250	3.40	9.00		100%
	6	0.0965	7.60		100%	0.0334	6.40	21.20		100%
	7	0.1403	84.60		100%	0.0456	9.60	54.00		100%
1	8	0.1917	201.60		100%	0.0677	9.20	41.40		100%
	9	0.2592	37.60		100%	0.0826	29.60	76.00		100%
	10	0.4843	434.80		100%	0.1318	64.60	241.40		100%
	11	0.6472	568.20		100%	0.3922	123.80	552.60		100%
	12	0.9159	712.00		100%	0.3083	156.40	547.80		100%
	13	10.9525	3145.80		100%	1.1175	419.00	1314.80		100%
	14	4.7581	4014.80		100%	1.1627	300.40	1043.60		100%
	15	657.1666	41153.60		100%	444.5906	1474.20	17828.00		100%
	20	2915.1011	110070.80		100%	840.0096	2431.20	32173.80		100%
2	5	0.0820	47.00		100%	0.0263	7.40	54.60		100%
	6	0.1226	44.10		100%	0.0451	11.90	84.80		100%
	7	0.1571	123.20		100%	0.0582	18.60	95.60		100%
	8	0.4895	480.80		100%	0.2000	98.40	457.40		100%
	9	0.5531	415.80		100%	0.3984	128.40	666.20		100%
	10	1.3820	915.40		100%	0.7600	174.40	1125.00		100%
	11	1.6639	835.60		100%	1.2961	235.80	1050.20		100%
	12	32.8139	12301.20		100%	8.2899	832.80	9301.60		100%
	13	143.7873	16259.40		100%	9.7330	4685.40	68409.20		100%
	14	1467.5540	44337.00	7.64%	80%	661.3465	3252.60	36310.60		100%
	15	3428.0761	423135.80	4.97%	80%	3424.9741	15712.80	179939.00	6.29%	60%
	5	0.0958	44.20		100%	0.0354	9.40	79.80		100%
	7	0.2645	414.60		100%	0.2772	189.70	1133.40		100%
	8	1.6716	2097.80		100%	1.1393	338.60	1894.20		100%
	9	3.7345	3827.40		100%	3.8655	407.60	3515.40		100%
0	10	5.9807	3465.20		100%	3.8294	333.80	2426.20		100%
3	11	713.2283	172376.20		100%	976.5382	61128.20	363205.60		100%
	12	1054.4171	479364.20	10 1507	100%	2828.2251	97800.80	576762.00	20.000	100%
	13	3323.6210	279362.20	13.45%	60%	4626.0085	116751.40	953914.60	20.98%	80%
	14	>7200	1383023.40	30.04%	0%	>7200	27120.40	102007.00	38.07%	0%
	10	>7200	14/3884.40	19.43%	100%	>7200	87730.20	392951.00	23.03%	100%
	0	0.0880	33.20		100%	0.0288	4.60	47.40		100%
	0	0.1088	307.20		100%	0.1797	95.80	1562.40		100%
	8	2.0333	1976.60		100%	1.1078	289.80	1562.40		100%
	10	4.4465	4930.00		100%	9.3933	444.00	28680.60		100%
4	11	460 2022	109141 90		100%	215 0120	6462 20	20000.00		10070
4	12	409.3033 9471 0740	190141.00	6 1507	100%	822 4400	105361 40	006147.00		100%
	12	4609 7707	403914.00	16.88%	40%	5134 5084	8477.00	163847.00	19.64%	40%
	14	>7200	807955 40	44 52%	4070	>7200	37016.40	192311.00	51.04%	4076
	15	>7200	948641 60	34 07%	0%	>7200	200/6 80	168779.80	13 330%	0%
	10	/1200	546041.00	04.01/0	070	/1400	49940.00	100119.00	-10.00/0	070

TABLE 1. Results of MTZ – MSTN and SEC – MSTN for  $\mathbb{R}^2$  instances.

## 4. BRANCH-AND-CUT SOLUTION ALGORITHM

In this section we describe the branch-and-cut solution algorithm that we propose for solving MSTN. The special structure of MSTN, with disjoint domains for each set of variables - x and u- and a bilinear objective function makes it possible to

			MTZ - N	1STN		SEC - MSTN				
r	n	CPU	#Nodes	GAP	%Solved	CPU	#SECs	#Nodes	GAP	%Solved
	5	0.0677	3.60		100%	0.0282	2.40	17.20		100%
	6	0.1049	11.80		100%	0.0429	3.00	14.00		100%
	7	0.2137	24.40		100%	0.0694	5.60	24.80		100%
	8	0.2439	52.40		100%	0.0813	6.20	38.40		100%
1	9	0.3733	166.80		100%	0.1298	13.40	127.40		100%
	10	0.3803	56.20		100%	0.1442	34.00	127.40		100%
	11	1.0249	281.40		100%	0.3568	27.60	336.20		100%
	12	0.6932	235.20		100%	0.2772	62.00	225.00		100%
	13	1.3241	763.40		100%	0.9351	113.60	819.60		100%
	14	4.1596	1112.00		100%	2.6353	200.80	1164.60		100%
	15	4.2952	1286.20		100%	2.5708	197.00	812.40		100%
	20	67.5323	6555.20		100%	8.9617	372.20	1441.00		100%
	5	0.0983	12.40		100%	0.0431	6.80	37.40		100%
	6	0.1479	27.40		100%	0.0497	4.70	35.30		100%
	7	0.2058	51.80		100%	0.0770	9.20	55.80		100%
	8	0.3084	211.40		100%	0.1645	49.80	263.00		100%
	9	0.8943	382.00		100%	0.4596	86.20	593.80		100%
<b>2</b>	10	0.5047	170.60		100%	0.2185	50.60	267.80		100%
	11	1.4917	653.40		100%	0.5416	134.00	679.60		100%
	12	3.2860	1814.40		100%	5.4726	462.80	2440.20		100%
	13	5.3095	1956.40		100%	5.6612	437.20	2344.40		100%
	14	16.8888	4485.20		100%	13.0737	1108.60	9084.40		100%
	15	100.5050	14664.20		100%	54.8965	1524.20	12674.20		100%
	5	0.1034	12.00		100%	0.0450	3.00	39.60		100%
	7	0.2737	199.30		100%	0.1663	79.70	428.00		100%
	8	1.0901	972.40		100%	1.6812	230.40	1323.80		100%
	9	15.9457	3589.40		100%	2.0036	295.00	3520.80		100%
	10	2.0609	1124.00		100%	2.2637	259.80	1459.20		100%
3	11	29.7077	5477.80		100%	34.5579	549.20	7713.00		100%
	12	330.0074	19946.80		100%	531.3279	1580.20	20383.00		100%
	13	1069.2640	37625.20		100%	668.1420	2349.60	30331.40		100%
	14	3875.3014	152561.80	15.19%	60%	2519.3367	11488.00	112377.40	6.87%	80%
	15	1001.7704	47758.80		100%	160.5466	4114.40	37114.80		100%
	5	0.0875	21.60		100%	0.0469	6.80	42.60		100%
	6	0.2094	134.20		100%	0.1156	28.00	255.40		100%
	8	0.8188	832.20		100%	1.1261	204.00	1188.60		100%
	9	2.8822	2408.60		100%	1.7530	329.40	4937.60		100%
	10	6.4525	3461.40		100%	7.0799	525.80	3539.00		100%
4	11	32.0012	9411.20		100%	37.8657	1084.40	9208.20		100%
	12	70.9765	12658.60		100%	37.6467	1104.00	11910.80		100%
	13	710.0275	100078.40		100%	1679.7648	52401.40	287336.00		100%
	14	4635.9384	287990.20	27.48%	60%	6433.5763	39467.20	192079.80	25.48%	40%
	15	5741.0396	115401.20	7.12%	20%	3609.2785	11392.80	75087.00	10.55%	60%

TABLE 2. Results of MTZ – MSTN and SEC – MSTN for  $\mathbb{R}^3$  instances.

apply well-known Benders-like decomposition methods [2, 21]. This type of wellknown solution schemes have been widely applied to problems with two sets of structural decision variables, in which the subproblem that results when fixing one of the sets of variables can be *efficiently* solved. Note that, as mentioned before, this requisite is satisfied in the case of MSTN.

In order to warrant the convergence properties of the approach, we also apply reformulation techniques to the bilinear objective function. For a given spanning tree  $\bar{x} \in ST_G$ , the "optimal" vertices and distances of its associated MSTN, can be computed by solving the following convex subproblem:

(PU<sub>x</sub>)  
$$u(\bar{x}) = \min \sum_{e \in E} u_e \bar{x}_e$$
s.t.  $u \in \mathcal{U}$ 

As already mentioned,  $(PU_{\bar{x}})$  is a continuous SOC problem, which can be efficiently solved with on-the-shelf solvers. Note also that the number of u variables in  $(PU_{\bar{x}})$  reduces to n-1, because only distances associated with the edges  $e \in E$ with  $\bar{x}_e = 1$  need to be computed. Hence, (generalized) Benders decomposition is a suitable methodology for solving the MSTN problem. The following result states explicitly the form of the Benders cuts that allow to use particular solutions of  $(PU_{\bar{x}})$  to solve MSTN.

**Theorem 4.1.** Let  $\bar{x} \in ST_G$  and  $u(\bar{x})$  its associated (PU<sub>x</sub>) solution. Then,

$$\Theta \ge u(\bar{x}) + \sum_{e:\bar{x}_e=1} \widehat{U}_e(x_e - 1) + \sum_{e:\bar{x}_e=0} \widehat{u}_e x_e$$

is a valid cut for MSTN, where, as before,  $\Theta = \sum_{e \in E} \theta_e$  with  $\theta_e \ge 0$ ,  $e \in E$ ; and  $\hat{U}_e$ 

and  $\hat{u}_e$  are upper bounds on the maximum and minimum values of the distance of edge e, respectively (for instance, the ones introduced after Example 2.1).

*Proof.* Let us consider the following equivalent reformulation of  $(PU_{\bar{x}})$  based on the Mckormick linearization of the bilinear terms of the objective function in the original MSTN formulation:

$$\begin{aligned} u(\bar{x}) &= \min \sum_{e \in E} \theta_e \\ (\text{RPU}_{\bar{x}}) & \text{s.t. } \theta_e \geq u_e + \widehat{U}_e(\bar{x}_e - 1), \qquad e \in E \\ \theta_e \geq \widehat{u}_e \bar{x}_e, & e \in E \\ u \in \mathcal{U}. \end{aligned}$$

Note that the reformulation  $(\text{RPU}_{\bar{x}})$  is a convex optimization problem, and Slater condition holds [33]. Hence, (necessary and sufficient) optimality conditions can be derived from the following Lagrangean function associated with  $(\text{PU}_{\bar{x}})$ :

$$L(\bar{x},\theta,u;\lambda,\mu,\nu) = \sum_{e\in E} \theta_e - \sum_{e\in E} \lambda_e(\theta_e - u_e + \widehat{U}_e(1-\bar{x}_e)) - \sum_{e\in E} \mu_e(\theta_e - \widehat{u}_e\bar{x}_e) + \nu^t G(u) + \lambda_e(u) + \lambda$$

where  $G(u) \leq 0$  are the constraints (only involving *u*-variables) defining  $\mathcal{U}$ .

Let  $\theta_e^*$ ,  $u_e^*$ ,  $e \in E$ , be an optimal solution to (RPU<sub>x̄</sub>) and  $\lambda^*$ ,  $\mu^*$  and  $\nu^*$  the associated optimal multipliers. Then,  $\lambda^*$  and  $\mu^*$  must satisfy:

(4.1) 
$$1 - \lambda_e^* - \mu_e^* = 0, \quad \forall e \in E$$

together with the complementary slackness constraints:

$$\lambda_e^*(\theta_e^* - u_e^* + \widehat{U}_e(1 - \bar{x}_e)) = 0, \quad \forall e \in E,$$
$$\mu_e^*(\theta_e^* - \widehat{u}_e \bar{x}_e) = 0, \quad \forall e \in E.$$

If  $\bar{x}_e = 1$ , then  $\mu_e^* = 0$ , since  $u^* \ge \hat{u}$  and  $\theta_e^* \ge u_e^*$ ; and by (4.1),  $\lambda_e^* = 1$ . Besides, if  $\bar{x}_e = 0$ , since  $u_e^* < \hat{U}_e$ , then  $\theta_e^* = 0$  and  $\lambda_e^* = 0$ . Thus, we conclude that:

(4.2) 
$$\lambda^* = \bar{x}_e \text{ and } \mu_e^* = 1 - \bar{x}_e, \quad \forall e \in E.$$

On the other hand, since  $u(x) = \Theta = \sum_{e \in E} \theta_e = \max_{\lambda \ge 0, \mu \ge 0} \min_{\theta, u} L(x, \theta, u; \lambda, \mu, \nu)$  also holds for any  $x \in ST_G$ , we have that

$$\begin{split} \Theta &\geq \min_{\theta, u} L(\bar{x}, \theta, u; \lambda^*, \mu^*, \nu^*) \\ &= \sum_{e \in E} \theta^*_e - \sum_{e \in E} \lambda^*_e(\theta^*_e - u^*_e + \hat{U}_e(1 - \bar{x}_e)) - \sum_{e \in E} \mu^*_e(\theta^*_e - \hat{u}_e \bar{x}_e) + \nu^{*t} G(u^*) \\ &= \sum_{e \in E} \theta^*_e - \sum_{e \in E} \lambda^*_e(\theta^*_e - u^*_e + \hat{U}_e(1 - x_e)) - \sum_{e \in E} \mu^*_e(\theta^*_e - \hat{u}_e x_e) + \nu^{*t} G(u^*) \\ &- \sum_{e \in E} \lambda^*_e(\hat{U}_e(1 - \bar{x}_e)) + \sum_{e \in E} \lambda^*_e(\hat{U}_e(1 - x_e)) - \sum_{e \in E} \mu^*_e(\hat{u}_e x_e) + \sum_{e \in E} \mu^*_e(\hat{u}_e \bar{x}_e) \\ &= u(\bar{x}) + \sum_{e \in E} \lambda^*_e \hat{U}_e(x_e - \bar{x}_e) + \sum_{e \in E} \mu^*_e \hat{u}_e(x_e - \bar{x}_e) \\ &= u(\bar{x}) + \sum_{e \in E: \bar{x}_e = 1} \hat{U}_e(x_e - 1) + \sum_{e \in E: \bar{x}_e = 0} \hat{u}_e x_e. \end{split}$$

This concludes the proof.

Note that, by construction, the above generalized Benders cuts imply that, we can compare the value of the subproblem  $(PU_{\bar{x}})$  associated with a given spanning tree  $\bar{x} \in S\mathcal{T}_G$ ,  $u(\bar{x})$ , with the value of the subproblem  $(RPU_x)$  associated with a different spanning tree  $x \in S\mathcal{T}_G$ , u(x). In particular, if there exist  $e_1, e_2 \in E$  with  $\bar{x}_{e_1} = 1$  and  $x_{e_1} = 0$ , and  $\bar{x}_{e_2} = 0$  and  $x_{e_2} = 1$ , then the value of u(x) is at least  $u(\bar{x}) - \hat{U}_{e_1} + \hat{u}_{e_2}$ . In other words, the difference between the values of the two subproblems is bounded by the maximum amount that can be saved (in the cost function) by removing  $e_1$ , plus the minimum gain that can be attained by adding  $e_2$ . Therefore, the relaxed master problem at the K-th iteration of the row-generation solution algorithm can be stated as:

(4.3) 
$$\Theta^* = \min \quad \Theta$$
$$\Theta \ge u(\bar{x}^k) + \sum_{\substack{e:\bar{x}_e^k = 1\\ x \in \mathcal{ST}_G.}} \widehat{U}_e(x_e - 1) + \sum_{\substack{e:\bar{x}_e^k = 0\\ e:\bar{x}_e^k = 0}} \widehat{u}_e x_e, \ k = 1, \dots, K_e$$

The reader may note that the cuts (4.3) can be interpreted as some form of lifting of the surrogated McCorminck inequalities (LIN – Mc), after projecting out the u variables in formulation (RL – MSTN).

Using the above cuts algorithmically, gives rise to the solution scheme described in Algorithm 1:

Algorithm 1: Decomposition Algorithm for solving MSTN.
<b>Initialization</b> : Let $x^0 \in ST_G$ be an initial solution and $\varepsilon$ a given threshold
value.
Set $LB = 0$ , $UB = +\infty$ , $\bar{x} = x^0$ .
while $ UB - LB  > \varepsilon \operatorname{do}$
(1) Solve $(PU_{\bar{x}})$ for $\bar{x}$ to get $u(\bar{x})$ .
(2) Add the cut $\Theta \ge u(\bar{x}) + \sum \widehat{U}_e(x_e - 1) + \sum \widehat{u}_e x_e$ to the current
$e:\bar{x}_e=1$ $e:\bar{x}_e=0$
master problem.
(3) Obtain the optimal value $\Theta$ to the current master problem, and its
associated solution $\bar{x}$ .
(4) Update $LB = \max\{LB, \bar{\Theta}\}$ and $UB = \min\{UB, \sum_{e \in E} u(\bar{x})_e \bar{x}_e\}$
end

The stopping criterion is that the gap between the upper and lower bound does not exceed the fixed threshold value  $\varepsilon$ .

**Theorem 4.2.** The decomposition-based solution scheme of Algorithm 1 terminates in a finite number of steps (for any given  $\varepsilon \ge 0$ ). Furthermore, if  $\varepsilon \le \min{\{\tilde{U}_{e_1} - \tilde{u}_{e_2} \ge 0 : e_1 \neq e_2 \in E\}}$ , it outputs an optimal MSTN.

*Proof.* The the finiteness of the number of underlying spanning trees of  $ST_G$ , the convexity of  $(PU_{\bar{x}})$  for any  $\bar{x} \in ST_G$ , and the linear separability of the problem assure the result by applying Theorem 2.4 in [21].

To avoid the enumeration of all spanning trees of G, and to reduce the number of iterations, several recipes can be applied. One of them is to start with a non-empty set of cuts which give a suitable initial representation of the lower envelope of  $\Theta$ . Hence, if  $\overline{ST}_G$  denotes the set of trees associated with the current set of constraints (4.3), the representation we use for the master problem is:

(4.4) min 
$$\sum_{e \in E} \theta_e$$
  
(4.5) s.t. 
$$\sum_{e \in E} \theta_e \ge u(\bar{x}) + \sum_{e:\bar{x}_e=1} \widehat{U}_e(x_e - 1) + \sum_{e:\bar{x}_e=0} \widehat{u}_e x_e, \forall \bar{x} \in \overline{ST_G},$$
$$\theta_e \ge \widetilde{u}_e x_e, \quad e \in E,$$
$$x \in ST_G.$$

Given that the master problem exhibits a combinatorial nature, the performance of a Benders-like algorithm can be improved by embedding the cut generation mechanism within a branch-and-cut scheme. This is the current trend nowadays [16, 17]. This requires to separate the optimality cuts in addition to any other generated cuts, at the nodes of the enumeration tree. Note that this approach is also valid in our case, as the cuts (4.5) are also valid if  $\bar{x}$  is the solution to a linear programming relaxation of a valid MST formulation.

4.1. **Computational Experiments**. The proposed decomposition approach has been tested over the same set of benchmark instances used to compared the compact formulations. Based on the results obtained in such a comparison, and also

to take advantage of the possibility of adding dynamically violated SECs within the branch-&-cut, we combine the decomposition approach with the classical SEC representation SEC – MSTN. In addition to the average statistics reported in the previous tables (CPU, #SECs, #Nodes, GAPs, and %Solved), we also report now the average number of Benders' type cuts, #BendersCuts, and the gap after the exploration of the root node of the branch-&-cut tree, %GAP<sub>0</sub>. Average results for the 4 scenarios are reported in Tables 3 and 4.

As can be seen, the computing times required by the decomposition approach are smaller than those obtained with the MINLP formulations for the small size radii scenario and also in the small-medium size radii scenario for the 3D case. However, the results obtained for the medium-large and large size scenarios reveal that the MINLP formulations have a better performance than the decomposition scheme. Note that the cuts induced by our approach depends of the available upper and lower bounds on the lengths of the edges in the graph. These bounds are tight for the small size radii scenarios, but far from being a representative value of the actual length of the edge in the remaining scenarios. Hence, a large number of cuts are needed to certify optimality of the solution in these cases.

### 5. A MATHHEURISTIC FOR MSTN

The results of the computational experiments section indicate that MSTN instances with up to less than 15 vertices can be optimally solved within the allowed time limit, but as the sizes of the instances increase the computing times become prohibitive. Below we present a mathheuristic alternative to obtain near-optimal solutions to larger MSTN instances. The main idea under the proposed algorithm is based on the observation that the problem is a biconvex problem, since fixing any of the set of variables the problem becomes an efficiently solvable optimization problem (in case x is fixed, the problem is a continuous SOCP, while if u is fixed, the problem is a standard MST problem).

The mathheuristic consists of two embedded loops. The outer loop is a multistart procedure. The input of each iteration in this loop is a spanning tree, which will be used in the initial iteration of the inner loop. The number of iterations of the outer loop is a parameter related to the initial spanning tree generation mechanism that we use, which will be explained later on.

The rationale of the inner loop is to alternate in solving subproblems in the solution spaces of the two main sets of variables (x and u). We proceed iteratively, and each iteration consists of solving a pair of subproblems, one in each space of variables. When solving the subproblem in one solution space we fix the values of the variables of the other space.

Formally, let  $(P_{\bar{x}u})$  and  $(P_{x\bar{u}})$  respectively denote the subproblems of the generic MSTN formulation  $P_{xu}$  of Section 3, when  $\bar{x}$  and  $\bar{u}$  are fixed. That is,

$$(\mathrm{PU}_{\bar{\mathbf{x}}}) \qquad \min \sum_{e \in E} u_e \bar{x}_e \qquad (\mathrm{PX}_{\bar{\mathbf{u}}}) \text{ and } \qquad \min \sum_{e \in E} \bar{u}_e x_e$$
  
s.t.  $u \in \mathcal{U}$  s.t.  $x \in \mathcal{ST}_G$ .

Figure 4 shows a flowchart of the inner loop of the mathheuristic. We start with a given spanning tree  $T^0$  associated with a solution  $x^0$ . In the k-th iteration, we compute the distances  $u(x^k)$  in the current tree  $T^k$  and update the vector  $\bar{u}^{k+1}$ 

r	n	CPU	#SEC	#BendersCuts	#NodesB%B	%GAP <sub>0</sub>	%GAP	%Solved
	5	0.0065	1.20	0.20	0.00	5.45%		100%
	6	0.0196	3.60	2.40	10.40	18.99%		100%
	7	0.0328	5.60	4.00	22.80	12.07%		100%
	8	0.0347	3.60	3.80	23.40	15.41%		100%
	9	0.0646	12.80	7.60	64.60	18.79%		100%
1	10	0.1796	26.60	23.40	180.00	20.06%		100%
1	11	0.5341	116.60	68.40	950.60	28.48%		100%
	12	0.6484	213.20	71.80	1129.00	32.67%		100%
	13	1.5531	246.20	167.60	2573.80	37.76%		100%
	14	1.6703	300.60	177.00	2204.20	32.39%		100%
	15	45.3193	1016.40	1637.40	23077.60	47.74%		100%
	20	333.5085	1628.60	3721.80	59876.80	39.75%		100%
	5	0.0464	4.20	6.40	25.60	29.32%		100%
	6	0.0730	6.70	11.40	50.90	24.67%		100%
	7	0.0678	12.20	10.80	78.20	28.19%		100%
	8	0.2743	21.60	43.60	311.60	41.06%		100%
	9	0.3111	55.20	46.80	492.20	30.63%		100%
<b>2</b>	10	0.4646	78.00	66.60	721.40	33.22%		100%
	11	1.3472	245.40	167.80	2382.60	35.11%		100%
	12	160.8519	864.80	3027.00	36569.60	61.72%		100%
	13	326.1787	1598.20	2800.40	50047.80	50.47%		100%
	14	226.5067	2024.20	6463.60	96243.00	43.07%		100%
	15	5824.7652	8023.00	18775.80	284590.80	73.80%	3.76%	20%
	5	0.1152	3.80	5.80	24.40	27.67%		100%
	7	0.4851	58.10	93.50	712.60	50.67%		100%
	8	3.2475	158.20	526.80	3963.60	59.22%		100%
	9	17.3417	521.00	1492.40	14560.00	67.32%		100%
	10	5.8312	226.20	595.00	5933.40	50.17%		100%
3	11	2603.6210	4308.40	12569.00	168712.00	75.77%	40.36%	80%
	12	>7200	5223.40	23172.40	275986.80	81.98%	22.01%	0%
	13	>7200	7191.60	20230.60	282031.60	85.37%	20.33%	0%
	14	>7200	15425.00	14481.80	311567.60	90.64%	53.59%	0%
	15	>7200	11379.40	13846.80	310549.80	83.69%	35.16%	0%
	5	0.0476	3.80	5.80	24.20	33.07%		100%
	6	0.3993	36.20	83.80	428.60	56.12%		100%
	8	2.9985	187.20	424.40	3055.80	62.99%		100%
	9	53.7040	418.00	2631.80	23586.40	67.46%		100%
	10	1013.3837	1444.00	7611.00	72987.20	82.73%		100%
4	11	4256.8194	4636.60	16430.60	204272.20	84.16%	30.36%	60%
1	12	6232.3367	6569.80	20400.00	250014.00	77.37%	16.60%	20%
1	13	>7200	8218.80	19321.40	299586.40	85.78%	29.58%	0%
1	14	>7200	13880.00	13080.80	336546.40	93.16%	71.25%	0%
1	15	>7200	16128.60	12538.00	326406.20	94.80%	50.14%	0%

TABLE 3. Average results for the decomposition approach for  $\mathbb{R}^2$  instances.

according to  $\bar{u}^k$  and  $u(x^k)$ . In the first iteration we use the distance lower bounds  $\bar{u}^0 = \tilde{u}$ . At each iteration k > 0 we first solve problem  $(PX_{\bar{u}^k})$  and then compute the vertices distances  $u(x^k)$  in its optimal tree  $T^k$ , by solving  $(PU_{x^k})$ . All components  $\bar{u}^k_e$  associated with edges  $e \in T^k$  are updated to the corresponding component of the distances vector  $u(x^k)$ . The remaining components remain unchanged. The procedure terminates when two consecutive iterations produce the same tree or a maximum number of iteration is attained.

For the sake of analyzing the quality of solutions obtained with the mathheuristic we introduce the notion of *partial optimal MSTN* adapting the notation in [35] for the general case of minimizing a non-separable function subject to disjoint constraints.

r	n	CPU	#SEC	#BendersCuts	#NodesB%B	%GAP <sub>0</sub>	%GAP	%Solved
1	5	0.0063	0.80	0.00	0.00	2.28%		100%
	6	0.0125	1.60	0.60	0.00	4.53%		100%
	7	0.0138	2.20	1.80	9.80	9.31%		100%
	8	0.0445	3.60	3.40	18.80	12.49%		100%
	9	0.0573	6.00	5.80	28.60	9.66%		100%
	10	0.0883	9.60	9.20	72.60	8.28%		100%
1	11	0.2478	30.20	17.20	162.00	17.26%		100%
	12	0.2455	59.00	25.00	314.20	16.00%		100%
	13	0.8280	87.60	85.20	1035.40	17.73%		100%
	14	1.1512	194.80	95.20	1535.20	11.92%		100%
	15	1.7121	264.00	130.20	1761.60	18.39%		100%
	20	8.2175	702.20	377.80	7398.60	16.68%		100%
	5	0.0218	3.80	2.40	7.80	12.34%		100%
	6	0.0292	2.40	3.30	12.50	8.57%		100%
	7	0.0388	4.20	4.60	18.80	18.30%		100%
	8	0.2397	24.00	33.40	247.00	23.13%		100%
	9	0.2389	26.00	32.60	304.00	18.73%		100%
2	10	0.2859	50.80	33.00	398.00	12.74%		100%
	11	0.5181	58.00	57.80	555.80	20.94%		100%
	12	4.8255	263.20	369.80	5574.80	28.77%		100%
	13	5.6111	498.60	635.80	9576.20	28.87%		100%
	14	11.3739	1388.00	1459.40	32630.40	27.78%		100%
	15	35.4121	1873.00	2982.00	67628.20	33.80%		100%
	5	0.0281	2.80	2.60	10.00	16.98%		100%
	6	0.2437	26.80	43.80	276.40	29.17%		100%
	7	0.2725	39.60	42.60	348.20	38.34%		100%
	8	1.5945	131.40	235.40	1915.20	49.20%		100%
	9	3.9492	292.40	1025.80	9022.00	45.81%		100%
3	10	2.5790	313.00	272.40	3468.00	26.01%		100%
	11	55.9248	689.40	1979.60	26140.60	42.86%		100%
	12	1258.5048	2060.40	8294.40	130089.80	47.82%	0.0107	100%
	13	3005.2253	5083.40	10824.20	212760.60	44.99%	3.81%	60%
	14	>7200	9029.40	15154.60	288000.20	53.37%	17.53%	0%
	15	1751.1580	9504.80	10049.00	243900.00	40.75%		100%
	5	0.0312	3.00	3.60	16.60	19.69%		100%
	6	0.1750	13.80	29.60	122.20	27.05%		100%
	7	0.6724	54.80	94.20	543.60	22.12%		100%
	8	1.6626	162.80	218.80	1898.40	46.48%		100%
	9	9.5678	326.60	916.20	8138.60	45.42%		100%
4	10	22.7335	576.60	1450.40	17267.40	47.61%		100%
	11	107.0304	1037.60	3051.40	40153.60	50.56%		100%
	12	1005.8061	1904.80	6533.00	99639.80	50.15%		100%
	13	999.9207	5066.20	12905.60	211964.00	50.13%	00 010	100%
	14	7200.3120	9951.60	14550.00	285772.40	70.62%	30.61%	0%
	15	6123.5383	12659.40	12203.20	266014.20	55.75%	16.35%	20%

TABLE 4. Average results for decomposition approach for  $\mathbb{R}^3$  instances.

**Definition 5.1** (Partial Optimum MSTN). Let  $\bar{x} \in ST_G$  and  $\bar{u} \in U$ .  $(\bar{x}, \bar{u})$  is said a partial optimum MSTN if:

$$\sum_{e \in E} \bar{x}_e \bar{u}_e \le \sum_{e \in E} x_e \bar{u}_e \quad and \quad \sum_{e \in E} \bar{x}_e \bar{u}_e \le \sum_{e \in E} \bar{x}_e u_e$$

for all  $x \in \mathcal{ST}_G$  and  $u \in \mathcal{U}$ .

Observe that a partial optimum MSTN  $(\bar{x}, \bar{u})$  implies that  $\bar{x}$  is a MST for the weights  $\bar{u}$  and that  $\bar{u}$  are the optimal distances with respect to  $\bar{x}$ . The following result states the partial optimality of the solutions generated by the proposed mathheuristic.

**Theorem 5.2.** The sequence of objective values produced at the inner loop of the mathheuristic, corresponding to a given initial solution, converges monotonically to a partial optimum MSTN.



FIGURE 4. Flowchart of the inner loop of the mathheuristic

*Proof.* Let  $f(x, u) = \sum_{e \in E} x_e u_e$  denote the objective function value associated with a given solution  $x \in ST_G$ ,  $u \in U$ . Let also  $x^1, \ldots, x^k \in ST_G$  and  $u^1, \ldots, u^k \in U$ be the solutions obtained in the first k steps of the alternate convex search for a given initial solution.

Observe that in the mathheuristic, for  $u^j$  given,  $x^{j+1}$  is obtained by solving  $(PX_{\bar{u}})$  with weights  $\bar{u} = u^j$ . Hence,

$$\sum_{e \in E} x_e^{j+1} \ u_e^j \le \sum_{e \in E} x_e \ \bar{u}_e^j, \forall x \in \mathcal{ST}_G.$$

Next, solving  $(PU_{\bar{x}})$  with  $\bar{x} = x^{j+1}$ , one obtains  $u(x^{j+1})$  and then  $u^{j+1}$  with:

$$\sum_{e \in E} x_e^{j+1} \ u(x^{j+1})_e = \sum_{e \in E} x_e^{j+1} \ u_e^{j+1} \le \sum_{e \in E} x_e^{j+1} \ u_e, \forall u \in \mathcal{U}.$$

Hence,  $f(x^k, u^k) \ge f(x^k, u(x^k)) \ge f(x^{k+1}, u^{k+1})$ , so the sequence  $\{f(x^j, u^j)\}_{j \in \mathbb{Z}_+}$ is monotonically non-increasing. Thus, since  $f(x, u) \ge 0$  for all  $x \in ST_G$  and  $u \in U$ , the sequence of objective values converges.

Let  $\Theta^* = \lim_{j \to \infty} f(x^j, u^j)$  and  $x^* \in ST_G$ ,  $u^* \in U$  such that  $f(x^*, u^*) = \Theta^*$ . Since  $ST_G$  and U are closed sets and f is continuous, we have that taking limits:

$$\Theta^* = \sum_{e \in E} x_e^* u_e^* \le \sum_{e \in E} x_e u_e^* \quad and \quad \Theta^* = \sum_{e \in E} x_e^* u_e^* \le \sum_{e \in E} x_e^* u_e.$$

Thus,  $(x^*, u^*)$  is a partial optimum MSTN.

Since only partial optimality of the solutions is assured at the end of each inner loop, it is possible that the mathheuristic gets trapped at a local optimum. Hence we have incorporated a multistart outer loop to allow escaping from local optimal. Note that the mathheuristic becomes an exact solution method if all possible spanning trees are considered as initial solutions. However, complete enumeration is prohibitive, even if the number of potential MSTs is finite (despite using varying weights). On the other hand, we have observed that (i) the mathheuristic is sensitive to the provided initial feasible solution, and; (ii) in many cases, a few changes over an initial standard MST with respect to the distances between the centers of the neighborhoods are enough to find an optimal MSTN solution. Hence,

we generate the set of initial spanning trees for the multistart procedure with an adaptation of the method proposed in [34], which is described in Algorithm 2. In principle, this method generates the whole set of spanning trees on a given graph (by increasing order values relative to a given weight vector). In our adaptation, we stop generating new spanning trees, when one of the following criteria is met: (1) a given number of MSTs has already been generated; or, (2) no improvement has been obtained, in the MSTNs obtained in the inner iterations, for a given number of outer iterations.

Algorithm 2: Initial solutions for the multistart procedure. Initialization:  $u_{vw}^0 = ||v - w||, \forall v, w \in V \text{ and } T^0 \text{ the MST}$  with respect to  $u^0, \mathcal{T} = \{T^0\}.$ for  $T \in \mathcal{T}$  do Let  $e_1, \ldots, e_{n-1}$  be the edges of T. for  $i = 1, \ldots, n-1$  do Construct the MST with respect to  $u^0, T_i$ , such that  $e_i$  does not belong to the tree but  $e_1, \ldots, e_{i-1}$  are part of it. Let  $c_i$  be the weight of  $T_i$ . end Choose  $T' \in \{T_1, \ldots, T_{n-1}\}$  with  $c(T') = \min_{i=1,\ldots,n} c_i$  and add it to  $\mathcal{T}$ . end

A series of computational experiments have been performed to analyze the computing times and the quality of the solutions obtained with the overall heuristic. We report results based on two batteries of benchmark instances. The first one is the same that was used in our previous experiments. Here the goal is to compare the quality of the solutions obtained by the exact and the heuristic methods. The second one contains larger size instances and the goal is to explore the limit of the mathheuristic. In the experiments we do not fix limits on the number of inner iterations but we set up the maximum number of trees generated (outer iterations) to  $100 \times |E|$ . Table 5 summarizes the obtained numerical results. We report average values of the computing times consumed the the mathheuristic (CPU) and the percentage deviation (%Dev) with respect to the optimal (or best-known) solutions obtained with the exact approaches. Observe that the quality of the solutions is extremely good, as the maximum %Dev obtained in all the experiments was 1.3086%. Furthermore, in most of the cases where the exact approaches did not prove the optimality of the best solution found, the heuristic produced a better solution. Indeed, many of the proven optimal solutions obtained with the other approaches, where also obtained with the mathheuristic. Moreover, in a few cases the mathheuristic gives slightly better solutions than those obtained by the exact methods which showed some precision difficulties caused by numerical instability. Tables 6 and 7 show the results for the largest instances. We report, apart from the average computing times, the percentage deviations with respect to available lower (%Dev LB) and upper bounds (%Dev UB) for the optimal value of the MSTN. Lower bounds were calculated by computing the MST with respect to the original graph in which the edge lengths are given as the minimum distance between the neighborhoods that contain the vertices of each edge, i.e.:

$$\bar{u}_e = \min\{d(y_v, y_w) : y_v \in \mathcal{N}_v, y_w \in \mathcal{N}_w\}, \quad \text{for } e = \{v, w\} \in E.$$

Upper bounds are computed as the optimal value of  $(PU_{\bar{x}})$ , when  $\bar{x}$  is the standard MST. Finally, we also report the percentage of instances (out of 5) in which the solution of the matheuristic coincides with the upper bound (i.e. the underlined MSTN equals the MST). As expected, the deviations with respect to the lower and upper bounds increases as the radii of the neighborhoods do. The same happens with the number of instances in which the solutions of the MSTN coincide with those of MST. In scenario 4, the instances with largest radii, the lower bounds are close to zero in most of the cases since almost all pairs of neighborhoods intersect, and several 100% deviations were obtained. The reader may observe that deviation with respect to lower bounds are few significative since these bounds are always rather far from the actual optimal solution. We would also like to emphasize that computing times for the three-dimensional instances are slightly larger than those obtained for the planar instances, due to the number of variables of the problems (PU<sub> $\bar{x}$ </sub>), that must be iteratively solved in the inner loop of the algorithm. However, the times do not seem to largely depend of the size of the neighborhoods.

#### 6. Conclusions

We analyzed the problem of finding minimum spanning trees with neighborhoods, where the neighborhoods are defined as SOC-representable objects and the lengths of the arcs in the graph are induced by a  $\ell_q$  norm. Two MINLP formulations are provided whose differences come from the representation of the subtour elimination constraints. We propose a decomposition-based methodology to solve the problem based on the efficiency of solving SOCP problems. Furthermore, a new mathheuristic procedure is applied to solve the problem exploiting not only the SOC-representability of the neighborhoods but also that the MST problems are easily solvable. The results of an extensive computational experience are reported to compare all formulations and procedures provided throughout this paper.

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		2-dimensi	onal instances	3-dimensional instances			
r	n	CPU	%Dev	CPU	%Dev		
	5	0.1004	0.0000%	0.1594	0.0000%		
	6	0.2068	0.0000%	0.2200	0.0000%		
	7	0.3368	0.0433%	0.3614	0.0001%		
	8	0.5220	0.0000%	0.7036	0.0000%		
	9	0.6982	0.0000%	0.6792	0.0195%		
1	10	1.2014	0.1768%	1.2254	0.0000%		
1	11	1.8868	0.2679%	2.1230	0.3749%		
	12	2.4382	0.0000%	2.3078	0.0000%		
	13	3.0136	0.1319%	4.1954	0.1223%		
	14	3.9986	0.1802%	4.0428	0.0527%		
	15	5.9238	0.3095%	5.4956	0.2659%		
	20	15.3978	0.2068%	15.4622	0.0565%		
	5	0.1788	0.0000%	0.2416	0.0001%		
	6	0.2603	0.0011%	0.3098	0.0000%		
	7	0.3972	0.1528%	0.5358	0.0000%		
	8	0.8566	0.0000%	1.3224	0.0000%		
	9	0.9240	0.6322%	0.9988	0.3318%		
<b>2</b>	10	1.4706	0.1666%	1.6722	0.0296%		
	11	2.0872	0.8081%	2.5434	0.3964%		
	12	3.1428	0.0212%	4.2852	0.2285%		
	13	3.7266	0.5755%	6.3750	0.3975%		
	14	5.6144	0.5838%	6.5618	0.0270%		
	15	9.1994	-0.0408%	10.2092	0.3245%		
	5	0.1710	0.0000%	0.2370	0.0000%		
	6	0.2134	0.0000%	0.6210	0.0000%		
	7	0.5969	0.1360%	0.7737	0.0713%		
	8	0.9008	0.1571%	1.3504	0.0271%		
	9	1.3432	1.3086%	2.3226	0.7177%		
3	10	1.8258	0.8340%	2.6464	0.4596%		
	11	3.0670	0.1899%	4.4142	1.1838%		
	12	4.3984	0.1122%	5.2298	0.0581%		
	13	4.9976	0.4673%	7.1142	1.2851%		
	14	6.7682	-0.1210%	10.2342	-0.1614%		
	15	8.2982	-0.0949%	11.2072	0.2390%		
	5	0.1664	0.0000%	0.2738	0.0000%		
	6	0.3942	0.1012%	0.4942	0.5379%		
	7	0.7893	0.0601%	0.9942	0.1123%		
	8	1.1640	0.0000%	1.6256	0.0353%		
	9	1.5462	0.7477%	1.8514	0.4004%		
4	10	2.2468	1.1261%	2.6576	1.3283%		
	11	3.2060	0.7875%	3.6996	0.6159%		
	12	4.5152	0.2935%	4.8816	0.1611%		
	13	5.0992	0.7808%	7.2430	1.0225%		
	14	6.8126	-0.1978%	9.6768	0.6739%		
	15	8.1124	0.0105%	11.6100	-0.2135%		

TABLE 5. Average Results for the mathheuristic.

1	$\cdot  V $	CPU	%Dev LB	% Dev UB	% MST
	20	14.5532	23.0877%	0.1201%	40.00%
	25	27.1624	27.6163%	0.2969%	40.00%
	30	54.5254	27.8230%	0.3004%	40.00%
	35	82.7320	28.8806%	0.1985%	40.00%
	40	122.8916	28.7590%	0.3342%	40.00%
	45	182.2026	38.7607%	0.1451%	80.00%
	50	255.4392	43.0832%	0.0912%	80.00%
	60	472.9626	40.6246%	0.2814%	20.00%
	70	724.8468	43.4054%	0.1118%	80.00%
	80	751.3728	47.7128%	0.3567%	40.00%
	90	1064.7958	49.2007%	0.0000%	100.00%
	100	1480.0034	53.4484%	0.1639%	80.00%
	20	16.4950	62.3051%	1.3996%	0.00%
	25	31.6210	77.3769%	0.3444%	20.00%
	30	59.5594	77.6920%	1.5311%	0.00%
	35	87.8010	86.6972%	2.4308%	0.00%
	40	145.0846	87.3522%	1.2426%	40.00%
ç	45	192.4576	84.7788%	0.7022%	60.00%
4	50	283.2516	91.5316%	1.0501%	40.00%
	60	525.9362	96.1926%	1.6971%	0.00%
	70	835.0496	96.2605%	0.8858%	20.00%
	80	779.3946	97.2727%	0.9087%	40.00%
	90	1122.9898	98.3883%	0.5728%	60.00%
	100	1548.9070	99.3069%	1.4232%	40.00%
	20	16.0632	90.6985%	2.2212%	20.00%
	25	32.1278	96.2322%	0.7643%	20.00%
	30	65.7792	97.5944%	1.0350%	0.00%
	35	90.1888	98.4009%	5.9840%	0.00%
	40	137.5042	99.0318%	2.0271%	0.00%
9	45	198.4974	99.0682%	1.0427%	40.00%
•	50	268.2828	99.8648%	2.2477%	20.00%
	60	502.3478	100.0000%	3.2364%	0.00%
	70	816.0300	100.0000%	2.7085%	20.00%
	80	756.5704	100.0000%	2.3165%	40.00%
	90	1116.6500	100.0000%	1.8877%	40.00%
	100	1530.6052	100.0000%	1.5370%	20.00%
	20	16.4998	97.9307%	2.7959%	20.00%
	25	33.8690	99.3203%	1.6366%	20.00%
	30	61.1976	100.0000%	2.6932%	0.00%
	35	89.4202	100.0000%	8.7080%	0.00%
	40	146.1266	100.0000%	3.3380%	0.00%
2	45	213.8344	100.0000%	3.0796%	20.00%
	50	282.9736	100.0000%	2.0663%	20.00%
	60	486.8964	100.0000%	4.5859%	0.00%
	70	763.0016	100.0000%	4.2135%	0.00%
	80	748.1272	100.0000%	4.5767%	0.00%
	90	1085.8690	100.0000%	3.2538%	20.00%
1	100	1668.2424	100.0000%	2.7675%	20.00%

TABLE 6. Average Results for the mathheuristic for large instances in the planar case.

r	V	CPU	%Dev LB	% Dev UB	% MST
	20	14.6272	10.3986%	0.0467%	80.00%
	25	40.6772	13.0944%	0.0378%	60.00%
	30	69.8356	10.6289%	0.0006%	80.00%
	35	106.5134	11.2375%	0.1286%	60.00%
	40	175.6634	11.0897%	0.1831%	40.00%
	45	262.2358	15.1212%	0.0322%	80.00%
1	50	370.5236	17.9594%	0.2323%	60.00%
	60	631.6412	14.9262%	0.0000%	100.00%
	70	1071.5590	18.0318%	0.1747%	60.00%
	80	1071.1360	17.2028%	0.1713%	60.00%
	90	1570.6312	17.1973%	0.0046%	80.00%
	100	2256.3462	20.5805%	0.1206%	60.00%
	20	24 0912	34 4738%	0.9106%	20.00%
	25	49 7172	47 0066%	0.4466%	20.00%
	30	81 0262	40 1495%	1 3887%	20.00%
	35	123 2108	45 9130%	0.4637%	60.00%
	40	211 2694	48 8337%	0.9941%	20.00%
	45	205 5366	52 4260%	0.9341%	60.00%
2	50	401 4358	55 8653%	0.5822%	60.00%
	60 60	743 1540	61 8838%	0.382270 0.2815%	60.00%
	70	1120 6448	68 2224%	0.201070	40.00%
	80	1139.0448	60 4113%	0.704070	40.0070
	00	1835 7320	09.411370 71 7028%	0.409370 0.5406%	40.0070
	100	2456 1402	71.192870 77.1601%	0.3400%	60.00%
	20	2430.1402	66 0737%	$\frac{0.109970}{2.4841\%}$	20.00%
	20	51 0204	76 22020	2.404170	20.0070
	20	01.9204	70.820370	2.830070	20.00%
	25	03.2004	10.101170 82.000207	0 220407	40.0070
	- 30 - 40	130.2374	03.292370	0.002470	40.00%
	40	207.1052	82.142370 85.760807	3.441970	0.0070
3	40	293.3924	85.7098%	1.1218%	20.00%
	00 60	431.9292	91.902070	1.020970	40.0070
	00	1162 2446	90.3082%	2.9933%	20.00%
	10	1103.3440	97.890370 07 = 67407	2.210370	40.007
	80	1231.3932	97.3074%	0.9325%	40.00%
	90	1770.0200	98.3331%	1.3740%	20.00%
	100	2357.2434	98.5889%	2.7997%	20.00%
	20	24.4800	90.5059%	4.3812%	0.00%
L	25	01.0444	93.0932%	2.9003%	0.00%
	30	84.3946	96.3750%	4.9004%	20.00%
L	35	134.4824	97.3869%	2.5519%	20.00%
	40	213.2442	98.0207%	5.4728%	0.00%
4	45	304.6368	99.5034%	1.9230%	0.00%
	50	415.3388	99.3344%	3.2609%	0.00%
	60	721.3308	99.9964%	2.7762%	20.00%
	70	1189.9664	100.0000%	3.0113%	0.00%
	80	1233.2842	100.0000%	2.1201%	20.00%
	90	1922.6220	100.0000%	2.3436%	0.00%
L	100	2412.5672	100.0000%	2.9934%	20.00%

TABLE 7. Average Results for the mathheuristic for large instances in the 3D case.

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