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Faster Exact Algorithms for Computing Steiner Trees in Higher Dimensional Euclidean Spaces

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Abstract The Euclidean Steiner tree problem asks for a network of minimum total length interconnecting a finite set of points in d-dimensional space. For $d \geq 3$, only one practical algorithmic approach exists for this problem — proposed by Smith in 1992. A number of refinements of Smith's algorithm have increased the range of solvable problems a little, but it is still infeasible to solve problem instances with more than around 17 terminals. In this paper we firstly propose some additional improvements to Smith's algorithm. Secondly, we propose a new algorithmic paradigm called branch enumeration. Our experiments show that branch enumeration has better performance than an optimized version of Smith's algorithm when $d \geq 3$; furthermore, we argue that branch enumeration has the potential to push the boundary of solvable problems further. All source code and data sets are available at `http://github.com/DIKU-Steiner/MPC15`.

Keywords Steiner tree problem · d-dimensional Euclidean space · exact algorithm · computational study

Mathematics Subject Classification (2000) 90-08 Computational methods · 52C45 Combinatorial complexity of geoetric structures

1 Introduction

Given a finite set of n points N in a d-dimensional space $\mathbb{R}^d$, $(d \geq 2)$, the *Euclidean Steiner tree problem* (ESTP) asks for a network T^* of minimum length interconnecting N. The vertices of T^* corresponding to points of N

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are called *terminals* while possible additional vertices in T^* are called *Steiner points*. T^* necessarily is a tree, and is referred to as a *Euclidean minimum Steiner tree* (EMST) for N. The ESTP in the plane ($d = 2$) has a history that goes back more than two centuries [4], and is known to be NP-hard [9], even when the terminals are restricted to lie on two parallel lines [16]. The generalisation to more than two dimensions was introduced by Bopp [3] in 1879; more recent mathematical treatments can be found in [10,13]. The problem in $\mathbb{R}^d$, $d \geq 3$, has applications to areas such as phylogenetics [6,7,5] and to the structure and folding of proteins [18,21].

An EMST T^* can be viewed as a union of *full* EMSTs whose terminals have degree 1. Steiner points in T^* (in any dimension) have degree 3. The three incident edges at a Steiner point are co-planar and each pair meets at an angle of 120^o. These degree conditions imply that full EMSTs spanning k terminals, $1 \leq k \leq n$, have $k - 2$ Steiner points.

The first exact algorithms for the ESTP in the plane ($\mathbb{R}^2$) were based on the following common framework [12]. Subsets of terminals are considered one by one. For each subset, all its full EMSTs are determined and the shortest is retained. Several tests are applied to these retained full EMSTs to decide if they can belong to an EMST for N. Surviving full EMSTs are then concatenated in all possible ways to obtain trees spanning N. The shortest of them is T^*.

The main bottleneck in this approach is the generation of full EMSTs. It has been observed [25] that substantial improvements can be obtained if full RMSTs are generated simultaneously across various subsets of terminals. Very powerful geometrical pruning tests identifying non-optimal full EMSTs can then be applied not *after* but *during* their generation. As a consequence of this speed-up, the concatenation of full EMSTs became a bottleneck of the EMST computation. A remedy was based on the observation that the concatenation of full EMSTs can be formulated as a problem of finding a minimum spanning tree in a hypergraph with terminals as vertices and subsets spanned by full EMSTs as hyperedges [22]. In practice, this problem can be solved efficiently using branch-and-cut techniques. The dramatic improvements of both the generation and concatenation of full EMSTs led to the development of GeoSteiner [23,24, 26] which can routinely solve problem instances with thousands of terminals in $\mathbb{R}^2$ in a reasonable amount of time. A similar methodology has been applied to other metrics and generalisations [11,15,27,28].

Significantly less improvement has been made on exact algorithms for the problem in $\mathbb{R}^d$, $d \geq 3$. Currently, only one practical algorithmic approach exists. It was proposed by Smith [19] in 1992. A couple of recent contributions [8,14], all based on Smith's algorithm, have pushed the boundary of solvable problems a little, but in practice it is still infeasible to solve problems for $d \geq 3$ with more than 17 terminals.

As observed by Fampa and Anstreicher [8], the bounds used in [19] do not correspond to rigorous lower bounds on the solution values of these problems, but are instead obtained from putatively near-optimal solutions. In addition, when a node fails to fathom the algorithm has no means to estimate the objective values associated with its potential children. As a result the terminal nodes are added in a fixed order, even though varying the order has the potential to substantially reduce the size of the branch-and-bound tree.

Our Contribution. In this paper we first describe and evaluate some improvements to Smith's algorithm. Then we describe a novel exact algorithm, a so-called a *branch enumeration* approach. The branch enumeration algorithm deviates significantly from Smith's algorithm. One of the advantages of the branch enumeration algorithm is that it is possible to apply stronger pruning tests early in the enumeration, e.g. based on the notion of bottleneck Steiner distances. We evaluate our new branch enumeration algorithm and our improved version of Smith's algorithm experimentally on a set of benchmark instances.

GeoSteiner [23,24,26] in the Euclidean plane can be viewed as a branch enumeration (to obtain a superset of full Steiner trees in the optimal solution) followed by the concatenation of these full Steiner trees (using branch and cut to solve the minimum spanning tree problem in a hypergraph). Prunning techniques in GeoSteiner are extremely powerful and make it possible to efficiently prune nonoptimal full Steiner trees. A branch enumeration algorithm has also been suggested to compute Steiner minimum trees in Hamming metric space [1]. Our approach to find Steiner minimum trees in high-dimensional Euclidean spaces is similar. However, pruning techniques in the Hamming metric space seem to be much stronger than in high-dimensional Euclidean spaces (but far from being as strong as in GeoSteiner when applied to the problems in the Euclidean plane).

Organisation of the Paper. In Section 2 we present some preliminaries on the ESTP. Smith's algorithm is introduced in Section 3. Its improvements are discussed in Section 4. Then in Section 5 we describe the branch enumeration algorithm. Computational results are presented in Section 6, and concluding remarks are given in Section 7.

2 Preliminaries

Consider a tree T in $\mathbb{R}^d$ that interconnects a set N of n points. We assume that T consists of a set of *vertices* (a superset of N) and a set of *edges* (straight line segments) connecting pairs of vertices. The *length* of T, denoted by $|T|$, is the sum of its edge lengths. The length of an edge (u,v) connecting points u and v is denoted by $|uv|$. The given points of N are called the *terminals*, and the other vertices, if any, are called *Steiner points* (see Fig. 1). The ESTP is to determine the shortest tree T^* for N. Steiner points in T^* have degree 3 while terminals have degree at most 3. Any tree satisfying these degree constraints is called a *Steiner tree* for N.

A *Steiner topology* $\mathcal{T}$ of a Steiner tree T for N is a specification of the interconnections in T, disregarding the positions of its vertices. Any Steiner topology can be transformed into a *full Steiner topology* (FST) where all terminals have degree 1. If $\mathcal{T}$ has a terminal t adjacent to two vertices v_1 and v_2,

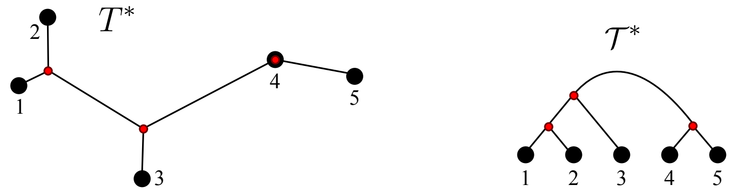


Fig. 1: The EMST of five terminals in $\mathbb{R}^2$. The terminals are shown as filled black circles, and the Steiner points are shown as smaller red circles. The topology $\mathcal{T}^*$ of T^* is shown to the right. Terminal 4 is connected to a Steiner point by a zero-length edge and therefore the Steiner point overlaps with terminal 4.

a new Steiner point s connected to t, v_1 and v_2 is added. If T has a terminal t adjacent to three vertices v_1, v_2 and v_3, a pair of Steiner points s_1 and s_2 is added. Steiner point s_1 is connected to s_2, v_1 and t. Steiner point s_2 is connected to s_1, v_2 and v_3.

The shortest Steiner tree for a given topology, $\mathcal{T}$, is called a *relatively minimal tree* (RMT) of $\mathcal{T}$. It always exists and is unique [12]. Its Steiner points may overlap with terminals and with other Steiner points because of zero length edges. Clearly, T^* is an RMT for its FST $\mathcal{T}^*$. Unfortunately, $\mathcal{T}^*$ is not known beforehand. Unless P=NP, the only feasible way to find it seems to be the enumeration of all FSTs, the determination of their RMTs and the selection of the shortest one as T^*.

The *bottleneck edge* between two terminals t_i and t_j of N is the longest edge on the path from t_i to t_j in the minimum spanning tree of N. The length of the bottleneck edge between t_i and t_i is referred to as the *bottleneck distance* and is denoted by $\beta(t_i, t_j)$. Bottleneck distances can be determined in polynomial time in a preprocessing phase. It is well-known [12] that no edge on a path between a pair of terminals t_i and t_j in the EMST can be longer than $\beta(t_i, t_j)$.

Consider a FST $\mathcal{T}$ for N. Let s be any of its Steiner points. Let r_i, r_j and r_k denote its adjacent vertices. When s is deleted, $\mathcal{T}$ breaks into three rooted binary trees or *branches* B_i, B_j and B_k rooted at r_i, r_j and r_k, respectively, see Fig. 2. Note that roots have degree 2 unless they are terminals. Furthermore the branches are *disjoint* in the sense that they do not share any terminals. The *depth* of a terminal in a branch is the number of edges separating it from the root of the branch.

Consider the FST $\mathcal{T}_i$ obtained by *splicing away* a non-terminal root r_i of B_i and connecting its adjacent vertices with each other. For notational convenience, let $\mathrm{RMT}(B_i)$ denote $\mathrm{RMT}(\mathcal{T}_i)$. Similar splicing away can be applied to non-terminal roots of B_j and B_k.

A pair of disjoint branches B_i and B_j rooted at respectively r_i and r_j can be combined into a branch $B = B_i \oplus B_j$ by adding a new Steiner point r as a root of B adjacent to r_i and r_j.

A triplet of disjoint branches B_i, B_j and B_k rooted at respectively r_i, r_j and r_k can be combined into a FST $\mathcal{T} = B_i \oplus B_j \oplus B_k$ by adding a new Steiner point r adjacent to r_i, r_j and r_k.

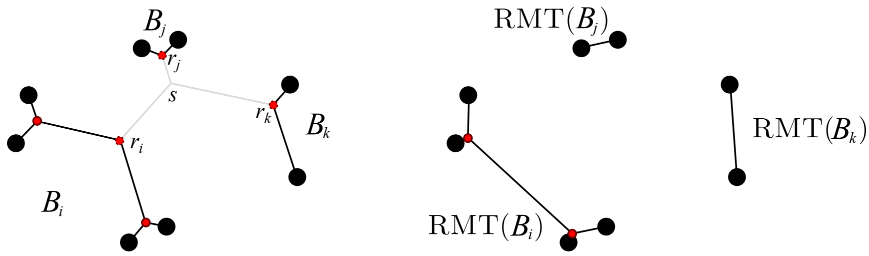


Fig. 2: Left: A FST that has been split in 3 branches B_i, B_j, and B_k by removing the Steiner point s. Right: The RMTs of each branch.

A new algorithm based on the enumeration of branches rather then the enumeration of FSTs for N will be described in Section 5. Root splicing will be used to prune branches that cannot be in the FST $\mathcal{T}^*$ of the EMST T^* of N. Disjoint triplets of the remaining feasible branches (whose union spans N) will generate feasible FSTs of N, including $\mathcal{T}^*$.

3 Smith's algorithm (Smith)

Smith's algorithm [19] enumerates FSTs of N. RMTs are then determined for each such FST. The shortest RMT encountered is an EMST T^* of N. The enumeration of FSTs is achieved by the following *expansion procedure*. Terminals are assumed to be in some fixed order $t_1, t_2, \ldots, t_n$. Assume that a FST $\mathcal{T}_k$ for $t_1, t_2, \ldots, t_k$, $3 \leq k < n$, is given. Note that only one FST exists for $k = 3$. Expand $\mathcal{T}_k$ into $2k-3$ FSTs, each with $k+1$ terminals, by inserting a new Steiner point s_{k-1} into every edge e of $\mathcal{T}_k$. In each expanded FST, s_{k-1} is adjacent to t_{k+1} and to the two vertices of e. This expansion process stops when $k = n$. It can be shown that every FST of N corresponds to exactly one unique sequence of such *expansions*. As described, the FSTs are generated in a breadth-first fashion. However, in order to obtain RMTs for all n terminals as quickly as possible, FSTs in [19] are generated in the best-first manner.

Given a FST $\mathcal{T}$ of N, arbitrary initial positions are assigned to its $n-2$ Steiner points. These positions are then recomputed iteratively by solving a system of $d(n-2)$ equations with $d(n-2)$ unknowns (corresponding to the locations of Steiner points). It can be shown [19] that the length of the tree reduces with each iteration and converges to RMT($\mathcal{T}$). The iterative procedure terminates if edges meet at Steiner points at angles within the interval $[2\pi/3-\epsilon, 2\pi/3+\epsilon]$ for an arbitrarily small constant $\epsilon > 0$. The reader is referred to [17] for the justification that a good approximation on the angles gives a good approximation of the length.

This iterative procedure can also be applied *during* the expansion process. Let $\mathcal{T}_k$ be a FST spanning k terminals, $3 \leq k < n$. Determine RMT($\mathcal{T}_k$). Suppose that it is not shorter than the shortest RMT of all n terminals encountered so far. The expansion of $\mathcal{T}_k$ can be stopped since any such expansion can only increase the lengths of RMTs of expanded FSTs. This algorithm will be referred to as SMITH.

Two improvements for SMITH have previously been suggested. Fampa and Anstreicher [8] used a conic formulation for finding a lower bound on a particular topology that eliminates the need to explicitly compute RMTs of children in the branch-and-bound tree. This was used to tighten lower bounds and guide the search. In the result-section we denote this method SMITH-FAMPA. Laarhoven and Anstreicher suggested a series of geometric criteria based on Voronoi-regions, bottleneck distances and lune-properties that could be used to discard partial topologies. Additionally they suggested exploring terminals starting with the one furthest from the point set centroid and going toward the center. In the result-section we denote this method SMITH-LAARHOVEN.

4 Smith's modified algorithm (Smith*)

Smith's algorithm adds terminals in fixed but arbitrary order when expanding FSTs. If the low index terminals are close to each other, the corresponding FSTs will have short RMTs. As a consequence, the expansion procedure will rarely stop before $k = n$. It has been suggested to index the terminals by their non-decreasing distance to their centroid [14]. We suggest a different distance-based indexing. Terminals t_1, t_2 and t_3 have to maximize the sum of their pairwise distances. The terminal t_k, $k = 4, 5, \ldots, n$, is farthest away from $t_1, t_2, \ldots, t_{k-1}$.

To obtain a reasonable upper bound (needed to stop the expansion process), the FST $\mathcal{T}_M$ of the minimum spanning tree of N is determined. This is achieved by introducing $c - 1$ Steiner points at terminals of degree c, $c \geq 1$. If $c \geq 3$, there are several ways of interconnecting these $c - 1$ Steiner points with each other and with the terminal. In the current implementation, an arbitrary interconnection pattern is chosen. The length of RMT($\mathcal{T}_M$) yields a good upper bound, denoted by UB, on the length of T^*. Given such good upper bound, the expansion of FSTs in the depth-first manner is no longer essential. Best-first expansion based on the lower bound together with the distance-based ordering of terminals results in the generation of fewer FSTs. This method is referred to as SMITH*.

The quality of lower bounds could be improved by using the conic formulations from the SMITH-FAMPA-method [8]. While smaller number of FSTs would be generated, the computation time increases significantly. Geometric criteria based on the lune-properties combined with the bottleneck distances were also used to speed up the expansion process by eliminating non-optimal FSTs [14]. However, the extra time spent on geometric computations makes the improvements minimal when compared to the distance-based sorting of terminals. None of these improvements are therefore included in the SMITH* algorithm.

5 Branch enumeration algorithm (Branch)

The approach of GeoSteiner [23] seems at first sight to be applicable to the ESTP in $\mathbb{R}^d$, $d \geq 3$. GeoSteiner has two phases. In the *generation phase*, full Steiner trees for all FSTs of all subsets of terminals are generated. Naturally, full Steiner trees that cannot be in T^* are pruned away. When FSTs are generated across different subsets, there are large groups of them that are very similar. The power of GeoSteiner rests partly in its ability to generate full Steiner trees with similar FSTs in a common pass and partly in its ability to prune away partially constructed FSTs. In the *concatenation phase*, GeoSteiner selects a subset of not pruned full Steiner trees that span all terminals and has the minimum total length. This problem can be formulated as the minimum spanning tree problem in a hypergraph. While this problem is NP-hard, a branch-and-cut algorithm seems to be quite efficient to solve problem instances involving full Steiner trees not pruned away during the generation phase.

Unfortunately, this is not the case. First of all, the generation of full Steiner trees for *all* subsets of terminals in $\mathbb{R}^d$, $d \geq 3$, is much more difficult than in $\mathbb{R}^2$. The determination of a full Steiner tree of a given FST with more than 3 terminals requires solving high-degree polynomials [19]. As a consequence, iterative numerical approaches are the only possibility. Such numerical approaches seem to block the generation of full Steiner trees across various subsets of terminals (unlike the $\mathbb{R}^2$ case). Finally, the geometrical non-optimality tests seem to be much weaker than in $\mathbb{R}^2$.

While the generation of full Steiner trees is very challenging for $d \geq 3$, the concatenation phase could be applied without any significant modifications. However, the lack of efficient pruning tests in the generation phase permits a huge number of non-optimal RMTs to survive causing the branch-and-cut concatenation algorithm to choke. These congestion problems become more and more serious as d grows.

The *branch enumeration algorithm* that is proposed here can be seen as a compromise between the approach used by GeoSteiner (generation of full Steiner trees of *all* subsets of terminals) and the numerical approach of Smith [19] described in Section 3 (generation of RMTs for FSTs with n terminals). Rather than enumerating RMTs for all FSTs for N, branches involving subsets of terminals are generated. Consider a FST $\mathcal{T}$ of N. As already mentioned in Section 2, removing a Steiner point breaks $\mathcal{T}$ into 3 branches. As will be seen in Subsection 5.3, every FST with n terminals contains a Steiner point whose removal creates three branches with at most $\lfloor \frac{n}{2} \rfloor$ terminals. This significantly reduces the number of branches that need to be generated.

The branch enumeration algorithm consists of three phases (see Algorithm 1). The *preprocessing* phase computes EMSTs for subsets with up to 8 terminals. These EMSTs are used in subsequent phases to prune away non-optimal branches and RMSTs. The second phase *generates* branches containing up to $\lfloor \frac{n}{2} \rfloor$ terminals. EMSTs obtained in the preprocessing phase together with RMTs of root spliced branches are used to prune away branches that cannot be in T^*. The third phase generates FSTs with n terminals by *concatenating* triplets of disjoint branches. The iterative procedure described in Section 3 is then used to determine their RMTs. The shortest RMT encountered is T^*.

Algorithm 1 Branch enumeration algorithm

Input: Set N of n terminals in $\mathbb{R}^d$.
Output: ESMT T^* of N.

1: **Preprocess:** Determine EMSTs of all subsets of terminals of size up to $\min\{8, \lceil \frac{n}{2} \rceil\}$, store them in $\mathcal{P}$, and order them by non-increasing length.
2: **Generate:** Enumerate sets $\mathcal{B}_k$ of feasible branches with k terminals, $k = 1 \dots \lfloor \frac{n}{2} \rfloor$ (pruning away non-optimal branches).
3: **Concatenate:** Combine triplets of disjoint feasible branches spanning N. Compute corresponding RMTs and let T^* be a shortest one.

5.1 Preprocessing phase

The maximum size κ of subsets of terminals for which ESMTs are determined in the preprocessing phase has a large effect on the number of branches that will be pruned away during their generation described in Subsection 5.2. As branches of up to size $\lceil \frac{n}{2} \rceil$ are generated, setting $\kappa = \lfloor \frac{n}{2} \rfloor$ ensures that for any branch it is possible to find a disjoint preprocessed tree. However, choosing $\kappa > 8$ makes the preprocessing phase computationally expensive. ESMTs are therefore generated using SMITH* for all terminal subsets of size $1, 2, 3, \dots, \kappa$, stored in $\mathcal{P}$, and finally sorted by non-increasing lengths.

5.2 Generating branches

Branches are generated by increasing number of spanned terminals. Branches of size k, $k = 1, 2, \dots \lfloor \frac{n}{2} \rfloor$, are stored in a set $\mathcal{B}_k$. It will be shown in Subsection 5.3 that only branches spanning up to $\lfloor \frac{n}{2} \rfloor$ need to be generated. A single terminal is a branch containing 1 terminal and is therefore stored in $\mathcal{B}_1$. The branches in $\mathcal{B}_k$, $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$, are generated by combining branches in $\mathcal{B}_l$ with branches in $\mathcal{B}_{k-l}$, $l = 1 \dots \lfloor k/2 \rfloor$. When $l = k - l$, care is taken to avoid generation of duplicate branches.

There are several criteria that can be used to reject a branch $B_k = B_l \oplus B_{k-l}$. First of all, B_l and B_{k-l} must be disjoint. This can be efficiently verified by bitwise AND on bit-strings representing subsets of terminals. Similarly, constructing the bitstring of B_k can be efficiently done using bitwise OR.

Assume next that t_i is a terminal in B_l while t_j is a terminal in B_{k-l}. Furthermore, assume that the depth of t_i in B_l is d_i and the depth of t_j in B_{k-l} is d_j. Let $d = d_i + d_j + 2$. Suppose that $|t_i t_j|/d > \beta(t_i, t_j)$ (see Fig. 3). Then B_k cannot be a part of $\mathcal{T}^*$ as it would contain an edge between t_i and t_j longer than the bottleneck distance between t_i and t_j.

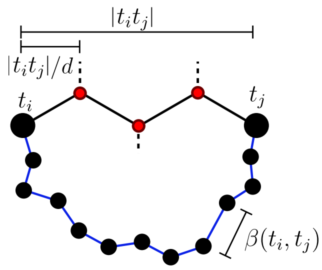


Fig. 3: A branch B_k with terminals t_i and t_j being $d = 4$ edges apart cannot be a part of $\mathcal{T}^*$ if any of these d edges are longer than the bottleneck distance $\beta(t_i, t_j)$. This will certainly be the case if $|t_i t_j|/d > \beta(t_i, t_j)$.

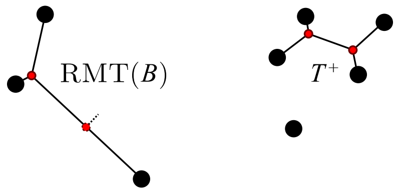


Fig. 4: The length of RMT(B) added to the EMST of any subset of terminals disjoint from $\mathcal{T}$ is a lower bound on $|T^*|$

Finally, suppose that RMT(B_k) spans the set of terminals N_k and the EMST T^+ for some non-empty subset of $N \setminus N_k$ satisfies

$$|\mathrm{RMT}(B_k)| + |T^+| \geq UB$$

where UB is an upper bound on the length of T^* (see Section 4), then B_k cannot be a part of $\mathcal{T}^*$. This is an immediate consequence of the following lemma and the fact that $UB \geq |T^*|$.

Lemma 1 *Let B_k be a branch of $\mathcal{T}^*$. Let N_k denote the terminals of B_k. Let T^+ be the EMST of a non-empty subset of $N \setminus N_k$. Then $|T^*| \geq |\mathrm{RMT}(B_k)| + |T^+|$.*

Proof. If $|N_k| = 1$ then $|\mathrm{RMT}(B_k)| = 0$ and the inequality trivially holds. Assume that $|N_k| \geq 2$. Let $B_k = B_i \oplus B_j$ with r_k, r_i and r_j being the roots of

B_k, B_i and B_j respectively. Let T_k^*, T_i^* and T_j^* be the parts of T^* corresponding to B_k, B_i and B_j respectively. Then

$$|T_k^*| = |T_i^*| + |r_i r_k| + |r_j r_k| + |T_j^*| \geq |T_i^*| + |r_i r_j| + |T_j^*| \geq |\mathrm{RMT}(B_k)|$$

where the first inequality is due to the triangle inequality and the second inequality is due to the fact that $\mathrm{RMT}(B_k)$ is the RMT of the FST obtained by splicing away r_k from B_k. Hence,

$$|T^*| = |T_k^*| + |T^* \setminus T_k^*| \geq |\mathrm{RMT}(B_k)| + |T^+|$$

since $T^* \setminus T_k^*$ is a tree spanning $N \setminus N_k$. □

Algorithm 2 Generate branches containing up to $\lceil \frac{n}{2} \rceil$ terminals

Input: Set N of n terminals in $\mathbb{R}^d$.
Input: Sorted list $\mathcal{P}$ of EMSTs for small subsets of N.
Input: An upper bound UB on $|T^*|$
Output: $\mathcal{B}_k, k = 1 \ldots \lceil \frac{n}{2} \rceil$

$\mathcal{B}_1 \leftarrow N$
for $k = 2$ **to** $\lceil \frac{n}{2} \rceil$ **do**
  $\mathcal{B}_k \leftarrow \emptyset$
  for $l = 1$ **to** $\lfloor \frac{k}{2} \rfloor$ **do**
    for all $B_l \in \mathcal{B}_l$ **do**
      for all $B_{k-l} \in \mathcal{B}_{k-l}$ **do**
        if B_l and B_{k-l} have a common terminal **then**
          $B_l \oplus B_{k-l}$ cannot be a part of $\mathcal{T}^*$
        end if
        for all pairs of terminals (t_i, t_j), $t_i \in B_l, t_j \in B_{k-1}$ **do**
          Let d_i and d_j denote the depth of t_i and t_j in respectively B_l and B_{k-l}.
          if $\frac{|t_i t_j|}{d_i + d_j + 2} > \beta(t_i, t_j)$ **then**
            $B_l \oplus B_{k-l}$ cannot be a part of $\mathcal{T}^*$
          end if
        end for
        $B_k \leftarrow B_l \oplus B_{k-l}$
        Find the longest ESMT $T^+ \in \mathcal{P}$ disjoint from B_k
        if $|\mathrm{RMT}(B_k)| + |T^+| \geq UB$ **then**
          B_k cannot be a part of $\mathcal{T}^*$
        end if
        Add B_k to $\mathcal{B}_k$.
      end for
    end for
  end for
end for
return $\mathcal{B}_k, k = 1 \ldots \lceil \frac{n}{2} \rceil$

5.3 Concatenation of branches

Consider a FST $\mathcal{T}$ of a set N of n terminals, $n \geq 3$. Let s be any of its $n-2$ Steiner points. When s (and its three incident edges) are removed, $\mathcal{T}$ splits into three branches B_i, B_j and B_k with respectively n_i, n_j, and n_k terminals, $n = n_i + n_j + n_k$. Assume that $n_i \geq n_j \geq n_k$.

Lemma 2 *$\mathcal{T}$ has a splitting Steiner point s such that $n_i \leq n_j + n_k$.*

Proof. Assume that $n_i > n_j + n_k$ for every Steiner points in $\mathcal{T}$. Pick a Steiner point s minimizing n_i. Let $s' \in B_i$ denote the Steiner point adjacent to s in $\mathcal{T}$. It exists since $n_i \geq 2$. Let n'_i, n'_j, and n'_k denote the number of terminals obtained by splitting $\mathcal{T}$ at s'. Then $n'_i = n_j + n_k$, $n'_j = x$ for some x, $0 < x < n_i$, and $n'_k = n_i - x$. Hence, n'_i, n'_j, and n'_k are all less than n_i, contradicting the choice of s. □

A split of any FST with $n_i \geq n_j \geq n_k$, $n = n_i + n_j + n_k$ and $n_i \leq n_j + n_k$ is called a *canonical split*.

Lemma 3 *$\lceil \frac{n}{3} \rceil \leq n_i \leq \lfloor \frac{n}{2} \rfloor$ in a canonical split of any FST with n terminals.*

Proof. To obtain the first inequality, observe that $n = n_i + n_j + n_k \Rightarrow n \leq 3n_i \Rightarrow \lceil \frac{n}{3} \rceil \leq n_i$. To obtain the second inequality, observe that $n_i \leq n_j + n_k = n - n_i \Rightarrow 2n_i \leq n \Rightarrow n_i \leq \lfloor \frac{n}{2} \rfloor$. □

Lemma 4 *An FST $\mathcal{T}$ with n terminals has exactly one canonical split unless n is even and $n_i = n/2$ in which case $\mathcal{T}$ has two canonical splits at adjacent Steiner points.*

Proof. Let B_i, B_j and B_k denote three branches of the canonical split at a Steiner point s. Consider another Steiner point $s' \in \mathcal{T}$. Assume first that $s' \in B_j$. Let $n'_i \geq n'_j \geq n'_k$ denote the number of terminals in the branches of this split at s'. Hence, $n'_i \geq n_i + n_k$ and $n'_j + n'_k \leq n_j$. Now $n'_i \geq n_i + n_k > n_j \geq n'_j + n'_k$ implies that the split is not canonical. Similar argument applies if $s' \in B_k$. Assume finally that $s' \in B_i$. Hence, $n'_i \geq n_j + n_k$. Now $n'_i \geq n_j + n_k \geq n_i \geq n'_j + n'_k$ implies that this split is canonical iff $n'_i = n'_j + n'_k$. This can happen if and only if $n'_i = n_i = n/2$. Hence, n has to be even and s and s' must be adjacent in $\mathcal{T}$. □

It is therefore only necessary to concatenate triplets of disjoint branches (B_i, B_j, B_k) with $n = n_i + n_j + n_k$, and whose individual sizes satisfy $\lceil \frac{n}{3} \rceil \leq n_i \leq \lfloor \frac{n}{2} \rfloor$, $n_i \leq n_j + n_k$ and $n_i \geq n_j \geq n_k$. See Algorithm 3 for a detailed description of the concatenation of triplets of branches.

6 Computational experiments

To benchmark our algorithms we generated and collected the 6 sets of problem instances shown in Table 1. The *Carioca* set was from the 2014 DIMACS challenge and the *Iowa* set from a previous publication by Fampa and Anstreicher [8]. The *Sausage* set contains d-sausages, which are linear concatenations of regular d-simplices, that have the lowest currently known Steiner ratio in dimensions 3 and up [20].

Algorithm 3 Concatenate triples of branches to obtain EMST T^*

Input: Sets of branches $\mathcal{B}_p, p = 1 \dots \lfloor \frac{n}{2} \rfloor$
Input: An upper bound UB on $|T^*|$
Output: T^*

$|T^*| \leftarrow UB$
for $i = \lfloor \frac{n}{2} \rfloor$ **to** $\lceil \frac{n}{3} \rceil$ **do**
  for $j = \min\{i, n-i-1\}$ **to** $\lceil \frac{n-i}{2} \rceil$ **do**
    $k \leftarrow n - i - j$
    for all disjoint triples of branches B_i, B_j, B_k with $B_i \in \mathcal{B}_i, B_j \in \mathcal{B}_j$ and $B_k \in \mathcal{B}_k$ **do**
      $T \leftarrow \mathrm{RMT}(B_i \oplus B_j \oplus B_k)$.
      if $|T| < |T^*|$ **then**
        $T^* \leftarrow T$
      end if
    end for
  end for
end for
return T^*

Set name	Dimensions	Terminals	Seeds	Set sz.	Point configuration
Cube	$d = 2 \dots 5$	$n = 10 \dots 15$	50	1200	Rand. in cube
Sphere	$d = 2 \dots 5$	$n = 10 \dots 15$	50	1200	Rand. on sphere
Carioca	$d = 3 \dots 5$	$n = 11 \dots 20$	5	150	Rand. in cube
Iowa	$d = 3 \dots 5$	$n = 10$	10	30	Rand. in cube
Solids	$d = 3$	$n = 4, 6, 8, 12, 20$	NA	5	Platonic solids
Sausage	$d = 2 \dots 5$	$n = 10 \dots 15$	NA	24	Simplex sequence

Table 1: Sets of problem instances used for benchmarking. The 'Cube' and 'Sphere' sets are generated, the rest are from known data sets.

Smith's algorithm (SMITH) described in Section 3, its modified version (SMITH*) described in Section 4 and the branch enumeration algorithm (BRANCH) described in Section 5, were implemented in C++ and run on an Intel Xeon X5550 2.67GHz CPU. All runs were stopped after 12 hours if they had not terminated. All source code, data files and instructions to build and run benchmarks are available online at `http://github.com/DIKU-Steiner/MPC15`.

To check correctness we compared the length of the ESMT for each of the methods BRANCH, SMITH*, and SMITH on 150 instances of random points in a unit square with $n = 10 \dots 12$ and $d = 2$. We also measured the distance with the numerically exact method GeoSteiner 3.1 [23]. For all instances the ESMT length obtained with BRANCH, SMITH* and GeoSteiner were identical down to a factor 1/10000 of the optimal length. The implementation of SMITH, however, returned suboptimal solutions 45% of the time due to a bug in the original code [19]. We fixed the bug and have made a corrected version and a description available online.

The iterative RMT calculation takes as input a tolerance, τ, that is used as a stopping criterion by terminating when $|T| \leq |RMT| + \tau$, where T is the current tree. The computation of τ used by Smith has not yet been proven to satisfy this criterion in all cases, but in practice it works when τ is sufficiently small. However, decreasing τ also affects the running time drastically. We therefore ran Smith, Smith*, and Branch on the 200 Cube instances with $n = 12$ and $d = 2, \ldots, 5$. For each instance we reported the CPU-time for $\tau = 0.1, 0.01, 0.001, 0.0001$ and divided it by the CPU-time for $\tau = 0.01$. The average of these values are shown in Table 2. The Smith algorithm has $\tau = 0.0001$, but its worth mentioning that a significant speedup could be obtained by increasing the tolerance to 0.01. Unfortunately, this also causes some examples to be solved incorrectly (those without checkmarks). Based on similar observations we set $\tau = 0.01$ for Branch and to $\tau = 0.001$ for Smith*.

Tolerance (τ)	0.1	0.01	0.001	0.0001
Branch	1.51	1.00	3.14	9.35
	✓	✓	✓	✓
Smith*	0.47	1.00	3.07	7.91
			✓	✓
Smith	1.37	1.00	2.54	8.80
			✓	✓

Table 2: Average relative CPU-times for different tolerance values based on the Cube instances with $n = 12$. Checkmarks indicate that all 200 instances could be solved to optimality.

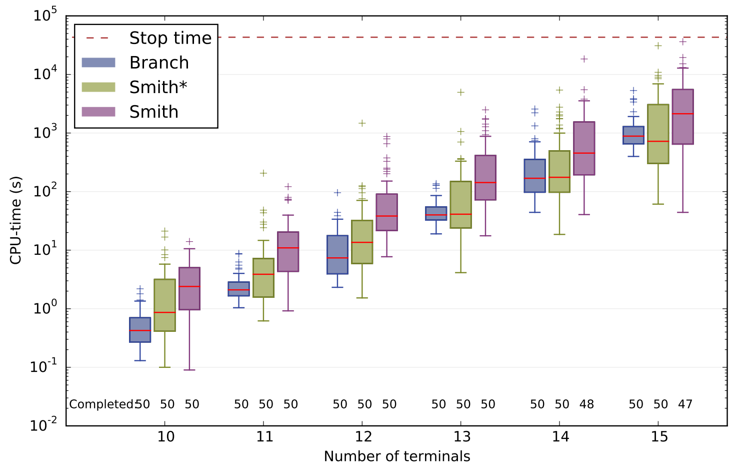


Fig. 5: Box-plot of CPU-times for Branch, Smith*, and Smith on random points, $d = 3$, in a unit cube (Cube set). Below each box is indicated the number of instances that finished within 12 hours.

Figure 5 shows distributions of CPU-times for the 300 problem instances with $d = 3$ from the *Cube* set. Figure 1 in the appendix shows similar running time distributions for $d = 2, \ldots, 5$. For $d \geq 3$, the Branch and Smith* implementations consistently outperform the original Smith algorithm. For many of the large instances ($n = 15$) Branch terminates within the prespecified time while Smith* does not. Appendix Figure 2 shows CPU-time distributions for the *Sphere* data set. Here Smith is more competitive but is still on average out-performed by Branch for $d \geq 3$. CPU-times and optimal ESMT lengths for the *Sausage*, *Smith* and *Solids* data sets are shown in Table 4 of the appendix.

Both Branch, Smith*, and Smith construct RMTs for various subsets of terminals in order to obtain reasonable lower bounds permitting pruning of non-optimal configurations as early as possible. In particular, Branch computes many such RMTs with up to 8 terminals in its preprocessing and generation phases. Note that the very straightforward way that preprocessing is currently done, the RMT of a particular topology may be computed multiple times. Additionally, the RMT of two distinct branches may also be identical. Using appropriate look-up tables to avoid redundant RMT computations would no doubt speed up Branch significantly.

Table 3 illustrates the strength of the different pruning criteria used in Branch. The 'Nothing' column indicates the number of branches that are explored if all pruning is disabled. The 'Preprocessing' column indicates the number of branches that are explored when all pruning methods are enabled. Using RMTs of branches as lower bounds is essential to be able to prune in the final concatenation phase (bottom rows in the table) but it is only when tightened using results from the preprocessing stage that branches can be pruned in the generation phase.

Table 4 compares Branch, Smith*, and Smith with two previous algorithms that solve the ESMT. The values for Smith-Fampa and Smith-Laarhoven are taken from [14]. For most instances, both Smith* and Branch show better performance.

Figure 6 illustrates the effects of changing the number of terminal subsets that are preprocessed. The Branch algorithm was run on three point sets with $d = 3$ and $n = 12, 13, 14$ and different values of κ. In all cases, setting $\kappa = \lceil n/2 \rceil$ gave the lowest CPU time. Lower values of κ resulted in very fast preprocessing, but weak lower bounds. This caused the concatenation phase to explode. Larger values of κ made the lower bound stronger, but required much more time for preprocessing. As a lot of redundant computations is performed in the preprocessing phase, this indicates that speeding up preprocessing and increasing κ might substantially improve the Branch algorithm.

7 Conclusions

Two new exact algorithms (Smith* and Branch) for solving the Euclidean Steiner tree problem in d-dimensional space, $d \geq 2$, have been proposed. One

Level	Nothing	Overlap	Bottleneck	Lowerbound	Preprocessing
8 random terminals in unit cube					
2	36	28	21	21	21
3	288	168	121	121	29
4	2 970	1 050	719	719	64
8	1 498 176	21 000	9 596	2 161	743
10 random terminals in unit cube					
2	55	45	32	32	32
3	550	360	246	246	50
4	7 040	3 150	2 034	2 034	77
5	100 650	26 460	15 810	15 810	108
10	12 560 296 100	3 508 785	1 183 316	65 609	7 274

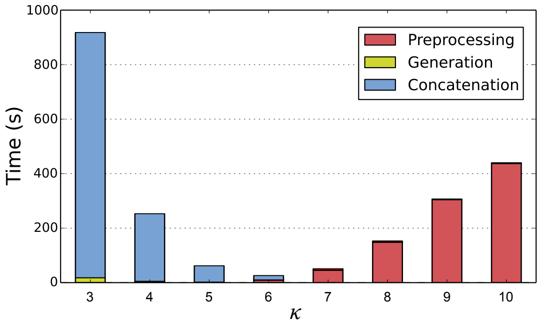
Table 3: The effect of different pruning criteria on the number of generated branches/full topologies in Branch algorithm. The level of a branch is the number of terminals it contains. 'Nothing' means that all combinations of branches are used in enumeration, including those with overlapping terminal sets. 'Overlap'-pruning discards all branches where the same terminal appears twice. 'Bottleneck'-pruning additionally uses the bottleneck criterion to prune. 'Lowerbound' prunes branches based on their lower bounds both in the generation and concatenation phases. 'Preprocessing'-pruning strengthens the lower bound of each branch by adding the lengths of disjoint optimal solutions from the preprocessing phase.

	n	10	10	10
	d	3	4	5
Smith	Nodes factor	1	1	1
	Time factor	1	1	1
Smith-Fampa	Nodes factor	**33.4**	**26.9**	**50.8**
	Time factor	3.1	2.8	4.4
Smith-Laarhoven	Nodes factor	3.5	6.1	3.7
	Time factor	3.6	6.4	3.8
Smith*	Nodes factor	19.9	17.5	6.6
	Time factor	**17.9**	**17.2**	**8.7**
Branch	Nodes factor	12.0	6.5	5.4
	Time factor	6.7	4.1	3.5

Table 4: Performance of known Steiner tree algorithms. Numbers indicate the improvement factor in nodes explored and CPU-time over Smith's original algorithm.

is an extension of the seminal algorithm by Smith while the other constructs branches in a bottom-up fashion. Computational studies show that both methods are faster than previous implementations of this problem.

It is worth noting that the use of branches in the branch enumeration method provides a more specific representation of partial solutions than the expanding topologies in Smith's algorithm. A branch can only be expanded by attaching to one particular edge, while expanding trees can have any edge split. This property has the potential to expose different and possibly stronger



(a) CPU times for $n = 12$ and varying values of κ broken down by algorithm phase.

$\kappa \backslash n$	12	13	14
5	62	881	1734
6	**25**	201	467
7	50	**166**	**320**
8	151	566	1076

(b) CPU times for different values of n.

Fig. 6: The CPU time for instances from the *Carioca* set with $d = 3$ where preprocessing finds EMSTs for subsets up to κ terminals. No matter what n is, setting $\kappa = \lceil n/2 \rceil$ results in the lowest total CPU time.

methods for fathoming partial solutions early. For instance, Laarhoven and Anstreicher [14] present a combination of lune-properties and bottleneck distances that could directly be used to prune in the very first steps of the enumeration. In general our findings suggest a need to identify tighter lower bounds and geometric criteria for excluding partial solutions in higher dimensions.

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